From theory to practice: Gaussian process metamodels for the sensitivity analysis of traffic simulation models. A case study of the Aimsun mesoscopic model.
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ABSTRACT
This paper discusses a metamodel-based technique for model sensitivity analysis and applies it to the Aimsun mesoscopic model. Throughout the paper it is argued that the application of sensitivity analysis is crucial for the true comprehension and correct use of the traffic simulation model while also acknowledging that the main obstacle to an extensive use of the most sophisticated techniques is the high number of model runs they usually require.

For this reason we have tested the possibility of performing sensitivity analysis not on a model but on its metamodel approximation. Important issues arising when estimating a metamodel have been investigated and commented on in the specific application to the Aimsun model. Among these issues is the importance of selecting a proper sampling strategy based on low discrepancy random number sequences and the importance of selecting a class of metamodels able to reproduce the inputs-outputs relationship in a robust and reliable way. Sobol sequences and Gaussian process metamodels have been recognized as the appropriate choices.

The proposed methodology has been assessed by comparing the results of the application of variance-based sensitivity analysis techniques to the simulation model and to a metamodel estimated with 512 model runs, on a variety of traffic scenarios and model outputs. Results confirm the powerfulness of the proposed methodology and also open up to a more extensive application of sensitivity analysis techniques to complex traffic simulation models.
INTRODUCTION

Over the last few decades, complex models have been developed in all scientific fields, often thanks to continually increasing computational capabilities. Design problems, process control and political choices increasingly rely on the results these models are able to provide. For this reason it is becoming crucially important to analyze a model, to understand how it works and, in particular, what influences its capacity to reproduce physical phenomena. Global sensitivity analysis is the family of tools to be used with this aim.

Together with uncertainty analysis, sensitivity analysis (SA) studies how the uncertainties in the model inputs affect the model response. In this picture, uncertainty analysis quantifies the output variability while sensitivity analysis describes the relative importance of each input in determining this variability (1,2).

The focus is, thus, on model uncertainty: "What makes modelling and scientific inquiry in general so painful is uncertainty. Uncertainty is not an accident of the scientific method, but its substance" (1). The main sources of model uncertainty can be considered, i) the (in)adequacy of the models to the reality and ii) the (uncertain) model inputs.

Uncertainty due to the inadequacy of models arises from a number of sources like the modelling basic assumptions, the structural equations, the level of discretisation, the numerical resolution method, etc. Reducing this part of uncertainty usually requires substantial modifications to the modelling structure and, therefore, can hardly be achieved by the model users, being mainly the responsibility of model developers.

On the contrary, the portion of the uncertainty due to uncertain model inputs rests almost totally on the shoulders of the model users. In order to reduce this part of the uncertainty, it is necessary to reduce as much as possible the uncertainty in the model inputs. Yet, different inputs can have a different influence on the model outputs and also the uncertainty they embody can affect the outputs in a different way. When the number of these inputs increases to several hundred, as is the case of many complex models available today, understanding which ones need our attention for their estimation becomes crucial. In this framework, sensitivity analysis plays a fundamental role, as it may direct the analyst towards the identification of the relative importance of each input. This is also demonstrated by the fact that sensitivity analysis has been also recognized in official guidelines of international institutions (3,4).

In addition, sensitivity analysis can be used to i) uncover technical errors in the model, ii) identify critical regions in the space of the inputs, iii) establish priorities for research, iv) simplify models and v) defend against analysis falsifications.

As models are becoming more complex, global sensitivity analysis techniques have made significant progresses in the last decade. Unfortunately it is common opinion that only a minority of sensitivity analysis practitioners make use of the most sophisticated techniques made available in the recent years (1). In fact, as discussed in the next section for what concerns sensitivity analysis of traffic simulation models, the most commonly adopted approach to sensitivity analysis still remains the One At a Time (OAT). OAT measures, are based on the estimation of partial derivatives, and assess how uncertainty in one factor affects the model output keeping the other factors fixed to a nominal value. The main drawback of this approach is that interactions among factors cannot be detected, since they require the inputs to be changed simultaneously. In addition, this approach pertains to a family of sensitivity analysis techniques usually referred to as “local sensitivity analysis”, used to derive information about the behaviour of the model around a certain point (for example around the solution of the calibration problems to ascertain the stability of such a solution) rather than exploring the input space. For this reason it should not be considered a good practice. However, its simplicity and parsimony makes it the preferred choice for practitioners (5).

The problem is that, even with the most sophisticated sampling strategies, the exploration of the input space required by any global sensitivity analysis approach requires many model runs to be performed. When the model is computationally expensive, which is fairly common in the applications, sensitivity analysis quickly becomes unfeasible. To deal with this issue, in recent years, some studies have made use of metamodels. Metamodels provide inexpensive emulators of complex and large computational models (6,7,8). The computational cost of estimating an emulator is generally dependent on the number of inputs, but the dependence is much weaker than that involving the calculation of commonly adopted sensitivity indices.
In the field of traffic simulation, metamodels have been recently adopted to verify the effectiveness of traffic model calibration procedures (9). The use of a metamodel was indispensible in assessing different calibration procedures, due to the huge amount of time otherwise required using the simulation model. In addition, in (9), the metamodel adopted, a type of Gaussian process metamodel proved to be able to reproduce, both globally and locally, the real objective function of the calibration problem, even with a small number of model simulations.

For this reason, in the present paper, we adopt a Gaussian process metamodel for the evaluation of variance-based sensitivity indices. In practice, indices are calculated based on the evaluation of the metamodel on several input-parameter combinations. Indices calculated in this way are then compared to those obtained using the traffic simulation models instead.

The procedure was tested on the mesoscopic version of the Aimsun simulation model (10) in five different synthetic traffic scenarios. The experience carried out shows that, even with a metamodel estimated on 128 simulations, sensitivity indices are approximately the same as those calculated with 36,864 simulations, with a consequent significant reduction of the total computation time. Key in this process is the definition of the sample of input parameters combinations. The sample, indeed, requires the provision of an optimal filling of the input space (8). To this aim, in the present study, we adopted the Sobol sequence of quasi-random numbers (11), which proved to be one of the sequences with the lowest discrepancy (that is the comparison between the intervals volume and the number of points within these intervals in the input space).

The paper is organized as follows. In the next section a brief overview of variance-based methods for sensitivity analysis is provided along with a discussion on the number of model evaluations required for their implementation. Then, in the third section the methodology for the metamodel-based sensitivity analysis is presented. The case study and the main results achieved are presented in the fourth and fifth sections. A concluding section closes the paper with reference to future research activities.

**VARIANCE-BASED METHODS ON THE SOBOL DECOMPOSITION OF VARIANCE**

Variance-based methods based on Sobol variance decomposition has been chosen in this application, being considered one of the most recent and effective global sensitivity analysis techniques. The original formulation of the method came from I. Sobol (12,13), who provided the analytical derivation and the Monte Carlo-based implementation of the concept. The latest setting for its practical implementation is by Saltelli et al. (6).

Given a model in the form:

$$Y = f(Z_1, Z_2, ..., Z_r)$$ (1)

with $Y$ a scalar, a variance-based first order effect for a generic factor $Z_i$ can be written as

$$V_{Z_i} \left( E_{Z_{-i}}(Y|Z_i) \right)$$ (2)

where $Z_i$ is the i-th factor and $Z_{-i}$ is the matrix of all factors but $Z_i$. Furthermore it is known that

$$V(Y) = E_{Z_i} \left( V_{Z_{-i}}(Y|Z_i) \right) + V_{Z_i} \left( E_{Z_{-i}}(Y|Z_i) \right)$$ (3)

Equation (3) shows that if $Z_i$ to be an important factor we need that $E_{Z_i} \left( V_{Z_{-i}}(Y|Z_i) \right)$ is small, that it is to say that the closer $V_{Z_i} \left( E_{Z_{-i}}(Y|Z_i) \right)$ to the unconditional variance $V(Y)$ the higher the influence of $Z_i$.

Thus we may define our first order sensitivity index of $Z_i$ with respect to $Y$ as:

$$S_i = \frac{V_{Z_i} \left( E_{Z_{-i}}(Y|Z_i) \right)}{V(Y)}$$ (4)

Sensitivity indices as in equation (4) can be calculated per each factor and per each factors combination. This, however, would need a huge amount of model evaluations. In order to reduce the efforts required, a synthetic indicator to be coupled with the first order sensitivity index is the total effects index, defined as follows (6):

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Total effects index of the input factor \(i\) provides the sum of first and higher order effects (interactions) of factor \(Z_i\). When the total index is \(S_{Ti} = 0\) the \(i\)-th factor can be fixed without affecting the outputs’ variance. If \(S_{Ti} \approx 0\) the approximation made depends on the value of \(S_{Ti}\). It is worth noting that while \(\sum_{i=1}^{r} S_i \leq 1\), \(\sum_{i=1}^{r} S_{Ti} \geq 1\), both being equal to one only for additive models.

**Variance-based methods. Implementation**

The calculation of the variance-based sensitivity indices presented in equations (4) and (5) can be performed in a Monte Carlo framework. This issue has been object of research in recent decades. Different approaches and strategies may provide results with different accuracy and efficiency. The approach adopted in the present work has been specified in (I.6) and can be summarized in the following points:

- two \((N, r)\) matrices of quasi-random numbers (II) are generated. Using the random numbers two matrices of values for the input variables of the model as in equation (1) are generated (called \(A\) and \(B\) in the following).

\[
A = \begin{bmatrix}
    z_1^{(1)} & z_2^{(1)} & \ldots & z_r^{(1)} \\
    z_1^{(2)} & z_2^{(2)} & \ldots & z_r^{(2)} \\
    \vdots & \vdots & \ddots & \vdots \\
    z_1^{(N)} & z_2^{(N)} & \ldots & z_r^{(N)} \\
\end{bmatrix} \tag{6}
\]

\[
B = \begin{bmatrix}
    z_1^{(1)} & z_2^{(1)} & \ldots & z_{r+i}^{(1)} \\
    z_1^{(2)} & z_2^{(2)} & \ldots & z_{r+i}^{(2)} \\
    \vdots & \vdots & \ddots & \vdots \\
    z_1^{(N)} & z_2^{(N)} & \ldots & z_{r+i}^{(N)} \\
\end{bmatrix} \tag{7}
\]

- a set of \(r\) matrices, \(C\), is obtained assembling \(r\) matrices equal to \(A\) except for the \(i\)-th column (with \(i\) varying from 1 to \(r\) among the \(r\) matrices) that is taken from \(B\).

\[
C_i = \begin{bmatrix}
    z_1^{(1)} & z_2^{(1)} & \ldots & z_{r+i}^{(1)} & \ldots & z_r^{(1)} \\
    z_1^{(2)} & z_2^{(2)} & \ldots & z_{r+i}^{(2)} & \ldots & z_r^{(2)} \\
    \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\
    z_1^{(N)} & z_2^{(N)} & \ldots & z_{r+i}^{(N)} & \ldots & z_r^{(N)} \\
\end{bmatrix} \quad \text{for } i = 1 \ldots r \tag{8}
\]

- the model is evaluated for all the \([N\cdot(r+2)]\) combinations of input variables as given by matrices \(A\), \(B\) and \(C\) so as to produce the vectors of outputs \(y_A = f(A)\), \(y_B = f(B)\) and \(y_{C_i} = f(C_i)\) for \(i=1\ldots r\). These vectors are sufficient for the evaluation of all the first order and total effects indices. For this reason the application of this technique for variance-based methods requires \([N\cdot(r+2)]\) model evaluations.

Sensitivity indices can be then evaluated using the following formulations (6):

\[
S_i = \frac{1}{N} \sum_{j=1}^{N} y_A^{(j)} \left( y_{C_i}^{(j)} - y_A^{(j)} \right) \tag{9}
\]

\[
S_{Ti} = \frac{1}{2N} \sum_{j=1}^{N} \left( y_A^{(j)} - y_{A+B}^{(j)} \right)^2 \tag{10}
\]
Since N usually varies from a few hundred to several thousand, the number of evaluation required by this efficient approach is not, in any case, negligible, especially for complex and expensive models.

In the field of traffic flow modelling, to the best of the authors’ knowledge, this method based on quasi-Monte Carlo sampling in the parameters space has been used only in Punzo and Ciuffo (14) in order to individuate the parameters which limit the calibration of two well-known car-following models. However, so far, no other studies in this context made use of this technique to perform global sensitivity analysis. The reason is mainly connected to the still high number of model evaluations required by the technique. In this light, when we move from car-following applications, like (14), in which each model evaluation requires less than a few seconds, to traffic model simulations, which may require several hours per model evaluation, the application of this technique, though efficient, quickly becomes unfeasible.

Nonetheless, renouncing the reliability and the robustness of the results achievable by variance-based sensitivity indices seems a too high price for practitioners in this field. For this reason we were wondering if the use of metamodels instead of the simulation model to carry out variance-based sensitivity analysis might represent the right compromise between accuracy of results and computation parsimony, namely, the right bridge between theory and practice. The question is, of course, related to the quality of the metamodel and of its estimation procedure. In the next sections we will deal with these issues.

**GAUSSIAN PROCESS METAMODELS FOR THE SENSITIVITY ANALYSIS OF COMPUTATIONALLY EXPENSIVE TRAFFIC SIMULATION MODELS**

As already stated, the intention of this paper is to provide a methodology for performing sensitivity analysis of a traffic simulation model using variance-based techniques on a metamodel estimated from a relatively small sample of evaluations of the simulation models itself.

The class of metamodel chosen is the Gaussian process metamodel. This class of metamodel extends the Kriging principles of geo-statistics to any experimental science by considering the correlation between two different samples (real or model-derived) depending on the distance between input variables (15,16). Numerous studies have shown that this interpolating model provides a powerful statistical framework for computing an efficient predictor of model response (17,18), also in the case of traffic simulation models (9). This general consideration, however, needs to be verified case by case, as any simulation model may hide peculiarities for which the principles on which Gaussian processes are based do not hold. In this light, several strategies can be adopted to estimate the best and most efficient surrogate for the simulation model. For further details, the interested reader may refer to (15,19).

In this paper we adopted a more simplistic approach. First of all, we consider a low-discrepancy sequence of quasi-random numbers. As already mentioned, the low discrepancy ensures good coverage of the input space. Any of these sequences has a recursive number R of generations in which the discrepancy is minimum. We start simulating the model on the first 2R elements of the sequence. With the results of the first R combinations a Gaussian process approximation of the model is estimated. Then the quality of the metamodel is assessed by comparing the outputs of the model in the second R inputs combinations with the predictions of the metamodel in the same R combinations. If model outputs and metamodel predictions match to a sufficient degree, then the metamodel can be used in the place of the model. Otherwise an additional set of R model evaluations is performed until the established quality criterion is met.

The proposed methodology is schematically presented in Figure 1. An important variable to be defined is the quality criterion. The closer the metamodel needs to be to the model, the higher the number of model evaluations required. The definition of the criterion is therefore very important and it’s strictly connected with the use of the metamodel. If the metamodel is used in place of the model in a design process or for a scenario analysis, then the quality required should be very high. On the contrary, if, as in (9), the metamodel is used to verify the effectiveness of a calibration procedure to be applied to the model, then the quality required might be lower. In the case of using a metamodel for the sensitivity analysis of a computationally expensive model it is not really necessary to have a perfect match between model evaluations and metamodel predictions but it is important that the metamodel is able to reflect the way an input affects the model outputs. In the experience carried out in the present paper, we have seen that, even with a not perfect metamodel the estimation of the sensitivity indices proved to be already satisfactory.
Figure 1. Flow chart of the metamodeling process validation methodology. When the validation condition is not satisfied a new set of inputs combinations is generated.

In the next section, the metamodel implemented, the validation criterion, the traffic model adopted and the low-discrepancy random sequence selected will be briefly described.

CASE STUDY: GAUSSIAN PROCESS METAMODEL FOR THE SENSITIVITY ANALYSIS OF THE AIMSUN MESOSCOPIC TRAFFIC SIMULATION MODEL

In the present section, the main elements of Figure 1, namely the i) low-discrepancy random sequence, ii) the traffic model, iii) the metamodel and iv) the validation criterion adopted in this paper are briefly presented.

Sobol’s quasi-random number sequence

The low-discrepancy random sequence used in this paper is the Sobol sequence, usually referred to as LPτ sequence. The Sobol sequence was introduced for the first time in 1967 by I.M.Sobol and it is considered one of the most suitable sequences to be used in Monte Carlo experiments and for the evaluation of variance-based sensitivity indices (1). Providing a description of the rationale behind the sequence is beyond the aim of the present paper. For further information the interested reader may refer to (1,11,20).

The implementation used for the derivation of the quasi-random sequences can be found in (21). As already mentioned, the minimum discrepancy of the sequence is achieved for the number of points $R$ equal to a power of two. For this reason, we started estimating the metamodel with $2^6 = 128$ inputs combinations.

Aimsun mesoscopic model

This section provides an overview of the Aimsun mesoscopic simulation model, describing its network representation and behavioural models, and focussing on car-following and gap-acceptance models.

Network Representation

The Aimsun mesoscopic model uses a node/section representation of the network based on a directed graph.

Basically, there are 3 geometric elements in the mesoscopic network representation:

- **Nodes**: in the mesoscopic representation they are treated as node servers, where vehicles are transferred from a section to a turning and then to their next section.
Turnings: the connections that vehicles use in their path. These turnings connect some/all lanes from the origin section to some/all lanes of the destination section. The turning speed as well as the turning length is used to calculate the turning travel time. All vehicles are assumed to travel without any restriction, namely at a free flow speed in turnings.

- Sections: the connectors between nodes. Each section has information about its geometry: number of lanes, speed limits and jam density.
- Centroids: the source of vehicles. They are used to generate vehicles.

**Behavioural models**

The mesoscopic level in Aimsun uses a vehicle-based representation of the traffic flow. The behavioral models are the following:

- Behavioural models in sections: car-following and lane-changing
- Behavioural models in nodes (node model): gap-acceptance and lane selection model

The car-following model implemented in the mesoscopic model relies on a simplified version of the Gipps car-following model (22) used for the microscopic level. The model is based on two components: acceleration and deceleration. The restrictions of acceleration and deceleration are simplified to obtain the following expressions:

\[
\begin{align*}
x(t, n) &\leq x(t - RT, n) + V \cdot RT \\
x(t, n) &\leq x(t - RT, n - 1) - s
\end{align*}
\]

where \( t \) is the simulation time, \( n \) is vehicle number ordered according to its arrival time at the lane, \( x(t,n) \) is the position of vehicle \( n \) at time \( t \), \( V \) is the maximum vehicle speed, that is the minimum between the vehicle’s max desired speed and the max speed of the section, \( s \) is the vehicle’s effective length (vehicle length plus the minimum distance between vehicles) and \( RT \) is the vehicle’s reaction time.

The original Gipps car-following model is used for calculating speed in the next simulation step. In the mesoscopic model, car-following and lane-changing models are applied to calculate the section travel time. This is the earliest time a vehicle can reach the end of the section, taking into account the current status of the section (that is, the number of vehicles in the section).

The number of vehicles in a section is bounded by the capacity of the section (SectionCapacity) defined as the number of vehicles that can stay at the same time in a section.

The Gap-Acceptance model is used to model give way behaviours. In particular the model is used when resolving node events in order to decide which of two vehicles in a conflicting movement has precedence.

The Gap-Acceptance model used in the mesoscopic approach is a simplification of the Gap-Acceptance model used in the microscopic simulator. The model takes into account the travel time from both vehicles to the collision point; then it determines how long the vehicles need to clear the node/intersection and, finally, it produces the decision.

The maximum give-way time parameters are used to determine when a driver starts to get impatient if he/she cannot find a gap. When the driver has been waiting more than this time, the safety margin (normally double the vehicle reaction time) is reduced linearly to 0.

**Case study**

The case study has been focused on the sensitivity analysis of the car-following and gap-acceptance models, and has been conducted using five different test networks, representing the main different configurations available in any type of network, either urban, non-urban or mixed, and cover all parameters involved in the behavioural models analyzed.

The different test networks are shown in Figure 2:

1. Roundabout
2. Give-way Intersection
3. Traffic-light intersection
4. On-Ramp
5. Merge-Diverge
 Parameters involved in the analysis are:
- Reaction Time: the time it takes a driver to react to speed changes in the preceding vehicle.
- Reaction Time at Stop: the time it takes a driver to react to a change in the respective traffic light. Only the first vehicle in this traffic light queue is affected by this reaction time at the traffic light - other vehicles use the normal reaction time.
- Vehicle Length: the mean length of vehicles in the traffic scenario
- Jam Density: the capacity of the link. When a lane reaches this value it is considered full and no more vehicles can enter the lane until the first vehicle leaves.
- Max Give-way time: when a vehicle is in a give-way situation, it applies the gap-acceptance model in order to cross.
- Max acceleration: the maximum acceleration, in m/s$^2$, that a vehicle can achieve under any circumstances. This acceleration is used only in the gap-acceptance model for estimating the time needed to get to the collision point.

Although not all the different parameters are expected to play a role in the different scenarios, in the analysis all these parameters have been included in all the scenarios.

In Figure 2, the different parameters have been reported along with their range of variability. These ranges are an input of the sensitivity analysis (referred to as “input factor distributions” in Figure 1) since, as no other information is available, the different parameters are expected to be uniformly distributed among them. The table includes the replication random seed; this is a number that determines the sequence of random numbers used during the traffic simulation (for example to simulate the arrival process in the network, to assign parameters to the different vehicles and so on). In practice it is one of
the main drivers of the model’s stochasticity. In common practice, its role is limited by simulating different replications of the same traffic scenario with different random seeds and thereby averaging the results. Since, in this analysis, we would also like to ascertain the share of the outputs’ variance explained by the stochasticity, the random seed has been considered as one of the model inputs. As a final remark, it is worth mentioning that, in the analysis, the traffic demand has been fixed to a value not causing traffic saturation with the default parameter values. As will be highlighted in the concluding section of the paper, the next stage of this research will see also the effect of changes in traffic demand being investigated.

**DACE (Design and Analysis of Computer Experiments) tool for Kriging approximations**

Although novel in the transportation field, Gaussian process (or Kriging) metamodels have become a popular mathematical method in several fields. For this reason, below we will provide only some elements to make the reader more familiar with the method, leaving the details to more specific articles and textbooks (the authors suggest the recent book of Kleijnen, 19, as a reference).

Kriging metamodels were first developed in geostatistics by Krige, even though the mathematical formulation was presented some years later by Matheron (23). A thorough reference in this field can be considered (24).

The simplest type of Kriging, the Ordinary Kriging (which is considered in this work and which is usually sufficient in practice, see 19,25) assumes that the output of a simulation model \( w(d) \) (being \( d \) the vector of the models’ variables) can be estimated by:

\[
 w(d) = \mu + \delta(d) \tag{12}
\]

where \( \mu \) is the simulation output averaged over the whole variables’ domain (or at least over the available experimental points) and \( \delta(d) \) is a zero mean stationary covariance process. It is worth knowing that, while in the Ordinary Kriging \( \mu \) is a constant value, in the Universal Kriging it is a regression model. In the case of a stochastic simulation model, it has been seen that equation (12) holds, being \( w(d) \) the average simulation output over different replications (25).

The output of a simulation model \( y(d) \) predicted by Kriging for a new variables’ combination \( d \) is provided by:

\[
 y(d) = \hat{\lambda}(d, D)'w(D) \tag{13}
\]

in which \( D \) is matrix of the variables’ combination for which the simulation output is known (the vector \( w(D) \)) and \( \hat{\lambda}(d, D) \) is the matrix of weights for the new variables combination \( d \) estimated using the old ones \( D \). \( \hat{\lambda}(d, D) \) values are not constant but decrease as the distance between \( d \) and \( D \) increase (and this is one of the main peculiarities of Kriging in respect to other regression models). The selection of the optimal weights is made using the Best Linear Unbiased Predictor (BLUP), which minimizes the Mean Squared Error of the predictor in equation (13). The solution may be proven to be:

\[
 \hat{\lambda}_0 = \Gamma^{-1} \left[ y + 1 \frac{1 - 1'\Gamma^{-1}y}{1'\Gamma^{-1}1} \right] \tag{14}
\]

being \( 1 \) the \( n \)-dimensional identical vector (\( n \) is the number of the old variable’s combinations in \( D \)), \( \Gamma \) the \( n \times n \) symmetric and positive semi-definite matrix with the covariances of the old outputs \( w(D) \) (\( cov(w_i, w_j) \) with \( i, j = 1, ..., n \)) and \( y \) the \( n \)-dimensional vector with the covariances between the \( n \) old outputs and the output for the variables’ combination to be predicted.

Finally, it can be proven that from equations (12), (13) and (14) it is possible to derive

\[
 y(d^*) = \hat{\mu} + y(d^*)\Gamma^{-1}(w - \hat{\mu}1) \tag{15}
\]

with
\[ \hat{\mu} = (1^T \Gamma^{-1} 1)^{-1} 1^T \Gamma^{-1} w \]

In simulation applications, the elements of \( y \) and \( \Gamma \) are estimated using a correlation function, which is the product of \( k \) one-dimensional functions (being \( k \) the number of variables or parameters of the simulation model). In Kriging applications, a popular function is the Gaussian correlation function (which has been used also here in the application). Using this, the covariances are calculated as follows:

\[
\text{cov}(w_i, w_j) = \prod_{g=1}^{k} \exp \left[ -\theta_g \left( |d_{i,g} - d_{j,g}| \right)^2 \right]
\]

in which \( \theta_g \) is a parameter of the correlation function for the variable \( g \), denoting the importance of the variable itself (the higher \( \theta_g \) is, the less effect the variable \( g \) has).

In order to find the best Kriging metamodel for a simulation model, it is therefore only necessary to estimate the \( k \)-dimensional vector of \( \theta_g \). This estimate is performed using a Maximum Likelihood Estimator. Unfortunately the constrained maximization required for this method is of not simple solution (25). In order to achieve the Gaussian process surrogate of the traffic simulation model, in the present work the Matlab toolbox DACE (26,27) has been used. This toolbox is freely available on the developer’s web-site.

**Metamodel validation criterion**

As already pointed out, different criteria may be used to validate the estimated metamodel, also depending on the specific application. For quantitative analyses, we suggest using one of the methodologies proposed in (15). Since, in the present paper, we are using the metamodel to carry out the sensitivity analysis of the model, in the authors’ opinion these quantitative approaches do not represent the most correct way to validate the metamodel. In fact, it is required that the metamodel reflects the input-output relationship and not that it is able to provide a perfect match with the model outputs. For this reason we used a visual approach in which we visually compared the input-output scatter plots coming from the metamodel and the model (using a different sample than that used for the metamodel estimation, in accordance with the methodology of Figure 1).

The reason for this choice is evident if we consider the scatter plots in Figure 2. Let us consider, for the sake of simplicity, just two possible input-output combinations. Pictures on the left refer to real model outputs whereas pictures on the right refer to the predictions of the metamodel estimated with 128 parameter combinations. If we compare, point-by-point, the different values, we may easily conclude that the metamodel is not able to strictly reproduce the model behaviour (in both cases). However, if we look at the two top pictures, we can easily recognize the following features: i) the outputs spread in the same range \([0,200]\) even if the metamodel shows a more oscillatory character; ii) the most important input-output relationship is achieved in the input range \([0,10]\) and the pattern in the two cases is approximately the same; iii) in both the cases the cloud is denser toward the upper and lower bounds of the outputs and less dense in the centre.

Similarly, in the two bottom pictures: i) in both the cases, most of the flow values are in the range \(4.500-5.200 \text{ veh/h}\), even if the metamodel shows a more oscillatory character, ii) the most important input-output relationship is achieved in the input range \([1.5,2]\) and the pattern in the two cases is approximately the same.

From these common features, in the authors’ opinion, one may expect that the results of the sensitivity analysis should not be totally different. As it will be discussed in the next section, this is totally reflected in the results of the sensitivity analysis.
Application of variance-based sensitivity analysis in the case study

As already pointed out, the calculation of the sensitivity indices from equations (9-10) relies on the choice of the Monte Carlo size $N$. There are no universal recipes for this choice. In order to assess if the indices calculated for a given $N$ are sufficiently stable, it is worth calculating their confidence interval. This can be easily carried out via a parametric bootstrapping \( (7) \). If the resulting confidence interval is sufficiently small, then the number of model evaluation can be considered sufficient.

In the present application the sensitivity analysis on the real model was carried out considering a dimension of the Monte Carlo experiment $N=2^{11}$ and thus a total of 36,864 simulations. The Kriging metamodel was instead estimated with a sample of $2^9$ simulations. The sensitivity indices for the metamodel are then calculated considering a dimension of the Monte Carlo experiment $N=2^{13}$. It is worth noticing that if the metamodel is able to reproduce the model input-output relationship, the evaluation of the sensitivity indices may be significantly more reliable, as they can be evaluated on a significantly higher number of model runs.

Both for the model and the metamodel, the sensitivity analysis was carried out considering four different model outputs – density, mean flows, mean delay time, mean travel time – both on the whole network and on each section of each network. This meant having, per each scenario, from 16 to 52 analyses, repeated on the real model and on the metamodel.

RESULTS

In the present section, results of the model sensitivity analysis for both the model and the metamodel, outputs are presented in a bar-plot graph indicating the confidence intervals. The superposition of first order (white bars) and total order (black bars) indices makes the reader immediately aware of the amount of variance each parameter accounts for per se and in combination with all the other
parameters. For the sake of the available space, per each scenario, only results of the sensitivity analysis for network density and mean travel time are presented. Results are shown in Figures 4-5 for the sensitivity analysis on the network density and on the network mean travel time respectively for the five scenarios. Per each figure, charts on the left show the sensitivity indices calculated on the simulation models, while charts on the right show the same indices for the metamodel predictions. In each chart, 90% confidence intervals for the sensitivity indices are also shown (grey lines).

Results clearly show the strength of the approach adopted. In four out of the five considered scenarios (namely, “Give Way”, “Merge Diverge”, “On Ramp” and “Traffic Lights”), the results of the analysis on the real model and the metamodel are significantly similar. In particular, in the four scenarios the parameters’ prioritization based on both first order and total order indices is always the same and the percentage error in the value of first and total order indices is never greater than 10%. In addition, 90% confidence intervals of sensitivity indices are always smaller for metamodel-based indices (being calculated on a higher number of model evaluations).

Problems arise with the “Roundabout” scenario. In this case, indeed, results are not only numerically different, but also the parameters prioritizations resulted differently. In particular, with both the outputs, a non-influential parameter, the “Reaction Time at Stop”, was found to be one of the most influential. The problem, in this case, is due to the fact that for certain parameter combinations, a gridlock occurs in the model. This causes a discontinuity in the input-output function that affects the performance of the metamodel. However, the charts for the roundabout scenario also appear to be unsatisfactory for the indices calculated on the simulation model: they reveal a totally different model behaviour with respect to the other scenarios with total indices much greater than first order ones. In sensitivity analysis practice this occurrence is not very common and usually warns against possible errors. In practice, gridlocks are likely to have affected the evaluation of sensitivity indices and therefore the results from the roundabout scenario are not considered reliable.

Besides the comparison between the indices calculated with the model and those with the metamodel, it is also interesting to comment on the results of the different analyses in order to understand the relative influence of the different parameters on the outputs of the model for different network configurations.

The following considerations hold:

1) In all scenarios the parameter with the maximum total sensitivity index and the first order sensitivity index is the “Reaction Time” parameter. This was expected as it is the main parameter involved in the car-following model. More interestingly in “On Ramp”, “Merge Diverge” and “Traffic Lights” scenarios, the Reaction Time alone accounts for almost the 90% of the variance of the mean Travel Time. This means that with a correct estimation of this parameter the model is able to predict the average travel time of this type of network configurations with an uncertainty of less than 10%.

2) The Vehicle Length also accounts for a certain share in the output variance for almost all network configurations. This is quite interesting, as this parameter is usually not considered in the calibration of traffic simulation models.

3) As expected, the Give Way Time parameters accounts for a significant amount of the output variance in the Give Way scenario.

4) The Reaction Time at Stop Parameter accounts for just a small amount of output variance in the Traffic Lights scenario. A priori, a higher influence of this last parameter might be expected, but analyzing the results, this parameter has this low influence as it is applied only to the first vehicle stopped at a red traffic light.

5) The Random Seed also accounts for some 10% of the output variance. This has to be considered when evaluating the uncertainty in the results of a traffic study.
FIGURE 3. Comparison of simulation-based (figures on the left) and metamodel-based (figure on the right) sensitivity indices for the five traffic scenarios on the mean density simulation output

- Give-way scenario
- Merge-diverge scenario
- On-ramp scenario
- Roundabout scenario
- Traffic-lights scenario
FIGURE 4. Comparison of simulation-based (figures on the left) and metamodel-based (figure on the right) sensitivity indices for the five traffic scenarios on the mean travel time simulation output.
CONCLUSIONS AND RECOMMENDATIONS

With the increasing complexity of the models involved in the decision-making process it is becoming of crucial importance to analyse them, understand how they work and, in particular, what influences their capability to reproduce physical phenomena. Global sensitivity analysis is the family of tools to be used with this aim.

Unfortunately it is common opinion that only a minority of sensitivity analysis practitioners make use of the most sophisticated techniques made available in the recent years. The problem is that, even with the most sophisticated sampling strategies, the exploration of the input space required by any global sensitivity analysis approach requires many model runs to be performed. When the model is computationally expensive, which is fairly common in the applications, sensitivity analysis becomes unfeasible. To deal with this issue, in recent years, some studies have made use of metamodels. Metamodels provide inexpensive emulators of complex and large computational models.

In this paper we have evaluated the possibility of performing the sensitivity analysis of the Aimsun mesoscopic simulation model on a Gaussian process metamodel estimated on a few hundred combinations of the Aimsun parameters. A key factor in a correct and efficient estimation of the metamodel is the selection of a low discrepancy sampling strategies. To this aim, Sobol sequences have been used.

The comparison of the results achieved using the model and a metamodel estimated on 512 parameter combinations showed the strength and the parsimony of the tested methodology, opening up to future spread of the most sophisticated sensitivity analysis techniques in the traffic simulation field.

Current research activities include the analysis of the combined impact of traffic demand and model parameters on traffic simulations, the different impact of different OD pairs (in order to simplify the OD estimation process) and so on. As usual, the ultimate objective of the work is to achieve a better understanding of traffic simulation models in order to improve their use among researchers and practitioners.

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