Algorithmic calibration of Land-Use and Transport Integrated models

Cédric Boittin Nicolas Gaud Vincent Hilaire

***Abstract*—Starting in the USA and now spreading to Europe, Land-Use Transport Integrated models meet a growing interest among urban planners and decision makers. However, with the development of microsimulation techniques, these models become more and more complex, and their calibration turns out to be a real problem, while no standard method exist to solve it. This paper proposes a calibration workflow for LUTI simulations. It also focuses on the variable selection in choice models: an essential aspect which, in practice, is often badly performed.**

I. Introduction

The management of the transportation facilities and the evolution of the urban land-use has been at all time a major stake in the cities' development. In the last century, many studies tackled these two aspects, and emphasis has been set on the relationships between them. It is now of common knowledge that land-use evolution induces a change in the transportation needs, and conversely. Since the 1950s, researchers have tried to simulate this interaction by developing Land-Use Transport Integrated (LUTI) models. Figure 1 illustrates those models' interactive nature and their complexity [1].

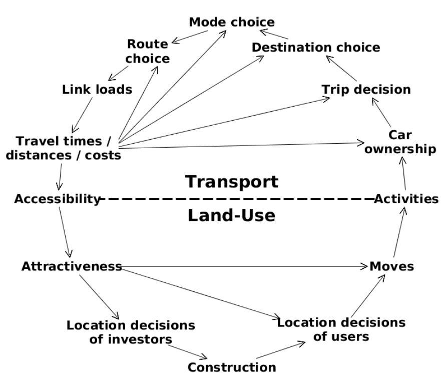

Fig. 1. *Land-Use/Transport feedback cycle (from [1])*

LUTI modeling is an interdisciplinary field, crossing scientific disciplines such as econometry, demography or transport engineering. The models are used as foundations for various simulation applications. Simulation results must be consistent with observations of the real world and can therefore serve as a basis for theoretical studies of the evaluation and forecasting of real systems behavior. An objective of LUTI simulations is to predict the evolution of an urban area, based on assumptions made in scenarios or policies considered in specific studies, and on a 20-30 year horizon. Eventually, the goal is to evaluate these policies or scenarios, and thus to determine the best option according to the simulation's results.

Though LUTI models use is growing, their spreading is slowed down because of the low confidence in their results. Indeed, with such complexity and size, it is hard to produce reliable forecasts. That is why the main focus in current LUTI research is about calibration and validation techniques. This paper contributes to LUTI models calibration, and in particular to variable selection which is often overlooked.

In section II, this paper will formally describe some of the inner processes upon which LUTI models are built, thus outlining the importance of the calibration problem, with the example of choice models. Next in section III, the usual practice for calibration of this type of model will be depicted. Last, section IV will define an algorithmic approach for variable selection based on the practical methods.

II. Background

Designing a LUTI model is a difficult task. First, the modeller must choose which aspects to take into account, so that the simulation may provide information which is relevant to the problem at hand. Then, each of the resulting submodels must be incoporated and scheduled in the global model. From there, it is possible to go further inside the submodels, and tune them with respect to the global scheme. Once everything is finely set up, one must validate that the model is an adequate representation of the target system. These steps are the usual workflow of designing simulation models [2]. However, given the heterogeneity of the submodels, their number, their inner interactions, and the size of the problems involved, it becomes exceptionally complicated and time-consuming.

Each submodel is a smaller simulation model of its own, and should be treated with the procedure mentioned above. In particular, every submodel should be properly calibrated. But, it is notorious that independent calibration of the submodels alone will not give accurate results on a global scale. Several types of approaches to solving this problem have been listed in [3]. Yet, the tools are missing for achieving it.

A. Calibration of LUTI models

Like any simulation model, LUTI models contain multiple parameters which are used to represent the characteristics and behavior of its components, and their interactions. Various calibration and validation steps prove to be essential to ensure that the proposed model is an acceptable approximation of the reality under certain conditions defined in the considered scenario, and this is especially true in the context of long-term predictions. In essence, calibration is the process of adjusting the parameters of the model so that its results are closer to the reality. The findings and conclusions based on uncalibrated or inappropriately calibrated models could be misleading and even erroneous. Thus, proper calibration is a crucial step in simulation [4], and this paper focuses on achieving it.

Even though the question remains critical, there is no standard process of LUTI models calibration. Instead, modelers refer to usual procedures for calibrating small parts of the model, with little care for the global scheme and for the specificities inherent to LUTI models. The authors' objective is to determine a methodology and the associated tools to help fix this problem, and thus contribute to the definition of a standard calibration process.

B. Utility

Discrete choice modeling is a key aspect in the LUTI field. LUTI models aim to simulate the decision making process of considered actors (companies, households, etc.). For example, a company's location choice influences the number of available jobs in an area, which in turn may attract people to relocate closer to this area, as well as inducing more trips to and from this area. With the relocation of the people, building construction is increased, thus influencing companies relocation.

Choice models are usually defined as Utility-maximization problems. The Utility function explains the behavior of an individual making a decision when confronted with several possibilities: it analyzes its alternatives and tries to evaluate them according to several criteria of different importance. Note that individual here is meant in a broad sense, that is an entity making decisions and not necessarily a person. Formally, Utility can be defined for each individual i and alternative j, as a function $u_{ij} = f(x, s)$ where s is a vector of individual characteristics influencing tastes, and x is a vector of observed attributes of a choice [5]. x and s correspond to the selection criteria the individual judges important. The choice model then amounts to an optimization of this utility. In practice, f is often expressed:

$$f(x, s) = A.x + B.s + \varepsilon_{ij} \tag{1}$$

with A and B vectors of real numbers, with the same sizes as x and s. The elements of A and B represent the relative importance an individual associates with each criterion. This representation of the Utility is called linear-in-parameters : each characteristic is weighted by a single parameter. It is neither possible, nor profitable that the whole decision process of the individual be fully tackled by the characteristics vectors. For modelling purposes, a random term ε is added to the expression of the utility so that it expresses the true utility. Of course, the random part is unknown to the modeler, who will have to make assumptions about its value. Most of the time, a probability distribution is assumed for ε, so that the the probability for the individual to choose each alternative can be more easily calculated [6].

For example, in the most commonly used choice model – the Multinomial Logit (MNL) – each ε_{ij} is assumed to be independently and identically distributed extreme value.

C. Means of action

Obviously, any model built upon the Utility function is primarily dependent on the quality of this function. As choice models are central in the LUTI field, their calibration is a key aspect. Following Equation 1 and given a particular distribution for the random variable ε, two means of action appear for calibration: the tuning of the weighting vectors A and B, and the composition of the characteristics vectors x and s. The latter is referred to as variable selection.

The optimization field provides a wide array of methods for the tuning of the weighting vectors. In the LUTI domain, this step is usually achieved by statistical methods of likelihood function maximization, as will be described in section III. It is called model estimation. Variable selection, in the other hand, is often performed ad-hoc by the modeller, without a rigorous procedure. In order to get good results, it is mandatory to pay due attention to this aspect. Current research trends have shown interest in managing it in a more consistent way, by means of sensitivity analysis [7]. A different approach, based on optimization algorithms, is proposed in section IV.

III. State of the Practice

A. Maximum likelihood Estimation

The usual estimation of choice models is performed statistically, by maximization of the likelihood function. The likelihood function is a function of the parameters of the model: it is equal to the probability of the observed outcomes given these parameters' values. Given the outcome x of a random variable X, and a probability distribution f depending on a parameter θ, the likelihood function is expressed as

$$L(\theta|x) = f_\theta(x) \tag{2}$$

The likelihood indicates how likely one value of θ is, given an outcome x. Its interest lies in comparing different values θ_i of θ: the θ_i with maximum likelihood will be the estimate. In practice, the logarithm of the likelihood function is often used instead of the pure likelihood, since it allows an easier calculation.

B. Statistical criteria

This kind of approach is particularly convenient: it allows a quick calculation of well-suited weighting vectors, and it offers several criteria which allow the comparison and evaluation of the output model. In particular, the maximum value of the log-likelihood is used as an estimator of the model goodness: two different parameter values can be sorted according to their maximum likelihood value. However, in order to keep the model as small as possible, it is often useful to penalize this value. Several derived criteria exist for achieving this: for example the Akaike Information Criterion (AIC) or the Bayesian Information Criterion (BIC, sometimes called Schwartz Information Criterion). The first one is expressed as

$$AIC = 2k - 2\ln L$$

where L is the likelihood of the model and k the number of parameters. The expression of the BIC resembles that of the AIC:

$$BIC = -2\ln L + k\ln N$$

with N the number of observations in the sample used for estimation. The BIC penalizes the number of parameters more than the AIC, especially in large samples. These two criteria, along with several others, allow comparing any two models, and can therefore be used in variable selection.

Maximum likelihood estimation is especially suitable to the estimation of choice models based on linear-in-parameters utility, such as in equation 1. This way, the likelihood function is globally concave, and it possesses only one local optimum, which is consequently the global optimum [6]. Very efficient techniques exist for reaching the optimum in these conditions.

Another useful criterion is the p-value. It is not related to the maximum likelihood estimation ; instead, it relies on a statistical hypothesis test. The hypothesis is that the parameter θ_i is irrelevant in regard to the other parameters θ_j. The test gives a confidence in the rejection of that hypothesis: if it is high enough, then the hypothesis can be rejected, which means the parameter is in fact relevant in the model. Several statistical tests exist for calculating p-values, such as the student's t test or the z-test. A good model should contain only relevant parameters.

C. Critics

These are really useful tools for estimating and comparing models. Still, they are not ideal. First, these methods are based solely on one given state of the system, while the model is supposed to capture the evolution of this system in time. The more the simulation advances in time, the more the estimated model is wrong: because it has been designed statically from a different state than the current.

Moreover, maximum likelihood estimation fully captures the different types of error in the input data, since it is based purely on it. In particular, the sampling of the data can severely bias the estimation. When running the estimated model multiple times, these errors successively add, which makes it hard for the model to be used in long-term predictions like we would like it to.

It is possible to counter, at least partially, these two problems: by integrating model estimation inside a more competent method of model calibration. Having two different terms is therefore relevant here : estimation can be seen as a preliminary step, which outputs a good candidate model for calibration. When calibrating, we use reference data, different from the input data used in the estimation. This way, it is possible to capture the dynamics of the system : its evolution is measurable by evaluating the difference between the two data sets.

D. Misuse of the methods

Even in the sole estimation of the models, the way statistical indicators are used in practical applications is questionable. Tools for calculating the estimated optimal parameter values exist, and they are efficient. But, no standard method for variable selection exist, and LUTI modellers often overlook it. Comparison using the available information criteria is commonly carried out, but only a few different selections are tested [8]. There is no guarantee of obtaining, or even approaching an optimal selection of variables.

Furthermore, since there is no standard in the realisation of this task, it is entirely up to the modeller to choose which different models he will test. The irregularity in the quality of the estimated models is therefore accentuated. Also, it makes the comparison between different applications even more difficult because of the additional inconsistency between estimation procedures.

An effort of standarization of the variable selection procedures could help answer those issues. A proposition is presented in the next section.

IV. Algorithmic calibration of LUTI simulations

The authors' objective is to contribute to a general framework for the full design of problem-tailored LUTI simulations, which would ideally bring solutions to every difficult aspect of the problem. This section stands as a first step in that direction, it is an attempt to answer the problematics raised in section II. A workflow of the calibration of a LUTI model is proposed, and its relevance is argumented.

A. Calibration workflow

The proposition of a standard process for LUTI models calibration consists in six steps performed in sequence, as pictured in figure 2. The process itself is relatively standard in simulation calibration [9], but it exploits some of the specificities of LUTI models.

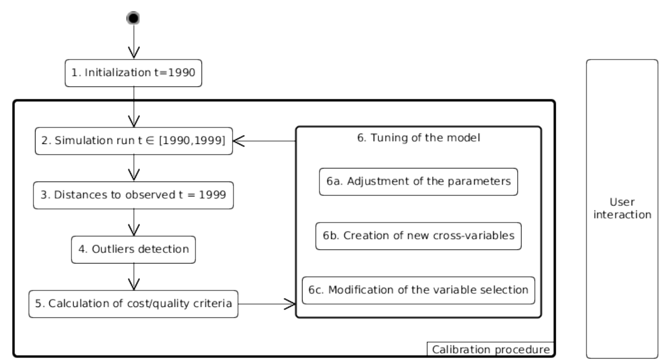

Fig. 2. *Calibration workflow*

In step 1, a first variable selection, and the associated parameters values, is determined. Both the variable selection and the parameters estimation should be decent, for their fine tuning in the next steps must be as quick as possible. Indeed, the full simulation run usually takes some time, and there is a necessity of running it a minimal amount of times. Step 1 does not need to be performed based on full simulation runs. Statistical estimation procedures can be used when available, or a simplified model can be worked out. Next, the step 2 consists in a succession of tasks, repeated until a pre-defined satisfaction criterion is met.

The tasks 2 and 3 are self-explanatory : the simulation is run on the current configuration, and several measures of distances are calculated. The expression of the distances depends on what is modelled and what is expected of the model. They should be precisely described. It is possible to measure distances associated with several different aspects of the model, for example, a households-related distance, and a companies-related distance. By fully tackling these aspects, the quality criteria gain in both precision and meaning.

Additionally, since the system is partitioned into several areas, a distance should be expressed for each one area. In task 4, the objective is to spot the zones or individuals for which the model is wrong, or less correct. It is optional, but given the size and the spatial dimension of the system, and the eventual voids in the available data, it is almost certain that the model will not evenly apply. Detecting those outliers benefits in two ways : it is a profitable information for the modeller, and it may serve the calibration process. For example, in task 5, the model is evaluated according to one or several quality criteria, which also have to defined. These criteria are mainly based on the distances calculated in task 3, but they can make use of the outliers detected in the previous task as well. It is advised to assign one quality criterion for each modelled aspect. This way, the calibration procedure gains in meaning and, more importantly, in adaptability.

The model is then tuned depending on those criteria, in task 6. As stated in in section II, there are two means of action : the adjustment of the parameters values (6a), and the modification of the variables selection. In order to modify the variable selection, it is possible to exchange some of the model's variables for some other among the available ones (6b), but also to create new ones. In particular, cross-variables are interesting to consider (6c). Cross-variables are the combination of two variables from the input set. Hopefully, they will capture an interesting feature of the system, which was unnoticeable from the raw data. In addition, user-interaction may be implemented (6d). This way, the user can check the results of calibration in real-time, and control the evolution of the calibration process. For instance, he can cut unpromising search directions, set static a desired portion of the model and later release it, or even input aspiring search directions for quick testing.

The proposed workflow has several advantages : it is general enough to be used either for one submodel, fixing the rest of the model, or globally with the parameters of all models. This allows for any kind of global calibration methods, as described in [3]. It also makes interaction with the modeller possible, during the calibration procedure. Calibration is essentially an optimization process. Techniques of interactive optimization exist and are meeting growing interest among the community [10]. In the case of LUTI models, which are inherently complex, it would have the triple advantage of reducing the computational complexity by guiding the search, increasing the confidence in the calibrated model – thus of its results – and improve the adaptability of the model by incoporating the modeller's desires into the model in an easier and integrated manner. It also permits the user to more precisely understand what is really happening during the calibration process, and hopefully to better understand the modelled system.

In the next part, a variable selection algorithm is presented. It is meant as a tool to solve the step 1 of the proposed workflow.

B. Variable selection algorithm

The biggest blank in LUTI model's calibration is the variable selection procedure. Here, we explain its difficulty, and propose a simple algorithm which will help performing this task in a more efficient, rigorous, and reliable manner.

The complexity of variable selection comes from its search space. The search space is $\mathcal{P}(V)$ the power set of V, with V the set of available variables. $\mathcal{P}(V)$ is the number of different subsets of any size in V. If the cardinality of V is n, then the cardinality of $\mathcal{P}(V)$ is 2^n. Its scanning is therefore a computationally challenging task, as n isn't limited to small values in LUTI applications. Moreover, its shape is very irregular, and chances are that it contains many local optima.

Still, an effort has to be done in that direction. In this paper, a first optimization approach to variable selection is proposed, which successively increases an initial random solution in order to get an acceptable one to input to the calibration process. Algorithm IV-B works as follows : until no improvement, remove variables from the model if it improves its quality, then add variables to the model if it improves its quality. By testing on the entire set of available variables, this procedures guarantees that the resulting model is a local optimum.

Algorithm 1 Local variable selection optimization

```
Algorithm variables
M : set of model variables
V : set of available model variables

function IMPROVE_MODEL(M)
    referenceObjective ← EVALUATE(M)
    improvement ← True
    while improvement do
        improvement ← False
        for m in M do
            M.remove(m)
            objective ← EVALUATE(M)
            if objective < referenceObjective then
                referenceObjective ← objective
                improvement ← True
            else
                M.add(m)
            end if
        end for
        candidates ← V − M
        for c in candidates do
            M.add(c)
            objective = EVALUATE(M)
            if objective < referenceObjective then
                referenceObjective ← objective
                improvement ← True
            else
                M.remove(c)
            end if
        end for
    end while
end function
```

This algorithm has several benefits. First, it ensures the resulting model does not have any local improvements. It is possible to use it as is, from any valid random solution, but also to test and improve a small subset of predefined models. It doesn't require too many evaluations of the model's quality, which can be rather time-consuming in LUTI applications. It is possible to use either likelihood-based criteria or a distance function as the model's quality. Interaction is not planned as it stands, but this kind of procedure could easily be tweaked to allow it. Being able to set fixed parameters could indeed be interesting for the modeller.

However, this algorithm does not guarantee to reach the global optimum – the best model according to the available data. The algorithm sticks to a local optimum, which can be far from the true optimal solution. That is why this local search procedure should be run iteratively, with several different initial solutions. This permits to widen the exploration of the search space, and increase the reliability of the resulting solution.

Section III also mentioned the p-values, as an indicator of (ir)relevance of a single variable in regard to the composition of the model. It might be added in the algorithm to ensure the consistency of the model : when comparing the objective of two models, make sure that the candidate one has a valid p-value for each variable, and discard it otherwise.

V. Conclusion

LUTI simulations involve a wide variety of submodels, and along with their heterogeneity, their inner interactions, and the size of the modelled systems, this makes for very complex models. Calibrating such models is therefore a difficult and critical task, especially since they are expected to produce reliable forecasts. Discrete choice submodels are an important element in LUTI simulation models, and their calibration necessitates to deal with two aspects: variable selection and parameter tuning. The statistics field provides competent tools for solving those problems, but variable selection is often overlooked and poorly performed.

This paper proposed a calibration process suited to LUTI models, with the associated methodological guidelines. To complete the LUTI simulations calibration methodology, a set of tools should be provided, and a first proposition has been made as an alternative to the available statistical methods of variable selection. A local optimization algorithm has several benefits: it allows testing and improving pre-defined models, and eases the comparison between two models by ensuring they don't have local improvements.

This work could be extended by adding interaction into the proposed variable selection process, and into the calibration of LUTI simulations in general. Interaction meets a growing interest in the optimization field, and could be really profitable to LUTI modelling since it would allow experts to infer their knowledge into the system in a most efficient manner.

Acknowledgments

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