Calibration of an Integrated Land-Use and Transportation Model Using Maximum-Likelihood Estimation

Parikshit Dutta, Elise Arnaud, Emmanuel Prados, Mathieu Saujot

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Abstract

The focus of this work is calibration of the land use module of an integrated land use and transportation model (ILUTM). The calibration task involves estimating key parameters that dictate the output of the land use module. Hence, an algorithm based on maximum likelihood estimation (MLE) is developed for calibration. Furthermore, the observed values of the outputs from the land use module are assumed to admit a Gaussian error.

The ILUTM methodology used here is TRANUS which is used to model the city of Grenoble in France. The aforementioned algorithm is then applied to calibrate the land use module of the Grenoble model. The covariance of the Gaussian error term is assumed to be unknown. It is represented as a function of the land use module inputs and "hyperparameters". The resulting MLE optimization problem has 111 parameters to be estimated, 90 of which are land use parameters and 21 are hyperparameters of the Gaussian covariance kernel. The performance of the proposed calibration methodology is then compared to traditional calibration techniques used for land use and transportation models, when applied to the Grenoble land use model. It is observed that the proposed method outperforms the traditional technique when compared based upon a given quantity of interest.

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Index Terms

Integrated land use and transportation, calibration and validation under uncertainty, maximum likelihood estimation, Gaussian process modeling, supervised learning.

1 INTRODUCTION

In recent years, due to constantly increasing environmental awareness, urban sustainability has become a key policy issue. The European Commission for Sustainable Development Strategy (EUSDS) has clearly identified environmental protection as one of the four objectives for sustainable development [1]. Moreover the 2009 review of EUSDS has emphasized the creation of a low carbon economy and fight against climate change, as major focus areas [2]. It is a well known fact that land use and transportation modeling plays a key role in the context of urban sustainability [3]. Hence, integrated land use and transportation modeling is important in order to create sustainable cities for future [4].

The integration of land use and transportation creates a complex system both temporally and spatially, which evolves in different scales [5]. Analyzing such systems, especially in presence of uncertainty is typically a difficult problem [6, 7]. Calibration plays a central role in such cases, as it helps us determine optimal parameters to create a reliable model. But it results in a problem which is hard to solve, since the parameters to be calibrated are large in number with hardly any prior information available about them. Also, the observed data set is erroneous and sparse [8]. Traditionally, calibration of such models is done manually, using expert opinion about variation of parameters gained through years of experience and practice [6, 9]. It is a well known fact that such a process is tedious and time consuming [10]. Moreover, it cannot be discounted that the method is not error free [11]. All these reasons emphasize the need of a better and comprehensive method of calibration, where the parameters to be calibrated can be estimated from the observed data, taking into account inherent errors.

For most mathematical models, if the number of parameters is large and the observed data is erroneous, calibration can be performed in maximum likelihood (ML) framework [12], where the state estimate is the parameter which maximizes the *likelihood*

function. However, up until now, ML framework has not been used to calibrate ILUTMs. Maximum likelihood estimation (MLE) yields estimates of the unknown quantities that maximizes the probability of obtaining the observed set of data. MLE has found application in myriad areas; from wireless communication systems [13] to psychometrics [14], and from astrophysics [15] to genetics [16]. MLE has several desirable properties; for example the estimate is *asymptotically efficient*, is *invariant* and is *consistent* [17, 18, 19]. Several other properties of MLE along with proofs can be found in the book by Sorenson [20]. This work uses MLE to estimate parameters of a nonlinear regression model, with erroneous outputs. The error in the outputs is assumed to follow a Gaussian process.

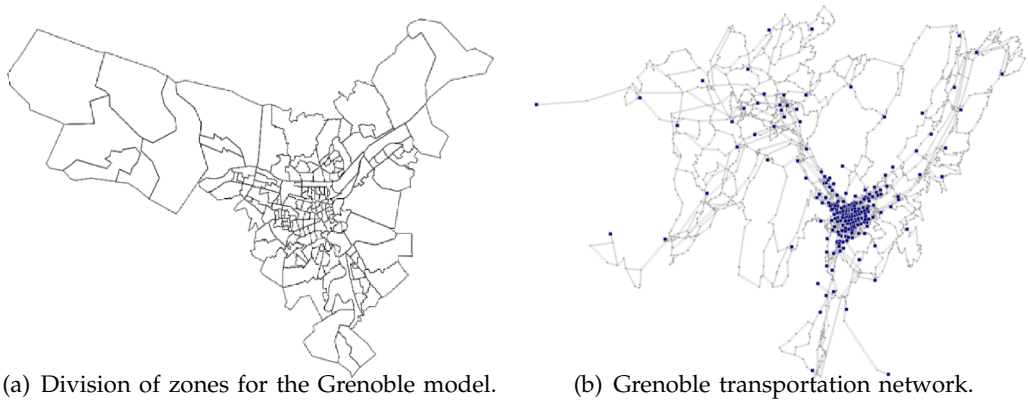
Gaussian processes has been widely used in statistics and machine learning communities for modeling natural processes for regression and classification [21]. The advantage of using Gaussian process is that the modeling technique is entirely data-based and is a generalization of nonlinear multivariate regression. The approach does not require the modeler to specify the structural relationships between independent and dependent variables. Instead, the modeler specifies the covariance structure of the outputs in terms of the input parameters and hyperparameters [22]. In a nonlinear regression setting, often the errors in observed outputs are modeled to follow a Gaussian process. In such cases, MLE can be used to estimate parameters [23, 24]. Use of Gaussian process to represent observation errors and subsequently estimating model parameters using MLE is often known as *krigging* [22]. In this work, we have modeled the outputs of the land use module of an ILUTM as a nonlinear regressor, whose error term follows a Gaussian process. Thereafter, the parameters of the land use module, and the "hyperparameters" of the Gaussian covariance kernel are estimated using MLE. Although the estimates obtained using the aforementioned algorithm, has all the advantages of a ML estimate, there are certain drawbacks to this technique. MLE is prone to "overfit" the given training data, and also it does not incorporate prior knowledge about the parameters [20]. The overfitting problem can be avoided by regularization of the MLE objective function. Moreover prior knowledge can be encoded if the parameters are estimated in a Bayesian setting [12]. However, land use module of an ILUTM has an unique nonlinear structure, with no known regularizer. On the other hand, *a priori* information in terms of expert opinion may be available and can be used to approximate a prior

probability density function (PDF) if Bayesian estimation is performed. However, it is a challenging task in itself to encode expert opinion in terms of prior PDF. In this work, prior knowledge about the land use parameters has been used to find appropriate ranges of parameters as well as the starting point for the nonlinear programming (NLP) solver, used to solve the MLE optimization problem.

A lot of work has been done on regarding uncertainty analysis in land use and transportation models [25, 6]. These research mainly focus on propagation of uncertainty during calibration of parameters and prediction of land use and transportation scenarios, and sensitivity analysis of the land use and transportation parameters. As far as parameter estimation is considered, Sevcíková *et al.* have used *Bayesian melding*, where they use maximum *a posteriori* estimation, to find optimal parameters in UrbanSim, an ILUTM [26]. Likewise, Clay *et al.* have investigated on multivariate uncertainty analysis along with validation exercises for MEPLAN [27]. But a comprehensive analysis, where the uncertainties have been modeled to follow a certain random process, and furthermore calibration in presence of uncertainties has largely been ignored. In this work we have taken into account uncertainties while analyzing the land use part of land use and transportation models. The observed data of the land use module is modeled to admit a Gaussian error. The land use and transportation modeling system used here is TRANUS. We have applied MLE to calibrate the land use part of TRANUS, which is used to model the city of Grenoble, France. TRANUS has been used by city planners and modelers to predict future land use and transport structures in many cities [28]. It uses several discrete choice logistic regression models, which are linked consistently with each other. Detailed description of the TRANUS modeling philosophy is omitted here and can be found in [28].

This paper has two key contributions. First, we show how the observation errors of the land use module of TRANUS can be modeled as a Gaussian process, which further enables the use of nonlinear regression techniques for parameter estimation. Secondly, we show that calibration of the land use module of TRANUS can be done by solving an optimization problem in ML framework. Further, we provide strong numerical results suggesting that the proposed calibration technique is superior than the traditionally used calibration methodology when applied to Grenoble model of TRANUS.

The rest of the paper is organized as follows: in Section 2, the technique of MLE is introduced, and calibration methodology using MLE is presented in context of land use models. In Section 3, the TRANUS land use algorithm is introduced, and a calibration algorithm is proposed using MLE. Finally in Section 4, we present the results of application of the proposed calibration algorithm on the land use model of Grenoble, France.



(a) Division of zones for the Grenoble model. (b) Grenoble transportation network.

Fig. 1. Figure representing division of zones in the Grenoble urban agglomeration. The left figure is a map of Grenoble urban area and shows how it is divided into geographical zones. The right figure shows how they are interconnected through transportation network. TRANUS finds the production values for each sector in table 1 in each zone. The figures are not to scale.

2 Calibration Using Maximum Likelihood Estimation

Consider a vector valued function $f : \mathcal{D}_y \times \mathcal{D}_\rho \mapsto \mathcal{D}_X$, and let $X \in \mathcal{D}_X$ $\rho \in \mathcal{D}_\rho$ and $y \in \mathcal{D}_y$ be the vector of outputs, parameters and input data respectively, where $\mathcal{D}_\rho \subset \mathbb{R}^p$, $\mathcal{D}_y \subset \mathbb{R}^n$ and $D_X \subset \mathbb{R}^q$, and $q, n, p \in \mathbb{N}$. p is the number of parameters in the model and n and q are sizes of input and output vectors respectively.

Let $X_o \in \mathcal{D}_X \in \mathbb{R}^n$ be the vector of random observed outputs. The calibration task involves finding the parameters ρ such that the outputs of the model X are consistent with the observations X_o. If the observations are modeled as in conventional nonlinear

regression analysis, then

$$X_o = f(y, \rho) + \eta, \tag{1}$$

where η is the error between observed and modeled behavior. Let us assume that $\eta \sim \mathbb{P}(\eta; \theta)$, where $\theta \in \mathcal{D}_\theta \subset \mathbb{R}^r$ are the parameters of the PDF of η also called the "hyperparameters".

In ML framework, we obtain the estimates of ρ and θ by maximizing the likelihood function. The parameters and the hyperparameters form an extended parameter space $\varphi = [\rho, \theta]^\top$, $\varphi \in \mathcal{D}_\varphi \subset \mathbb{R}^{r+p}$, from which the optimal estimates are found. In other words, the estimate φ, maximizes the probability that the modeled behavior is in agreement with the observations, hence

$$\hat{\varphi} = \text{argmax}_{\varphi \in \mathcal{D}_\varphi} L[\varphi | X_o; y], \tag{2}$$

where $L(\cdot|\cdot)$ is the *likelihood function* and $\hat{\varphi}$ is the *ML estimate*. Likelihood function gives us the conditional probability of observing X_o given the parameters φ and the input data y, which can be written as $\mathbb{P}(X_o|\varphi, y)$. Hence, it is a function of φ for a given value of X_o and y.

If there are s independent and identically distributed (i.i.d.) observations, $X_o^1, \ldots, X_o^s$, obtained from s input sets, i.e. $y^1, y^2, \ldots, y^s$, it is customary to find $\hat{\varphi}$ that maximizes the joint density of the i.i.d. samples, in other words,

$$\hat{\varphi} = \text{argmax}_{\varphi \in \mathcal{D}_\varphi} \prod_{i=1}^{s} L(\varphi | X_o^i; y^i).$$

In practice, it is easier to optimize the logarithm of the likelihood function, especially if the PDF of the observation process belongs to the exponential family. Then resulting function is called the *log likelihood* function. Thus, the optimization problem is given as

$$\hat{\varphi} = \text{argmax}_{\varphi \in \mathcal{D}_\varphi} \sum_{i=1}^{s} \log \left[L\left(\varphi | X_o^i; y^i\right) \right]. \tag{3}$$

The ML estimation problem is generally solved as an unconstrained optimization problem. However, in the presence of constraints between input parameters a constrained optimization problem can be solved. In such cases the optimization problem is written

as,

$$\max_{\varphi \in \mathcal{D}_\varphi} \quad \sum_{i=1}^{s} \log \left[L\left(\varphi | X_o^i; y^i\right) \right],$$

subject to

$$g(\varphi) \leq 0, \qquad h(\varphi) = 0, \qquad \varphi \in [\varphi_l, \varphi_u], \tag{4}$$

where $g(\varphi)$ and $h(\varphi)$ are bounded nonlinear functions. The calibrated parameter $\hat{\varphi}$ is obtained by solving the above optimization problem.

2.1 MLE of a Nonlinear Model with Gaussian Error

If the model outputs are $X = f(y, \rho)$ and $X \in \mathcal{L}_2$, then it is customary to assume that η follows a zero mean Gaussian process, hence $\eta \sim \mathcal{N}(\eta; 0, \Sigma(\theta))$, where θ are the hyperparameters of the Gaussian covariance kernel, $\Sigma(\theta) \in \mathbb{R}^{q \times q}$. Assuming $\varphi = [\rho, \theta]^\top$, from (1) the conditional PDF of the observations given the inputs and the parameters, can be written as,

$$\mathbb{P}[X_o | \varphi, y] = L\left(\varphi | X_o; y\right) = \frac{1}{\sqrt{(2\pi)^q |\Sigma(\theta)|}} e^{-\frac{1}{2}[X_o - f(y,\rho)]^\top \Sigma(\theta)^{-1} [X_o - f(y,\rho)]}. \tag{5}$$

where $\mathbb{P}[X_o | \varphi, y]$ is the conditional PDF of the observations (X_o) given the parameters ($\varphi = [\theta, \rho]^\top$) and $L\left(\varphi | X_o; y\right)$ is the likelihood function. q is the size of the output vector. If there are s i.i.d. observations, the likelihood function will be the product of s terms having same form as (5). The constrained MLE objective function in (4) is then given by,

$$\min_{\varphi \in \mathcal{D}_\varphi} \quad \sum_{i=1}^{s} \left[\frac{1}{2} \left[X_o^i - f(y^i, \rho) \right]^\top \Sigma(\theta)^{-1} \left[X_o^i - f(y^i, \rho) \right] \right] + \frac{s}{2} \log\left(|\Sigma(\theta)| \right). \tag{6}$$

The estimated parameter $\hat{\varphi}$ is the argument that minimizes the above optimization function subject to the constraints in (4).

2.2 Special Case for Land Use Models

Let $f(\cdot, \cdot)$ be the land use model and X_o be the observed data corresponding to outputs of the model. The constraints on the parameters are linear and are generally given by

inequalities. Hence, the MLE optimization problem in (4) can be formulated as,

$$\min_{\varphi\in\mathcal{D}_\varphi} \quad \sum_{i=1}^{s}\left[\frac{1}{2}\left[X_o^i - f(y^i,\rho)\right]^\top \Sigma(\theta)^{-1}\left[X_o^i - f(y^i,\rho)\right]\right] + \frac{s}{2}\log\left(|\Sigma(\theta)|\right),$$

subject to,

$$\mathcal{A}\rho \leq b, \tag{7}$$

where $\mathcal{A}\in\mathbb{R}^{h\times p}$ represents the linear constraint matrix and $b\in\mathbb{R}^h$ is a vector. Note that we have included the upper and lower bound information of the parameters in matrix $\mathcal{A}$. An example of how matrix $\mathcal{A}$ is constructed will be given in Section 4. The objective function in (7) can be augmented to form the Lagrangian from where the first order necessary conditions for optimality can be derived. Let $\mu\in\mathbb{R}^h$ be the Karush Kuhn Tucker (KKT) multipliers. Then using properties of matrix derivatives and utilizing the fact that the objective function is a scalar, the derivative of the ML objective function can be obtained,

$$\begin{aligned}\frac{\partial L(\varphi|X_o;y)}{\partial\varphi} &= -\sum_{i=1}^{s}\left[\frac{\partial f(y^i,\rho)}{\partial\varphi}^\top \Sigma(\theta)^{-1}\left[X_o^i - f(y^i,\rho)\right]\right] + \mathcal{A}^\top\mu + \frac{s}{2}\,\mathbf{Tr}\left[\Sigma(\theta)^{-1}\frac{\partial\Sigma(\theta)}{\partial\varphi}\right]\\ &\quad -\frac{1}{2}\mathbf{Tr}\left[\Sigma(\theta)^{-1}\frac{\partial\Sigma(\theta)}{\partial\varphi}\Sigma(\theta)^{-1}\sum_{i=1}^{s}\left[X_o^i - f(y^i,\rho)\right]\left[X_o^i - f(y^i,\rho)\right]^\top\right].\end{aligned} \tag{8}$$

Elementary matrix operations used to derive the above equation can be found in Appendix A and a discussion on how the derivatives are calculated is in Appendix C. At optimality, the first order optimality conditions and the complementary slackness condition must be satisfied. Moreover the optimal solution must satisfy the constraints too. Hence, the optimal solution is obtained by solving the following system of equations simultaneously,

$$\begin{aligned}\sum_{i=1}^{s}\left[\frac{\partial f(y^i,\rho^*)}{\partial\varphi^*}^\top \Sigma(\theta^*)^{-1}\left[X_o^i - f(y^i,\rho^*)\right]\right] - \mathcal{A}^\top\mu^* - \frac{s}{2}\,\mathbf{Tr}\left[\Sigma(\theta^*)^{-1}\frac{\partial\Sigma(\theta^*)}{\partial\varphi^*}\right]&\\ +\frac{1}{2}\mathbf{Tr}\left[\Sigma(\theta^*)^{-1}\frac{\partial\Sigma(\theta^*)}{\partial\varphi^*}\Sigma(\theta^*)^{-1}\sum_{i=1}^{s}\left[X_o^i - f(y^i,\rho^*)\right]\left[X_o^i - f(y^i,\rho^*)\right]^\top\right] &= 0, \quad \text{(first order optimality,)} \qquad (9a)\\ \mu^\top\mathbb{I}(\mathcal{A}\rho^* - b) &= 0, \quad \text{(complementary slackness,)} \qquad (9b)\\ \mathcal{A}\rho^* &\leq b, \quad \text{(primal feasibility,)} \qquad (9c)\\ \mu &\geq 0, \quad \forall\mu, \quad \text{(dual feasibility,)} \qquad (9d)\end{aligned}$$

where $\mathbb{I} = \mathbb{I}_{h\times h}$ in (9b) is the identity matrix. The above problem can be solved by using an appropriate NLP solver. For the current work, we have used NLP solvers based on sequential quadratic programming.

3 CALIBRATION OF TRANUS LAND USE MODEL

The land use model of TRANUS [28] is based on random utility theory [29]. Typically it combines traditional input output model with multinomial logit model for allocation of activities and land use. The final output is obtained by recursively solving a set of nonlinear algebraic equations. An intense mathematical description of the model can be found in [29, 30].

Input-output models characterize interactions between market elements, aggregated into *economic sectors*. The model calculates flow of commodities or services between sector, giving rise to productions and demand. For a multiregional model, flow can occur between different regions, adding a spatial element. The different regions are called *geographical zones*. If the region of interest is a city then an example of a geographical zone may be a *neighborhood near an university* or *near an industry* in the city and economic sectors can be *students* or *industry workers*.

The inputs to a multiregional input-output model are *final demand* and *primary inputs* for each sector and zone. From these inputs the *intermediate demands* are calculated. To meet the intermediate demand, *production* of services and commodities is required. The total production for a sector in a zone is essentially seen as the output of the model. If the multiregional input output structure is determined by a multinomial logit model, we have the random utility based multiregional input output (RUBMIO) model.

In this work we calibrate the parameters of the TRANUS land use algorithm which is based on RUBMIO theory.

3.1 Description and Governing Equations for TRANUS

In the literature there are several descriptions of TRANUS [31, 30], which are not exactly identical but share the same principles. The differences are in fact rather minor. Here, we use the mathematical equations detailed in Ref. [30].

Let us have M economic sectors and J geographical zones. Let $Y_i^m \in \mathbb{R}^{M\times J}$ represent the matrix of final demand of sector $m \in \mathbb{N}[1, M]$ in zone $i \in \mathbb{N}[1, J]$. Consider the tensor of *technical coefficients*, $a_j^{mn} \in \mathbb{R}^{M\times M\times J}$, which is a function of υ^{mn}, the demand elasticity of sector m with respect to goods produced in sector n; and P_j^n, which is the price of sector n in zone j. a_j^{mn} is denoted by function described as $a_j^{mn} = \mathbb{F}(P_j^n, \upsilon^{mn})$ (Chapter 5 in Ref. [30]). In TRANUS framework, the demand elasticity υ^{mn} is further a function of $\underline{\mathcal{X}}^{mn}$ and $\overline{\mathcal{X}}^{mn}$ which are the maximum and minimum requirement of sector n per unit of sector m respectively; and δ^{mn} which is the elasticity of sector m with respect to cost of sector n (Chapter 6 in Ref. [30]). Let us also, consider the *utility function tensor* $V_{ij}^n \in \mathbb{R}^{M\times J\times J}$ which is calculated as follows:

$$V_{ij}^n = \vartheta^n \xi_j + t_{ij}^n, \tag{10}$$

where ξ_j is the value of land (real estate) in zone j, t_{ij}^n is obtained from the transport model and is the *transport disutility* for sector n for transportation from production zone i to consumption zone j and ϑ^n is a parameter for regulating the importance of ξ_j^n as compared to transport disutility (Chapter 6 in Ref. [30]).

The intermediate demands and final production outputs of TRANUS are calculated using a nested multinomial logit model. Let us consider that the random dispersion parameter of the multinomial logit model is given by $\beta^n \in \mathbb{R}^M$. Looking at how a_j^{mn} and V_{ij}^n are calculated, we can say that the primary inputs to the land use model consists of $\underline{\mathcal{X}}^{mn}$, $\overline{\mathcal{X}}^{mn}$, δ^{mn}, P_j^n, β^n, ϑ^n, ξ_j and t_{ij}^n.

The intermediate demand in the first iteration is given by

$${}^1D_{ij}^{mn} = Y_i^m a_j^{mn} \frac{\exp\left(-\beta^n V_{ij}^n\right)}{\sum_k \exp\left(-\beta^n V_{kj}^n\right)}, \tag{11}$$

where ${}^1D_{ij}^{mn}$ represents the amount of commodities or services of sector n required in zone j due to the final demand of m in zone i at the first iteration. Hence the total requirements for sector n in zone j is then

$${}^1R_j^n = \sum_i \sum_m {}^1D_{ij}^{mn}. \tag{12}$$

As mentioned earlier, the calculation of intermediate demand is done iteratively. Hence for successive iterations, if $n, m \in \mathbb{R}^M$ are economic sectors and $i, j \in \mathbb{R}^J$ are geographical

zones, the requirement of n^{th} sector located in j^{th} zone in r^{th} iteration is

$$ {}^{r}R_j^n = \sum_i \sum_m {}^{r}D_{ij}^{mn}, \tag{13} $$

$$ \text{where, } {}^{r}D_{ij}^{mn} = {}^{r-1}R_i^m a_j^{mn} \frac{\exp\left(-\beta^n V_{ij}^n\right)}{\sum_k \exp\left(-\beta^n V_{kj}^n\right)}. \tag{14} $$

If the equilibrium is achieved after p iterations then the total amount of sector n in zone j required to be produced is given by

$$ {}^{p}X_j^n = \sum_{r=1}^{p} {}^{r}R_j^n + Y_j^n, \tag{15} $$

where ${}^{p}X_j^n$ is the total production of sector n in zone j and the output of TRANUS land use model.

3.2 Traditional Calibration Methodology

Traditionally ILUTMs are calibrated manually, using feedback from past experience. This is a very cumbersome job and needs expertise based on practice. In practice, calibration of ILUTMs like TRANUS is difficult to achieve, as correcting the parameters to obtain an optimal solution is a delicate task. This calibration method is performed by trial-and-error, where some goodness of fit metric is numerically computed and used to guide the modeler. The calibration can typically take up to 6 months for a medium size model (about 100 geographic zones, about 10 sectors).

3.3 Calibration Algorithm Using MLE

In this work, we apply MLE to calibrate primary inputs of the land use module of TRANUS. The land use module of TRANUS is represented in a similar way as (1), where $f(\cdot,\cdot)$ is the TRANUS land use algorithm and X_o are the observed land use production values. It can be shown that under certain conditions, the outputs of RUBMIO models like TRANUS are $\mathcal{L}_2(\mathbb{P})$ regular (see Appendix B). Hence, the errors in observations are modeled to follow a Gaussian process.

$\underline{\mathcal{X}}^{mn}$, $\overline{\mathcal{X}}^{mn}$, δ^{mn}, ϑ^n and β^n constitute the space of parameters (ρ); and the input space (y) consists of Y_j^n, P_j^n, ξ_j and t_{ij}^n. The parameters are estimated given the inputs and the

observed land use production outputs. Moreover η is modeled as a Gaussian process with unknown covariance. The hyperparameters (θ) of the Gaussian covariance kernel are estimated by solving the MLE optimization problem.

It is well documented that land use and transportation models suffer from lack of data [11, 32]. This is true for most TRANUS models, including the current application. The government agencies collect land use data from population and transportation statistics, maintain them in a form which is not readily usable as inputs and outputs of the land use module of TRANUS. To obtain a set which is compatible with the land use module, data integration is required, which in effect reduces the amount of data available as observation replicates [33]. Even obtaining the said data is difficult, expensive, as well as time consuming. For example, for the present work, integration of data took around 6 months of time. Hence, often the modeler is left with only a single set of replicate. In such cases, constituting the MLE objective function is a difficult task.

To circumvent this problem we have adopted an approach where the observation replicates are created from a single set of observed land use outputs. In other words, let us have M economic sectors and J geographical zones. Then we have a matrix of $M \times J$ land use data available to work with. At first we divide the zones (columns) into *training* and *test* zones, by selecting them randomly. Then within test and training sets, observed output of each sector is assumed to be an i.i.d. observation. However, for a given sector observed output of a zone is assumed to be dependent on outputs of other zones of the same sector. Hence given a zone, observations for each sector within that zone are independent, but given a sector, observations for zones within that sector are not independent. To describe the approach mathematically, let the observed data for sector n and zone j be given by X^n_{oj} and the corresponding inputs be $y = y^n_j$, where $n = 1, \ldots, M,\ j = 1, \ldots, J$. Let the number of training zones be J_{tr} and test zones be J_t, where $\mathbb{N}[1, J_{tr}] \subset \mathbb{N}[1, J]$ and $\mathbb{N}[1, J_t] \subset \mathbb{N}[1, J]$. Then the training data is is given by $\bar{\mathbf{X}}_\mathbf{o} = \{\bar{X}^n_{oj}\} = \{X^n_{oj}\}^{J_{tr}}_{j=1}$ and the test data is given by $\tilde{\mathbf{X}}_\mathbf{o} = \{\tilde{X}^n_{oj}\} = \{X^n_{oj}\}^{J_t}_{j=1},\ \forall\, n \in \mathbb{N}[1, M]$. Amongst training sets we have

$$\mathbb{P}\left(\bar{X}^1_{oj}\bar{X}^2_{oj}\ldots\bar{X}^M_{oj}|\varphi, y\right) = \mathbb{P}\left(\bar{X}^1_{oj}|\varphi, y\right) \times \mathbb{P}\left(\bar{X}^2_{oj}|\varphi, y\right) \ldots \times \mathbb{P}\left(\bar{X}^M_{oj}|\varphi, y\right),\ \forall\, j = 1, \ldots J_{tr},$$

and similarly for test sets:

$$\mathbb{P}\left(\tilde{X}^1_{oj}\tilde{X}^2_{oj}\dots\tilde{X}^M_{oj}|\varphi,y\right)=\mathbb{P}\left(\tilde{X}^1_{oj}|\varphi,y\right)\times\mathbb{P}\left(\tilde{X}^2_{oj}|\varphi,y\right)\dots\times\mathbb{P}\left(\tilde{X}^M_{oj}|\varphi,y\right),\ \forall j=1,\dots J_t.$$

This describes the independence of sectors for a given zone j. But, within training and test sets the following is true,

$$\mathbb{P}\left(\bar{X}^n_{o1}\bar{X}^n_{o2}\dots\bar{X}^n_{oJ_{tr}}|\varphi,y\right)\neq\mathbb{P}\left(\bar{X}^n_{o1}|\varphi,y\right)\times\mathbb{P}\left(\bar{X}^n_{o2}|\varphi,y\right)\dots\times\mathbb{P}\left(\bar{X}^n_{oJ_{tr}}|\varphi,y\right),\ \forall n=1,\dots M,$$

and

$$\mathbb{P}\left(\tilde{X}^n_{o1}\tilde{X}^n_{o2}\dots\tilde{X}^n_{oJ_t}|\varphi,y\right)\neq\mathbb{P}\left(\tilde{X}^n_{o1}|\varphi,y\right)\times\mathbb{P}\left(\tilde{X}^n_{o2}|\varphi,y\right)\dots\times\mathbb{P}\left(\tilde{X}^n_{oJ_t}|\varphi,y\right),\ \forall n=1,\dots M,$$

which shows dependence of zones for a given sector n.An important point to note is J_t is fixed to a certain value while J_{tr} is varied, hence we always have $J_{tr}+J_t\leq J$.

Although the methodology described above is not ideal, our goal here is obtain best possible approximation of i.i.d. observation replicates from the limited data available. Due to the connection of land use module to transportation network there is a production demand and supply loop between geographical zones of a given sector, which leads to strong correlation between them. However, from prior knowledge of TRANUS implementation, we can say that the production output of economic sectors for a given zone are weakly dependent on each other [28, 34]. Hence, the aforementioned approach is justified. A generic way of obtaining observation replicates from the available data will be addressed in our future work.

At first the initial guess for the MLE optimization problem in (7) is obtained by randomly sampling the parameter space using Monte Carlo sampling (accept-reject procedure) to get N_s number of samples. The ML objective function is then calculated after obtaining the outputs from TRANUS. While sampling, an uniform distribution is assumed on the parameters and the parameter ranges are obtained from expert opinion. The accept-reject procedure makes sure that for each sample the constraints on the parameters are not violated. The sample providing the lowest objective function value, in (7) with $s=M$, is considered as the initial guess. Point to note here is that to get the initial guess, no distinction is made between test and training zones and each of the s observations is of size J.

To obtain the optimal parameter values from the training set, a NLP problem is solved, which is formulated according to (7), with constraints upon the land use parameters taken into account. Let the calculated land use assignment values be denoted by $\tilde{\mathbf{X}}$, for all sectors and all test zones. The calibration task is achieved if the square of the $\mathcal{L}_2$ norm of the error between observed and calculated values, also called the *quantity of interest* (*QoI*), for the test set is less than a prespecified value (Q_d).

$$Q = ||\tilde{\mathbf{X}} - \tilde{\mathbf{X}}_o||_2^2 < Q_d. \tag{16}$$

The whole algorithm is shown in Algorithm 1.

For the TRANUS run during optimization, parameters (ρ) for all the sectors and zones are considered. However, TRANUS takes in the inputs (y) for only the zones that are considered as training sets, during training; or inputs for test sets, when the test cases are run. The rest of the inputs are assumed to be zero. Similarly, while evaluating the MLE objective function only the outputs (X) of the training sets are compared to their respective observations (X_o), while training; and the outputs of the test sets are compared to the observations of the test sets after they have been run.

4 Application to Calibrate the Grenoble Model

In this section, we have applied the proposed algorithm based on MLE to calibrate the TRANUS model of Grenoble, France [6]. The results obtained from the proposed model are compared to a traditionally calibrated model of Grenoble, against the *QoI* given in (16). It is observed that, the proposed MLE based algorithm improves the calibration results significantly.

4.1 Description of the Land- Use Model

The Grenoble model considers 21 economical sectors. The economic sectors consists of employment, population and real estate. The real estate represents work place or residence for the population, and population tends to choose the place of residence based upon employment. The sectors that are used for the Grenoble model is given in Table 1. The data for calibrating the land use model are obtained from INSEE[1],

1. Institut National de la Statistique et des Etudes Economiques

Algorithm 1 TRANUS calibration using MLE

Require: $M, J \in \mathbb{N}$, ▷ Sector and zone definitions.

X_{oj}^n ▷ Observed production values.

φ_l, φ_u ▷ Parameter ranges.

y_j^n ▷ Input values.

$f(\cdot,\cdot)$ ▷ TRANUS land use structure.

J_{tr} ▷ Training zones.

J_t ▷ Test zones.

Q_d ▷ Desired *QoI* value.

$\{\varphi_k\}_{k=1}^{N_s} \leftarrow$ MC[Uniform(φ_l, φ_u)]. ▷ Get samples assuming uniform distribution on parameters using accept reject procedure.

$\mathbf{X}_o = [X_{oj}^n]\ \forall j = 1, \ldots, J;\ n = 1, \ldots, M.$ ▷ Vector of all observations.

for $k = 1$ to N_s **do**

  $L_k(\varphi_k|\mathbf{X}_o; y) \leftarrow L[\varphi_k|\mathbf{X}_o; y]$. ▷ $L_k(\cdot|\cdot)$ refers to the augmented Lagrangian of (7) for k^{th} sample.

end for

$\varphi_0, K_0 \leftarrow \text{argmin}_{k\in[1,N_s]}\, L_k[\varphi_k|\mathbf{X}_o; y]$. ▷ Get the initial guess. K_0 is the index.

$\mathcal{K}_0 =$ **NULL** ▷ Rejected initial guess set.

repeat

  $\bar{\mathbf{X}}_o \leftarrow \{X_{oj}^n\}_{j=1}^{J_{tr}}$ ▷ Get the data in training zones (J_{tr}).

  $\hat{\varphi} \leftarrow \text{argmin}_{\varphi\in\mathcal{D}_\varphi}\, L[\varphi|\bar{\mathbf{X}}_o; y] \leftarrow \text{NLP}(L[\varphi|\bar{\mathbf{X}}_o; y], \varphi_0)$ ▷ **Calibration**. Using (7)

  $\tilde{\mathbf{X}}_o \leftarrow \{X_{oj}^n\}_{j=1}^{J_t}$, ▷ Get the data in test zones (J_t).

  $\tilde{X}_j^n \leftarrow f(y_j^n, \hat{\varphi})\ \forall j \in [1, J_t], n \in [1, M]$, ▷ Run TRANUS for test zones.

  $\tilde{\mathbf{X}} \leftarrow [\tilde{X}_j^n]\ \forall j = 1, \ldots, J_t;\ n = 1, \ldots, M$ ▷ Vector of calculated test outputs

  $Q \leftarrow ||\tilde{\mathbf{X}} - \tilde{\mathbf{X}}_o||_2^2$ ▷ **Validation**. Q is the *QoI*

  if $Q > Q_d$ **then**

    $\mathcal{K}_0 \leftarrow [\mathcal{K}_0, K_0]$ ▷ Augment the set of rejected initial guesses.

    $\varphi_0, K_0 \leftarrow \text{argmin}_{k\in[1,N_s]\setminus\mathcal{K}_0}\, L_k[\varphi_k|\mathbf{X}_o; y]$ ▷ Get the initial guess.

  else

    $\varphi_{optimal} = \hat{\varphi}$ ▷ Do nothing, optimality reached.

  end if

until $Q < Q_d$

AURG[2], UNEDIC[3] and EMD[4], for the year 2010. These data have been processed to obtain population and employment by type and by zone as well as the prices of the real estate. The sector classification is based upon the kind of data available and how important is a sector towards land use and policy decisions.

TABLE 1
Description of the sectors.

Sector number	Description	Sector Type
1	Industrial employment	Employment
2	Public employment	Employment
3	Offices, research & development employment	Employment
4	Retail employment	Employment
5	School employment	Employment
6	Household income (rich)	Population
7	Household income (above average)	Population
8	Household income (below average)	Population
9	Household income (poor)	Population
10	Students	Population
11	Individual housing	Real estate
12	Apartment Housing	Real estate
13	Land for economic activities	Real estate
14	Land for shops in urban area	Real estate
15	Social housing	Real estate
16	University	Employment
17	Retail employment (less frequent)	Employment
18	Supermarket employment	Employment
19	Retired income (rich)	Population
20	Retired income (poor)	Population
21	Land for other commercial ventures	Real Estate

2. Agence d'Urbanisme de la Région Grenobloise

3. Union Nationale Interprofessionnelle pour l'Emploi dans l'Industrie et le Commerce

4. Enquète Ménage Déplacement

4.2 Description of the Transportation Network

The Grenoble urban agglomeration is divided into 225 geographical zones, and the transport network is composed of 2413 nodes. The data of the transport network are obtained from the SMTC[5]. The transport data on peak hours are mainly gathered from SMTC, AURG, INRETS[6] and the survey EMD made on Grenoble in 2010. The transportation network along with the geographical zones for the Grenoble model is shown in Fig. 1. In this work we do not calibrate the transportation network. The transportation model parameters are assumed to be known and constant throughout the calibration process of the land use model. However, in future we do plan to calibrate both land use and transportation parameters together.

4.3 Calibration of the Grenoble Model Using MLE

For the Grenoble model, the parameters that are assumed to be unknown are the cost elasticity parameters (δ^{mn}), the minimum and maximum requirement parameters ($\underline{\mathcal{X}}^{mn}$, and $\overline{\mathcal{X}}^{mn}$), the scaling parameter ϑ^n and the dispersion parameter (β^n) (please refer to Section 3 for their definitions). Amongst 210 possible choices of m and n, 22 of δ^{mn} and 21 each of $\underline{\mathcal{X}}^{mn}$, and $\overline{\mathcal{X}}^{mn}$ are assumed to be uncertain. For the other parameters, amongst 21 choices, 8 of β^n and 18 of ϑ^n are uncertain parameters. Hence, in all, there are 90 land use parameters which are to be estimated. The choice of uncertain parameters is based upon expert opinion about the TRANUS Grenoble model and its parameters. As for the covariance of the Gaussian model, it is assumed that the error between observed and calculated total production (X_j^n) for each sector is uncorrelated to each other. The covariance kernel is constructed based on the independence structure given in Section 3.3. For computational simplicity, in the Gaussian covariance kernel, each sector is assumed to be represented by a single hyperparameter, hence the number of hyperparameters to be estimated are 21. If referred to Section 2, $p = 90$ and $r = 21$. The number of outputs and inputs depend on number of test or training zones used,

5. Syndicat Mixte des Transport en Commun

6. Institut National de REcherche sur les Transports et leur Sécurité

hence $n = q =$ number of training/ test zones$\times$number of sectors. s is the number of independent observations which here is the number of sectors, 21.

Several experiments are performed to obtain the structure of the covariance kernel, which would give the lowest value of MLE objective function, while satisfying the constraints. If θ^n is the hyperparameter for sector n, the structure of the Gaussian covariance kernel that gives us the best result is given by, $\Sigma_{ij}(\theta^n) = \alpha\theta^n$, with $\theta^n > 0$, $i, j = 1, \ldots, J_{tr} \times M$ while training and $i, j = 1, \ldots, J_t \times M$ when test sets are used and $n = 1, \ldots, M$ is the hyperparameter number. The parameter $\alpha = 1$, for $i = j$ and $\alpha = 0.1$, for $i \neq j$. Hence, the total number of parameters to be estimated is 111.

The constraint matrix $\mathcal{A}$ for the MLE of TRANUS Grenoble model mainly consists of bounds on the cost elasticity parameters, δ^{mn}. The total number of constraints on the elasticity parameters are 16. They are given in (17a) to (17g). The superscripts here refer to sector numbering as given in Table 1.

$$\delta^{6,11} \leq \delta^{7,11}, \quad \delta^{7,11} \leq \delta^{8,11}, \tag{17a}$$

$$\delta^{6,12} \leq \delta^{7,12}, \quad \delta^{7,12} \leq \delta^{8,12}, \quad \delta^{8,12} \leq \delta^{9,12}, \tag{17b}$$

$$\delta^{8,16} \leq \delta^{9,16}, \tag{17c}$$

$$\delta^{20,11} \leq \delta^{21,11}, \quad \delta^{20,12} \leq \delta^{21,12}, \tag{17d}$$

$$\delta^{6,11} \leq \delta^{6,12}, \quad \delta^{7,11} \leq \delta^{7,12}, \tag{17e}$$

$$\delta^{8,16} \leq \delta^{8,11}, \quad \delta^{8,11} \leq \delta^{8,12}, \quad \delta^{9,16} \leq \delta^{9,12}, \tag{17f}$$

$$\delta^{20,11} \leq \delta^{20,12}, \quad \delta^{21,16} \leq \delta^{21,11}, \quad \delta^{21,11} \leq \delta^{21,12} \tag{17g}$$

The constraints come directly from the TRANUS mathematical description in Ref. [31], and expert opinion about elasticity parameters of the Grenoble model.

4.3.1 Computational Aspects

The Monte Carlo simulations to generate the initial guess sets, were done in *Grid5000* which has around 7000 active cores, equipped with Intel Xeon and AMD Operaton processors [35]. The time taken to run one simulation of TRANUS Grenoble model is 10 minutes. 2000 Monte Carlo sets are generated to get the best initial guess, with batches of 80 sets generated in parallel. Figure 2 shows how the total computational

time varies with number of cores used, for one batch of 80 Monte Carlo sets. Ideally the scaling should be linear. However the graph here takes into account delays due job scheduling in *Grid5000*, message passing and other network based delays, which explains the nonlinear behavior of the graph.

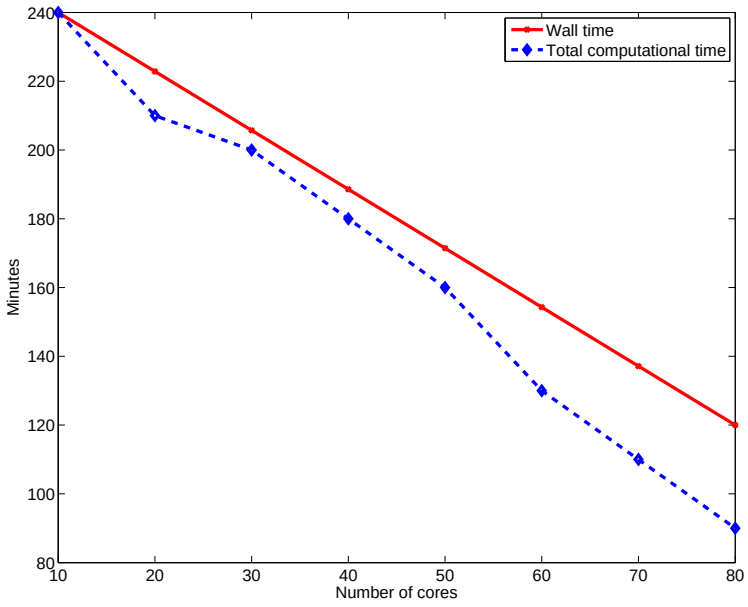


Fig. 2. Computational time comparison to run 80 Monte Carlo sets for TRANUS Grenoble model. We can see that the computational time taken (dashed line) almost scales linearly with number of processors (cores) used.

Large scale NLP solvers were used to solve the optimization problem. The software used here is OpenOpt, which is written in Python programming language [36]. The NLP solver uses line search methods based on sequential quadratic programming. The optimization problem has not been scaled here. It is our future goal to develop a scalable algorithm for calibrating land use and transportation models.

4.3.2 Comparison to Traditionally Calibrated Model of Grenoble

In this work we compare the calibrated model of Grenoble using the proposed algorithm and one calibrated traditionally. The description of the traditionally calibrated model of

Grenoble is not discussed here and can be found in Ref. [28] and in some parts of Ref. [6].

First we show that the calibration algorithm proposed here is consistent. As the ML estimator is asymptotically efficient, the estimate is expected to be closer to the true solution as the number of training sets are increased. Hence the *QoI* value for the test sets should decrease. Figure 3 shows plot of the *QoI* for the test cases w.r.t increase in number of training zones. It is observed that *QoI* decreases as number of training sets are increased. Hence, we can say that the proposed algorithm is able to consistently estimate the land use parameters.

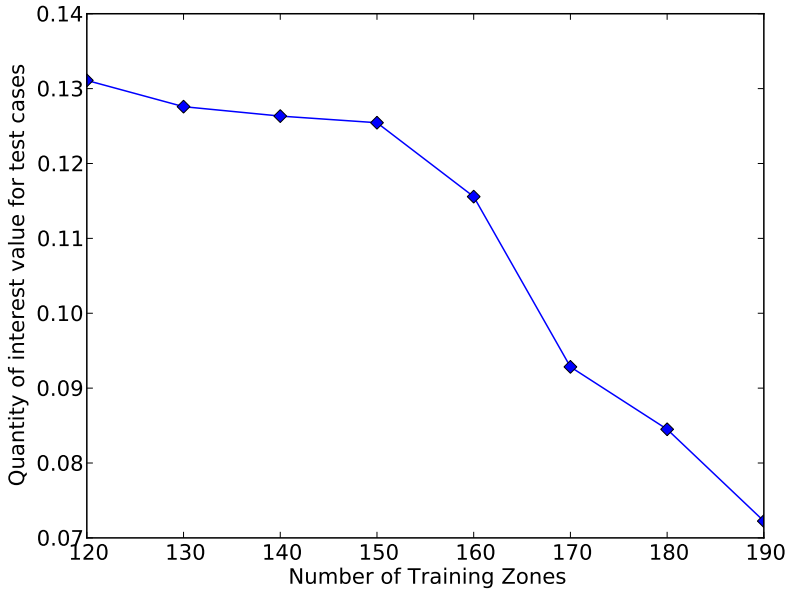


Fig. 3. Figure showing the plot of the quantity of interest (for the test cases) vs. the number of training zones. It can be seen that the quantity of interest decreases as number of training cases increase.

The traditional calibration technique yielded a *QoI* value of 9.42, which is almost 70 times more than the worst *QoI* value obtained using the proposed algorithm. Hence, it can be said than the proposed calibration algorithm outperforms the traditional calibration technique, when compares using the *QoI* in (16).

4.3.3 Likelihood Ratio Test

Due to Gaussian process approximation, the proposed calibration methodology has more parameters to be calibrated than the traditional approach. The additional parameters are the hyperparameters of the Gaussian covariance kernel. The proposed method, is expected to perform better than the traditional technique as it has more "degrees of freedom". The extra degrees of freedom are supposed to help in yielding a better approximation of the true land use and transportation scenario. So, for proper comparison, we have performed a *likelihood ratio test* between the traditional and proposed models. Detailed discussion on likelihood ratio test can be found in Ref. [37].

For the likelihood ratio test we consider all the 225 zones as training zones. The null hypothesis H_0, is that the traditionally calibrated model is better than the one calibrated using proposed method and is accepted at a significance level $\alpha = 0.05$. The degrees of freedom for the test is 21. Let the traditionally calibrated parameters be $\check{\varphi}$ and the ones obtained using the proposed method be $\hat{\varphi}$. The test statistic is obtained as,

$$X^2 = -2\log\left[\frac{L(\check{\varphi}|X^n_{oj};y)}{L(\hat{\varphi}|X^n_{oj};y)}\right] = 18.5597 > \mathcal{X}^2_{0.95,21} = 11.591,\ j \in \mathbb{N}[1,225], n \in \mathbb{N}[1,21].$$

Hence, the null hypothesis is rejected. In other words, this means that for the current application, chance of the traditionally calibrated model being better than the proposed model is less than 5%.

4.3.4 10-fold Cross Validation

In this section, we use 10-fold cross validation technique to verify if the MLE based calibration algorithm is consistent and is able to reduce the variance in mean square error. Interested readers are directed to Ref. [38] for a detailed treatise on cross validation.

For the validation experiment, observation replicates are chosen assuming a similar independence structure amongst sectors and zones as described in Section 3.3. In this work, the number of observation replicates is M, which is the number of sectors. Folds are chosen from the available replicates, hence each fold has a size of $\frac{M}{10}$ approximately. Furthermore, we vary the number of zones in a single fold. We investigate if proposed calibration methodology is able to reduce the *mean squared error* variance for the test fold, as the number of zones is increased. Given a fold, the zones are chosen randomly from

the available J zones. For the k^{th} fold, if the set of zones is represented by $J_f(k) \subset \mathbb{N}[1, J]$, and the observation replicates are $M_f(k) \subset \mathbb{N}[0, M]$, then the mean squared error is given by,

$$MSE(k) = \frac{\sum_{n \in M_f(k)} \sum_{j \in J_f(k)} (X_j^n - X_{oj}^n)^2}{\#J_f \times \#M_f}, \tag{18}$$

where $\#\mathcal{S}$ refers to the number of elements in set $\mathcal{S}$. Rest of the symbols have their usual meaning.

In Fig. 4 we have plotted the variation of the mean square error as the number of zones in a fold ($\#J_f$ in (18)) is varied. We select ten folds from the available 21 observations sectors with $\#M_f$ fixed to 2. The fold for which MSE is calculated is the test fold. We can see that as the number of zones increase the proposed technique is able to reduce the mean as well as converge the $\pm 3\sigma$ limits of MSE for the test fold. It can be said that as the number of zones in a fold is increased, the confidence in the parameter estimates obtained by the proposed methodology increases.

An important point to note is that for the same number of zones the results in Fig. 4 is worse than that in Fig. 3. This happens because for the cross validation we use only $\#M_f = 2$ replicates per fold, however for the algorithm presented in Algorithm 1 all the 21 replicates are considered.

4.3.5 Confidence Intervals of Estimation

Figure 5 shows plots for confidence interval of the estimate obtained by solving the MLE optimization problem. The confidence intervals are computed using the normal approximation of the estimation error, where the standard error is the square root of the inverse of the Fisher information matrix [39]. The parameters $\underline{\mathcal{X}}^{mn}$ and $\overline{\mathcal{X}}^{mn}$, have the units of X_j^n, which in the present case is the unit of population or real estate depending upon the sector. However δ^{mn}, β^n and ϑ^n are dimensionless. An important point to note here is that, similar to Section 4.3.3, all the 225 zones are used for training in this case.

The red lines represent 95% confidence intervals and the green lines represent range of initial uncertainty in the parameters. It can be seen the 95% confidence intervals are more localized than the initial uncertainty for most of the parameters. Hence, it can be said that, MLE is able to reduce the dispersion of uncertainty effectively for majority

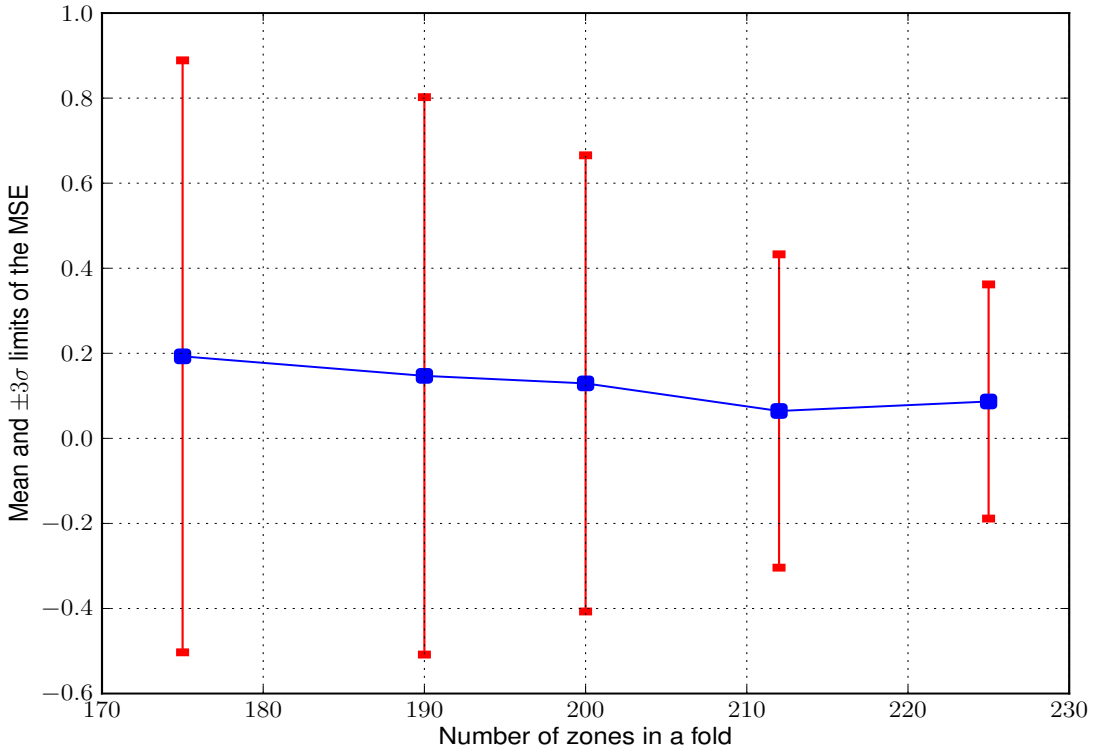


Fig. 4. Figure showing the plot of mean (blue line) and $\pm 3\sigma$ limits (red bars) for MSE of the test fold. It can be seen that as the number of zones in a fold increases the mean decreases and $\pm 3\sigma$ limits converge.

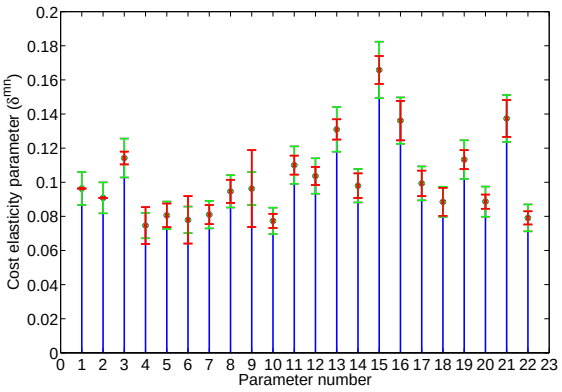
of the parameter space. In other words, the proposed estimation methodology could capture the localization of uncertainty effectively.

Comparison to the confidence intervals of the traditionally calibrated model could not be done for the Grenoble model, as it was not possible to obtain such an opinion, and is a subject of future research.

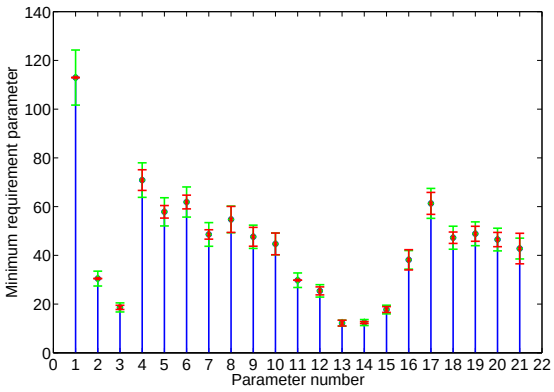
5 Conclusion and Future Research Direction

In this work we present an algorithm to calibrate the land use module of an integrated land use and transportation model. The algorithm developed solves an optimization problem based on maximum likelihood estimation to get the calibrated parameters, and approximates the error in the observed data to follow a Gaussian process.

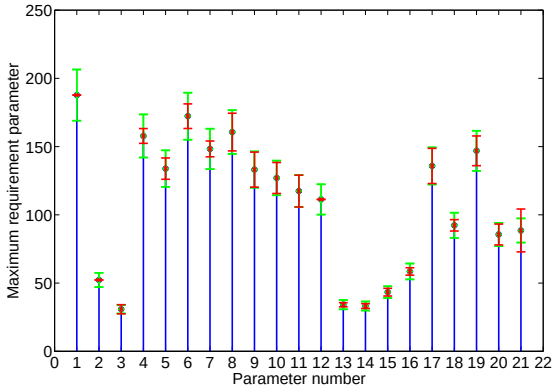
The proposed algorithm is then applied to calibrate the parameters of the Grenoble model of TRANUS, which is an integrated land use and transportation model. The



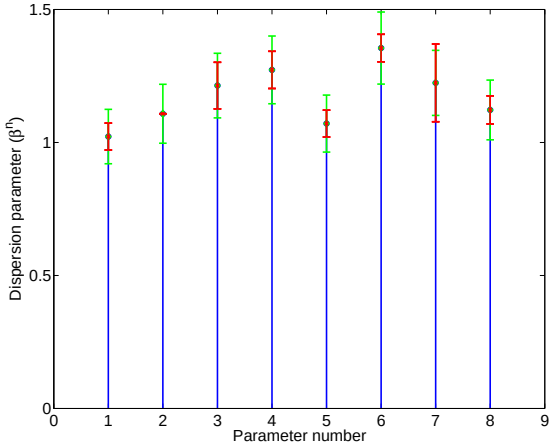
(a) Elasticity parameter (δ^{mn}).



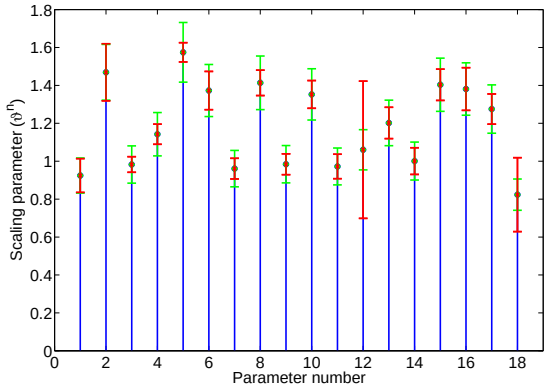
(b) Minimum requirement parameter ($\underline{\mathcal{X}}^{mn}$).



(c) Maximum requirement parameter ($\overline{\mathcal{X}}^{mn}$).



(d) Dispersion parameter (β^n).



(e) Scaling parameter (ϑ^n).

Fig. 5. Plot of the parameters estimates obtained using MLE and 95% confidence intervals (red lines) and initial uncertainty (green lines). $\underline{\mathcal{X}}^{mn}$ and $\overline{\mathcal{X}}^{mn}$ have the same units as X_j^n. Rest of the parameters are dimensionless.

performance of the algorithm is then compared to the traditional calibration technique, which is based on expert opinion; against a prespecified *quantity of interest*. It was found that the proposed calibration methodology outperforms the traditional method.

In future, our first aim is develop a generic way of solving the MLE optimization problem for the TRANUS Grenoble model. The current method uses one data set to create observation replicates and also assumes an independence structure between economic sectors. Our goal is to obtain replicates such that the independence assumption can be relaxed. Also in future, we will like to calibrate the model using Bayesian estimation. Prior PDFs of the land use parameters, can be obtained using expert opinion and the data. Moreover, we expect to calibrate the transportation and land use model together, using techniques of maximum likelihood estimation as well as in Bayesian framework. Validation over time is also important to evaluate the prediction capabilities of the calibrated model using data from future, which is one of our future goals too.

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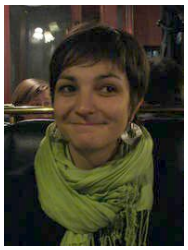

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