A COMPARISON OF METHODS FOR ANTICIPATING AND UNDERSTANDING UNCERTAINTY OF OUTPUTS FROM TRANSPORTATION AND LAND USE MODELS

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ABSTRACT: Uncertainty is important to appreciate in the outputs of complex and dynamic urban systems. This study demonstrates three methods for uncertainty propagation in transportation and land use models: Local Sensitivity Analysis with Interaction (LSAI), Monte Carlo (MC) methods, and Bayesian Melding (BM) method. Two case study settings are used to illustrate how these methods work, allowing for inter-method comparisons. LSAI can provide the sign of change implied by the changes in exogenous variables, the relative importance of the change in exogenous variables, and the decomposition of the change of output into the individual and interaction changes in exogenous variables. The computing time for multiple model runs is determined by the number of (groups of) exogenous variables. However, that approach obtains only point estimates, while MC and BM can deliver the entire distribution of each output. However, the MC and BM meethods require an understanding of the uncertainty of all model inputs and parameters. MC methods can be used to solve problems with probability structures, or non-probabilistic problems. It is straightforward to obtain a model's output distributions via random sampling from the distributions of inputs and parameters. However, MC methods require a large number of samples (and thus full model runs), especially for more accurate results. Both LSAI and MC only solve the deterministic problems, while BM can solve both deterministic and stochastic problems, explicitly. BM can estimate the posterior distribution of outputs from prior probability distributions and likelihoods of inputs and parameters. However, BM can be extremely expensive in terms of computing time, since it requires several hundred runs of the model. Moreover, all outputs must be known at an intermediate point (in time, typically), to allow foror intermediate validation.

Key words: Uncertainty Propagation, Transportation and Land Use Models, Local Sensitivity Analysis with Interaction (LSAI), Monte Carlo (MC) methods, Bayesian Melding (BM)

INTRODUCTION

Scientific computing involves large-scale simulations to represent real-world phenomena like evolution of cities and their traffic patterns. With improvements in computing capabilities and more efficient algorithms, simulation results can better represent real-world conditions. Models allow for accurate forecasts over longer prediction periods. Predictions are typically affected by uncertainties in input data and model parameters, and by incomplete knowledge of underlying behaviors (Cheng, 2009). Models (and the systems they represent) are often explicitly stochastic (Sevcikova et al., 2014), with random components generated and used through the predictive process. It is very important for system design optimization and policy-making to capture and represent this uncertainty information appropriately in model results. Much work has been done, in areas as diverse as hydrology (e.g., Christensen, 2003; Neuman, 2003; Korving et al., 2003), climate change (e.g., Andrew and Francis, 2000; Casman et al., 1999), and land use forecasting (e.g., Pradhan and Kockelman, 2002; Waddell, 2002; Waddell et al., 2003).

Uncertainty quantification is the process of representing imperfectly known or understood inputs and parameters, propagating this variability through the model system and then characterizing the uncertainty in model results. The outcome usually comes with attached “error bars” to indicate uncertainty ranges. Probability density and mass functions (PDFs and PMFs) are useful to describe the statistics of the uncertainty.

In order to carry out a probabilistic analysis of a system, one must first identify sources of uncertainty (e.g., Morgan and Henrion, 1990; Dubus et al., 2003). Pradhan and Kockelman (2002) reviewed the literature on the sources of uncertainty in land use-transportation models and examined the impact of uncertainty in the land use component of a partially integrated land use-transportation modeling system called UrbanSim. Sevcikova et al. (2007) reviewed the key sources of uncertainty for UrbanSim land use modeling outputs, such as measurement errors on inputs (like population and jobs by neighborhood), systematic errors from miscalibrated measurement tool or from sampling procedures that are not completely random, uncertainty about model structure, and uncertainty about model input parameters and model stochasticity or randomness. They focused on how to propagate this uncertainty through complex models if inputs and parameters uncertainties are known.

Probabilistic analysis is one way to represent uncertainty (Papoulis, 1991). In this approach, uncertainties associated with model inputs are described by probability distributions, the objective being estimation of the outputs’ probability distributions (Pradhan and Kockelman, 2002). Probabilistic methods include analytical and sampling based methods (for example, the Monte Carlo and Latin Hypercube methods, Fourier Amplitude Sensitivity Test (FAST) methods, reliability based methods, and response surface methods) (Pradhan and Kockelman, 2002).

The objective of this study is to demonstrate and compare methods for uncertainty propagation in complex transportation and land use models. Detailed reviews of three distinctive and reasonably exhaustive methods are given, including two small application examples, enabling comparisons of these methods.

METHODS FOR ANTICIPATING UNCERTAINTY IN TRANSPORTATION AND LAND USE MODELS

A variety of different methods for anticipating and understanding output uncertainties were investigated here. Top methods for forecasting uncertainty in land use and transportation model outputs are Local Sensitivity Analysis with Interaction (LSAI), the Monte Carlo (MC) method, and Bayesian Melding (BM). This paper uses two reasonably transparent transportation settings to illustrate and compare these methods.

Local Sensitivity Analysis with Interaction (LSAI)

While building and using numerical simulation models, sensitivity analysis is an invaluable tool. Sensitivity analysis is the study of how uncertainty in the output of a mathematical model or system (numerical or otherwise) can be apportioned to different sources of uncertainty in its inputs (Saltelli et al., 2008). Modelers may conduct sensitivity analyses for a number of reasons including the need to determine (Hamby, 1994): (1) which parameters require additional research for strengthening the knowledge base, thereby reducing output uncertainty; (2) which parameters are insignificant and can be eliminated from the final model; (3) which inputs contribute most to output variability; (4) which parameters are most highly correlated with the output; and (5) once the model is in production use, what consequence results from changing a given input parameter. There are many different ways of conducting sensitivity analyses; however, in answering these questions the various analyses may not produce identical results (Iman and Helton, 1988).

Conducting sensitivity analyses by presenting details on the types of sensitivity analyses utilized for various modeling situations, Hamby (1994) summarized many of the methods available. Hamby (1995) compared the assessment of several methods and intended to demonstrate calculation rigor and parameter sensitivity rankings resulting from various sensitivity analysis techniques.

Sensitivity analyses are often referred to as either "local" or "global". A local analysis addresses sensitivity relative to point estimates of parameter values, while a global analysis examines sensitivity with regard to the entire parameter distribution. Local sensitivity analysis is the assessment of the local impact of input factors' variation on model response by concentrating on the sensitivity in the vicinity of a set of factor values. Such sensitivity is often evaluated through gradients or partial derivatives of the output functions at these factor values, so other inputs' values are held constant when studying the local sensitivity of a specific input. Such approaches have been used in evaluating large environmental systems, including climate modeling, oceanography, and hydrology (Cacuci, 2003, Castaings et al. 2007).

Kockelman et al. (2008) ran a Gravity-based Land Use Model (G-LUM) over three alternative scenarios, with total employment counts (EMP), household counts (HH) and link impedances or travel times (TT) increased by 50%, utilizing each set one at a time. Borgonovo et al. (2014) used their G-LUM model to illustrate LSAI techniques and found that the endogenous variables respond almost additively to variations in the model inputs over the given scenarios. Changes in the base year employment assumptions strongly influence future job and land use pattern predictions

To overcome the limitations of local methods (like linearity and normality assumptions, and emphasis on local variations), Saltelli et al. (2008) use a new class of statistical methods for understanding uncertainty. In contrast to local sensitivity analysis, their method is called "global sensitivity analysis" because it considers the entire range of inputs variations. Saltelli et al. (2008) first used a small test network to demonstrate how local sensitivity analysis works when interaction is nontrivial. They then used global sensitivity analysis to analyze the variance of model outputs, and more specifically, how input variations influence the variance of outputs.

Sensitivity analysis can be essential for deriving insights from decision-support models in a wide range of applications. In linear programming settings (where outputs are a result of optimization), Wendell (2004) used simultaneous variations in objective function coefficients to develop a tolerance sensitivity approach. Besides linear programming, the works of Borgonovo and Apostolakis (2001) and Borgonovo (2008) addressed the joint sensitivity of generic model outputs for small changes in all inputs (including parameters). Saltelli and Tarantola (2002) defined group sensitivity indices in the context of a global sensitivity analysis. As far as finite changes are concerned, Borgonovo (2010) introduced sensitivity measures for individual exogenous variables. To find sensitivity measures for specific input factor sets (typically, sets of parameters), one then needs to extend Borgonovo's (2010) results to group variations. Borgonovo and Peccati (2011) proved that a change in model output is decomposed as a function of factors with the same structure of the parameter decomposition (Rabitz and Alis, 1999). Based on this finding, they introduced factor finite change sensitivity indices (FCSI) for model parameters and investigated the relationship between the factor FCSI's and parameter FCSI's. Knowledge of the FCSI's enables analysts to quantify the contributions of factors, the relevance of their interactions and identify the key-drivers of scenario results. Borgonovo and Peccati (2011) merged scenario analysis and high-dimension model representation (HDMR) theory. Perturbation techniques entail the requirements of smoothness (differentiability) in model outputs and of small changes in independent variables. In a variety of managerial applications, however, parameters undergo finite variations, inducing discrete/non-smooth changes in decision-support criteria.

Monte Carlo Methods

MC techniques have been widely used for uncertainty propagation due to the conceptual simplicity and ease of implementation. In MC techniques, one samples random variables, runs an ensemble of simulations, and simply presents the distribution of outputs, for all uncertainty statistics. A well-known drawback of MC is its slow convergence rate. A reasonable result usually requires a large number of ensemble runs, which is computationally expensive for large-scale systems. More efficient approaches need to be developed to represent and propagate uncertainties in large-scale simulations (Cheng, 2009).

Zhao and Kockelman (2002) conducted a study of the propagation of uncertainty in 4-step travel demand models. They used Monte Carlo simulation and sensitivity analysis to quantify variability in model outputs. Their results suggested that uncertainty is compounded over the first three stages of a transport model, resulting in a magnification of errors at later stages. However, traffic assignment, the final step of the model, reduced these variations back to the initial input levels. The authors hypothesized that this was due to a centralizing tendency of compounded travel choices, and congestion feedbacks in the shortest-path search algorithm.

Harvey and Deakin (1995) conducted a similar study, in which they considered uncertainty in population growth, fuel price and household income levels in the STEP models of the Los Angeles (LA) region. They found that plausible ranges of the input variables resulted in percentage changes in total VMT of 25% below to 15% above the original prediction.

A study conducted by Thompson et al (1997) examined the impact of higher-than-projected population estimates on emission trends for metropolitan regions in California. They found that levels of CO, ROG and NO_x were below projected attainment year levels, even for high growth scenarios, as a result of fuel and motor vehicle emissions control programs. Rodier and Johnston (2002) identified plausible error ranges of ± 2% for population and employment growth projections. Their results suggest that while plausible error ranges for household income and fuel prices may not be a significant source of uncertainty, plausible errors in population and employment projections are likely to cause significant errors in predictions.

Method of Bayesian Melding

Pradhan and Kockelman (2002) examined the propagation of uncertainty in the context of UrbanSim. However, this study analyzed only the sensitivity to a small sample of selected input values and explored the effect of these changes on outputs, in addition to simple stochastic simulation error from variation in random seeds.

Another approach to extrapolate prediction accuracy for land-use models was taken by Pontius and Spencer (2005). Their method used models calibrated at different time points to stimulate the present land-cover change. They estimated how accurately the model will predict the future through a measure derived by a validation with empirical data. This method was specific to simulation models that have categorical outcomes and stochasticity was not taken into account. Furthermore, none of the above studies generated any statistical inferences, nor any new methodology to calibrate a stochastic model system with respect to uncertainty. However, Sevcikova et al. (2007) helped develop and then apply the method of Bayesian melding by extending an earlier method (developed for macro-level deterministic simulation models) to agent-based stochastic models. This method encodes all available information about model inputs and outputs in terms of prior probability distributions and likelihoods, and used Bayes' theorem to obtain a posterior distribution for any quantity that is a function of model inputs and/or outputs. They compared it with a simpler method that uses repeated runs of the model with fixed estimated inputs and concluded that the simple (repeated runs) method gave distributions of quantities of interest that were too narrow, while BM gave well-calibrated uncertainty statements. They also pointed out a practical problem with their approach for larger cities/regions, UrbanSim can take a long time to run, so the BM method can be very computationally intensive, since it requires several hundred runs of the model.

Thus they provided various ways in which it may be possible to reduce the time required (see (Sevcikova et al., 2007) for more details). However, simply repeating a simulation multiple times does not result in an accurate assessment of uncertainty (Sevcikova et al., 2007). Based on work by Sevcikova et al. (2007, 2011), Sevcikova et al. (2014) described the first incorporation of uncertainty assessment into the development of an official land use forecast published by a metropolitan planning organization (MPO). They demonstrated how the BM methodology for assessing uncertainty could be used to support application of an academically founded land use model, which had been adopted into practical use by a public planning agency and then used in an official land use forecast. The methodology itself is not specific to land use models, of course; it can be applied to any simulation models that fit into its forward-in-time framework.

Introduction to Local Sensitivity Analysis with Interaction

A mathematical model is used to denote the input-output mapping as

$$y = f(\mathbf{x}), f\colon \Omega_{\mathbf{x}} \longrightarrow \mathbb{R} \tag{1}$$

where y is the endogenous variable of interest, $\Omega_{\mathbf{X}} \subseteq \mathbb{R}^K$ and $\mathbf{x} = (x_1, x_2, \cdots, x_K)$, $\mathbf{x} \in \Omega_{\mathrm{X}}$ is the vector of the exogenous variables. K is the number of factors whose variation is of interest. Here, the input components $\mathrm{x_i}$ $(i = 1,2,\cdots,K)$ are supposed to be independent.

Therefore, the base-case output of the simulation $\mathrm{y}^0 = f(\mathbf{x}^0)$ can be obtained by the simulation with exogenous variables to a base-case scenario, $\mathbf{x}^0$. Similarly, different outputs depending on alternative values of the endogenous variable, $y^s = f(\mathbf{x}^s)$, where $s = 1,2,\cdots,S$. The analyst knows the response of the endogenous variable in each scenario, although he/she has no information about the sources of change (Borgonovo et al, 2014). The change from scenario 0 to scenario 1 of the exogenous variables induces the change $\Delta \mathrm{y} = \mathrm{y}^1 - \mathrm{y}^0$ in the endogenous variable. And the change can be decomposed by using by a multivariate Taylor expansion of $\Delta \mathrm{y}$ when supposing that $f(\mathbf{x})$ is r times differentiable at $\mathbf{x}^0$ (Saltelli and Tarantola, 2002; Saltelli et al., 2004; Borgonovo et al, 2014):

$$\begin{aligned}&\Delta \mathrm{y} = \mathrm{y}^1 - \mathrm{y}^0 = \\ &\textstyle\sum_{s=1}^{K} f_s'(\mathbf{x}^0)\Delta \boldsymbol{x}_s + \sum_{s,t=1}^{K} f_{s,t}''(\mathbf{x}^0)\Delta \boldsymbol{x}_s \Delta \boldsymbol{x}_t + \cdots + \\ &\textstyle\sum_{s_1=1}^{K}\sum_{s_2=1}^{K}\cdots\sum_{s_r=1}^{K} f_{s_1,s_2,\cdots,s_r}^{r}(\mathbf{x}^0)\Delta \boldsymbol{x}_{s_1}\Delta \boldsymbol{x}_{s_2}\cdots\Delta \boldsymbol{x}_{s_r} + o(||h||^r)\end{aligned} \tag{2}$$

Then, one obtains

$$\Delta \mathrm{y} = f(\mathbf{x}^1) - f(\mathbf{x}^0) = \textstyle\sum_{k=1}^{K} \Delta_k f + \sum_{k<t}^{K} \Delta_{k,t} f + \cdots + \Delta_{1,2,\cdots,K} f \tag{3}$$

where

$$\begin{cases} \Delta_k f = f\left(x_k^1, \mathbf{x}_{\sim k}^0\right) - f(\mathbf{x}^0) \\ \Delta_{k,t} f = f\left(x_k^1, x_t^1, \mathbf{x}_{\sim(k,t)}^0\right) - \Delta_k f - \Delta_t f - f(\mathbf{x}^0) \end{cases} \tag{4}$$

and where $\left(x_k^1, \mathbf{x}_{\sim k}^0\right)$ denotes that the kth element of the $\mathbf{x}$ vector, x_k^1 is set at the value it assumes in Scenario 1, while all other variables are at their Scenario 0 values. Based on such a decomposition, finite-change sensitivity indices can be computed as follows:

$$\varphi_{k_1,k_2,\cdots,k_r}^{r} = \Delta_{k_1,k_2,\cdots,k_r} f \tag{5}$$

where $k_1, k_2, \cdots, k_r$ denotes a group of r indices ($r \le K$) and $\varphi_{k_1,k_2,\cdots,k_r}^{r}$ is the portion of $\Delta \mathrm{y}$ due to the interaction of exogenous variables corresponding to the selected indices.

Particularly, the first-order finite-change sensitivity indices are $\varphi_k^1 = \Delta_k f$ and the total-order indices are $\varphi_k^T = \Delta_k f + \sum_{k<t}^{K} \Delta_{k,t} f + \cdots + \Delta_{1,2,\cdots,K} f$, where φ_k^T is the total contribution of x_k to Δy, and is the sum of the individual contribution of x_k, plus all the contributions due to the interaction of x_k with the remaining exogenous variables. Thus, the index $\varphi_k^I = \varphi_k^T - \varphi_k^1$ represents the effect of interactions associated with x_k (Borgonovo et al, 2014).

According to the definition of φ_k^T, it can be computed by

$$\varphi_k^T = f(\mathbf{x}^1) - f\left(x_k^0, \mathbf{x}_{\sim k}^1\right) \tag{6}$$

where $f(\mathbf{x}^1)$ is the value of the endogenous variable in scenario 1 and $f\left(x_k^0, \mathbf{x}_{\sim k}^1\right)$ is the point obtained with all exogenous variables at scenario 1 but x_k that remains at the base case scenario.

As discussed in the literature (e.g., Saltelli and Tarantola, 2002; Saltelli et al., 2004), the sign of the first order indices (φ_k^1) is the sign change in y due to the individual change in x_k. The sign of $\varphi_{k_1,k_2,\cdots,k_r}^{r}$ is the sign of the interaction between the exogenous variables x_{k_1}, x_{k_2} and x_{k_r}. The total-order indices (φ_k^T) are the appropriate sensitivity measures, since they deliver not only the individual importance of the factors, but also account for interactions. The magnitudes of $\varphi_{k_1,k_2,\cdots,k_r}^{r}$ provide the natural sensitivity measures.

All finite-change sensitivity indices can be computed by use of 2^K simulations if there are K (or group of) exogenous variables whose variations are of interest. The triplet $(\varphi_k^1, \varphi_k^I, \varphi_k^T)$ can be computed at the cost of $2K$ simulations, instead of 2^K. This computational burden reduction result makes the sensitivity measures applicable also to complex simulation codes.

Introduction to Bayesian Melding

Figure 1 shows the basic concept of BM developed for deterministic models (Sevcikova et al., 2014). There is a prior distribution of model inputs $q(\Theta)$from which one draws input values Θ_i for $i = 1, \dots, I$. The model runs I times from the base year to the present year and for each input Θ_i. It produces as output the quantity of interest, Φ_i. The model can be viewed as a mapping, M, from the space of inputs to the space of outputs, which is denote by $\Phi = M_\Phi(\Theta)$. The "present" time is defined as a time point with observed data available. The observed data is denoted by y and used to compute a weight ω_i for each input Θ_i: $\omega_i = L(\Theta_i)$. Here, $L(\Theta_i)$ is the likelihood of the model outputs given the observed data, $L(\Theta_i) = \text{Prob}(y|\Phi_i)$. For each of the I runs, the model is run forward until a future time when making a prediction. The results by running the ith model are denoted by Ψ_i. The posterior distribution of Ψ is approximated by a discrete distribution with values Ψ_i having probabilities proportional to ω_i.

The primary BM stages or steps are as follows (Sevcikova et al., 2007):

- As before, draw a sample $\{\Theta_1, \Theta_2, \dots, \Theta_I\}$ of values of the inputs from the prior distribution $q(\Theta)$.
- For each Θ_i, run the model to obtain Φ_i
- Compute weights $\omega_i = L(\Theta_i)$. Here, an approximate posterior distribution of inputs with values $\{\Theta_1, \Theta_2, \dots, \Theta_I\}$ and probabilities proportional to $\{\omega_1, \omega_2, \dots, \omega_I\}$ are obtained.
- The posterior distribution of Φ is no longer approximated by the set $\{\omega_i\}$ but now has a finite mixture distribution of the form

$$\pi(\Phi) = \prod_{i=1}^{I} w_i p(\Phi|\Theta_i) \tag{7}$$

In (7) the conditional distribution $p(\Phi|\Theta_i)$ has an assumed parametric form that reflects the additional sources of variation.

The posterior distribution of Ψ has a similar form, namely

$$\pi(\Psi) = \prod_{i=1}^{I} w_i p(\Psi|\Theta_i) \tag{8}$$

TWO TEST EXAMPLES

To illustrate the different methods for uncertainty propagation in transportation and land-use models, we use Example 1 for LSAI and MC applications and Example 2 for BM application.

Example 1 is as the following small test network (Fig. 2).

Example 1. The test network (Fig.1) is a simple travel demand model (TDM), which consists of 3 nodes (O is the origin, D1 and D2 are destination), 4 links. $(*,*)$ denotes the free-flow travel time and capacity on each link.

The equations for this TDM are as follows:

$$Z = x_1 x_2 + x_3 \tag{9}$$

$$Z_{12} = Z * \frac{e^{x_4 * GC_{12}}}{e^{x_4 * GC_{12}} + e^{x_4 * GC_{13}}} \tag{10}$$

$$Z_{13} = Z - Z_{12} = Z * \frac{e^{x_4 * GC_{13}}}{e^{x_4 * GC_{12}} + e^{x_4 * GC_{13}}} \tag{11}$$

$$GC_{12} = min\{LC_1, LC_2\} \tag{12}$$

$$GC_{13} = min\{LC_3, LC_4\} \tag{13}$$

$$LC_i = \gamma * \text{time} + \text{Toll} * t_f \tag{14}$$

where Z denotes number of trips generated, Z_{1j} denotes number of trips going from the original node O to destination node j (j=D1,D2), GC_{1j} denotes generalized cost going from O to j(j=D1,D2), LCi

denotes generalized cost on link *i*, (*i*=1,2,3,4). This assumes the travelers have the same value of time (VOT), which is $\gamma = \$6/\mathrm{hour}$ (Chen et al., 2015). Toll is priced by using links (HT=$0.55/mile for links 1 and 3; LT=$0.20/mile for links 2 and 4 as Chen et al. (2015)). Network traffic assignment is based on user equilibrium (Sheffi, 1985). The BPR function is adopted as the form: $\mathrm{time} = t_f(1 + \alpha * \left(\frac{v}{c}\right)^{\beta})$, where t_f is the free-flow travel time (and the distance of link), v is the traffic flow on the link, and c is the capacity of link, and α and β are volume/delay coefficients. The traditional BPR values for α and β are 0.15 and 4.0, respectively. But for a small urban area using default parameters and wishing only to use a single volume-delay function, NCHRP Report 365 (Martin 1998) suggested larger values, of 0.84 and 5.5, respectively. These larger values are applied here. The parameters used in the test examples are illustrated in the following table:

LSAI is applied on the test example by increasing all exogenous variables by 10%. The change of each model's outputs (traffic flow on links) from $\mathbf{x}^0$ to $\mathbf{x}^1$ can be decomposed into 15 terms that account for the individual changes in x_1, x_2, x_3, x_4, to their interactions in pairs, and in the residual term that contains their overall and residual interactions. Here, $2^4 = 16$ simulations are needed on the model. If we compute the first-order indices, the total-order indices and the effect of interactions associated with every exogenous variable, only $2 * 4 = 8$ simulations are needed. The *i*-th order indices as well as their sum and the total-order indices are illustrated by Figs. 3-4. The elasticity of the first-order indices and the total-order indices are also shown in Fig. 5, where elasticities are computed as $\frac{\Delta \mathrm{v}/\mathrm{v}}{\Delta \mathrm{x}/\mathrm{x}}$

Fig. 3(a) shows that increasing parameter x_3 by 10% will lead to the largest increase of traffic flows on links 1 and 2. While increasing input x_1 by 10% will lead the largest increase of traffic flows on links 1 and 2. Increasing x_4 by 10% will lead to a decrease of traffic flows on links 1 and 2. The individual effect of x_1 is the most important on the traffic flow of links 3 and 4. The individual effect of x_4 is the most important on the traffic flow of links 1 and 2. Fig. 3(b) shows that the interaction between the parameters x_2 and x_3 will lead to the largest increase of traffic flows on all links among all second order interactions. Other interactions (besides the interaction between x_1 and x_3 is 29.2) are all very small (the absolute values are all less than 15). The signs of second-order indices are negative, such as the interactions between x_2 and x_4, and x_3 and x_4 on links 1 and 2, the interaction between x_1 and x_4 on links 3, the interactions between x_1 and x_2, x_1 and x_3, and x_1 and x_4 on links 4. Fig. 3(c) shows that almost all third order indices will lead to a negative effect on the traffic flows on all links except the third-order interactions among x_1, x_2 and x_4, and among x_1, x_3 and x_4 have positive effects on the traffic flows on links 3 and 4. The interactions among x_1, x_2 and x_3, and among x_2, x_3 and x_4 have almost same effect on the traffic flows on all links. The interactions among x_1, x_2 and x_4, and among x_1, x_3 and x_4 have very small (positive or negative) effects on the traffic flows on all links. Fig. 3(d) shows that the fourth-order index has positive effects on all links. The fourth-order index has the largest effect on the traffic flow in link 4, and the smallest effect on the traffic flow on links 1 and 3.

Fig. 4(a) shows that the sum of the third-order index has non-positive effects on all links (zero for link 1, negative for other links). The sums of other order indices positively affect all links. Of all the sums of the order indices with positive effects on all links, the sum of the fourth-order has the biggest effect on the traffic flow on links 1, 2, and 3, while the sum of the first-order has the biggest effect on the traffic flow on link 4. Figure 4(b) shows that the total-order indices positively affect all links. Input x_1 and parameter x_3 have almost identical and the most impactful effect on traffic flows on all links. x_2 is the second. x_4 is the third. Fig. 4(c) shows the effect of interactions associated with $x_1, x_2, x_3,$ and x_4. The effect of interactions associated with every exogenous variable is almost the same on the traffic flows on each link. Compared with the first-order indices in Fig. 3, the effect of first-order indices is less than that of interaction on the traffic flows on links 1, 2, and 3, while the effect of first-order indices is less than that of interaction on the traffic flows on link 4. The effect of interactions associated with x_2 and x_4 is almost same as that of the total-order indices on traffic flows on all links.

Fig.5 shows the elasticities of the first-order and total-order indices. They have the same trend with the first-order index and the total-order index in Fig. 3(a) and Fig. 4(b), which resulted from the same increasing of exogenous variables in this test example.

The Monte Carlo method was applied with the test example by randomly generating 16 different sets of model inputs and parameter values, and then drawing randomly from their associated probability distributions. In general, the number of simulation runs needs to be large enough to obtain robust and accurate results. Here, we randomly choose 16 different sets of inputs and parameters. Final link flows were obtained from the converged UE assignment results. Table 2 provides the mean, standard deviation (SD), and coefficient of variation (CoV) for the four links' traffic flows.

The coefficients of variation of the traffic flows on links 2 and 4 are larger than 0.10, which suggests the final uncertainty may be compounded and end higher than any input or parameter uncertainty. The coefficients of variation of the traffic flows on links 1 and 3 are smaller than 0.06, which suggests the final uncertainty is lower than any input or parameter uncertainty.

For better understanding and interpretation of the results, ordinary least squares (OLS) regression was used to identify model inputs that are key contributors to uncertainty in model output (Table 3), which characterizes the linear relationship between inputs and outputs.

MC methods involve random sampling from the distribution of inputs, and successive model runs until a statistically significant distribution of outputs is obtained. These can be used to solve problems with probability structures, or non-probabilistic problems such as finding the area under a curve. However, these methods require a large number of samples. In order to achieve computational efficiency, methods that sample the input distribution in an efficient manner have been introduced. One such variant of the standard Monte Carlo method is the Latin Hypercube (LH) sampling method (McKay et al., 1979; Eglajs and Audze, 1977; Iman et al., 1980, 1981). In this method, the range of probable values for each input parameter is divided into ordered segments such that the parameter space, consisting of all uncertain parameters, is partitioned into cells having an equal probability. Thus, parameter estimates are sampled in an efficient manner, since each parameter is sampled only once from each of its possible segments. The advantage of this approach is that it allows representation of the extremes of the probability distribution of the outputs.

Example 2. To illustrate how BM method works, an integrated land-use and transportation model is presented by the following equations:

$$x_1^{t_j} = (1+\delta)^{\Delta t} x_1^{t_{j-1}} \ (j = 1,2,\dots), \text{ where } \Delta t = t_j - t_{j-1} \tag{15}$$

$$Z^{t_j} = x_1^{t_j} x_2 + x_3 \tag{16}$$

$$Z_{12}^{t_j} = Z^{t_j} * \frac{e^{x_4 * GC_{12}}}{e^{x_4 * GC_{12}} + e^{x_4 * GC_{13}}} \tag{17}$$

$$Z_{13}^{t_j} = Z^{t_j} - Z_{12}^{t_j} = Z^{t_j} * \frac{e^{x_4 * GC_{13}}}{e^{x_4 * GC_{12}} + e^{x_4 * GC_{13}}} \tag{18}$$

$$GC_{12}^{t_j} = min\{LC_1^{t_j}, LC_2^{t_j}\} \tag{19}$$

$$GC_{13}^{t_j} = min\{LC_3^{t_j}, LC_4^{t_j}\} \tag{20}$$

$$LC_i^{t_j} = \gamma * time + Toll * t_f \tag{21}$$

where Z^{t_j} denotes number of trips generated at time t_j, $Z_{1D}^{t_j}$ denotes number of trips going from O to D(D=D1,D2) at time t_j, $GC_{1D}^{t_j}$ denotes generalized cost going from an O to D (where D=D1 or D2) at time t_j, $LC_i^{t_j}$ denotes generalized cost on link i,(i=1,2,3,4) at time t_j, ${x_1}^{t_j}$ denotes the total number of population in zone O at time t_j. Other notation is the same as those provided in Example 1.

In this example, Equation (15) is a simple land-use model (LUM), while Equations (16)–(21) describe a simple TDM. LUM reacts to travel network changes and such. But there's not nearly as strong a link from TDM to LUM as there is from LUM to TDM because it's hard to move one's home & to construct new buildings, for example – and we don't want to destroy old buildings. Thus, in this land-use and transportation model, we only research the interaction of land-use model on TDM because only the outputs of the land-use model acts as an inputs for a TDM without feedback of TDM to LUM. Outputs from LUM act as inputs for a TDM; and where travel times from the traffic-assignment stage of the TDM are fed forward into the subsequent years LUM.

We randomly choose 16 samples, and ran the model 3 times for each set of inputs & parameters. Therefore, *I=16;J=3;K=4.* Starting from t_0 = 2010, we will use t_1 = 2015 as "present" year and run the simulation forward until t_2 = 2020. According to the steps of BM, the $\hat{\sigma}_i^2$, â,and $\hat{\sigma}_\delta^2$ are computed as follows: $\hat{a}$ =0.18; $\hat{\sigma}_\delta^2$ =6.65. Because, $y_k|\Theta_i \sim N(\hat{a}+\widehat{\mu_{ik}}, v_i)$ with $v_i = \hat{\sigma}_i^2 + \frac{\hat{\sigma}_\delta^2}{J}$, ω_i being computed by the following equation:

$$\omega_i = p(y|\Theta_i) = \prod_{k=1}^{K} \frac{1}{\sqrt{2\pi v_i}} exp\left[-\frac{1/2(y_k - \hat{a} - \widehat{\mu_{ik}})^2}{v_i}\right] \qquad (22)$$

In order to compute the posterior distribution of the traffic flow on link *k*, the propagation factors b_a and b_v are set to 15/15, equal to $\frac{2015-2010}{2020-2015}$.

The posterior distribution of the traffic flow on link *k* is given by a mixture of normal distributions, as follows:

$$\pi(\Psi_k) = \sum_{i=1}^{I} \omega_i N(\hat{a}b_a + m_{ik}, (\hat{\sigma}_i^2 + \frac{\hat{\sigma}_\delta^2}{J})b_v) = N(\sum_{i=1}^{I} \omega_i(\hat{a}b_a + m_{ik}), \sum_{i=1}^{I} \omega_i(\hat{\sigma}_i^2 + \frac{\hat{\sigma}_\delta^2}{J})b_v) \qquad (23)$$

where $m_{ik} = \frac{1}{J}\sum_{j=1}^{J} \Psi_{ijk}$.

The distribution of the traffic flow on link *k* is given by N($\boldsymbol{\mu_k}, \boldsymbol{\sigma}$), where $\sigma = 1110, \mu_1 = 912, \mu_2 = 862, \mu_3 = 1540,$ and $\mu_4 = 646$.

CONCLUSIONS

In this paper, two small land use-transportation examples were used to demonstrate how LSAI, MC and BM methods of uncertainty characterization really work, and to compare these three methods' strengths and weaknesses. LSAI was to obtain interaction effects of exogenous variables due to changes in endogenous values. MC involved simply sampling the distribution of inputs and parameters, and running the models several times until a statistically significant distribution of outputs was obtained. BM helped put the analysis of simulation models on a solid statistical basis with calibration. Moreover, the feedback from traffic assignment to trip distribution was used in these test examples.

To summarize the findings, LSAI has a direct interpretation in terms of comparative statics, since it relies on the computation of derivatives and relative changes across small input shifts. This method can provide the sign of change implied by the changes in exogenous variables, the relative importance of the change in exogenous variables and the decomposition of the change of output into the individual and interaction changes in exogenous variables. LSAI's computing time requires about 2,000 simulations simply to obtain the first-order indices, the total-order indices, and the effect of interactions associated with *K* (groups of) exogenous variables and 2^K simulations to obtain all interaction effects. Moreover, LSAI only obtains point estimation, while MC and BM can provide distributions of needed outputs. MC methods involve random sampling of the distribution of inputs, and successive model runs until a statistically significant distribution of outputs is obtained. These methods can be used to solve problems with probability structures, or non-probabilistic problems such as finding the area under a curve. It is straightforward to obtain output distributions via random sampling of the distribution of inputs and parameters. However, such activities require a large number of samples. As with LSAI, MC only solves the deterministic problems while BM can solve both deterministic and stochastic problems. The BM method was proposed as a way of putting the analysis of simulation models on a solid statistical basis. The basic idea is to combine all the available evidence about model inputs and model outputs in a coherent Bayesian way, to yield a Bayesian posterior distribution of the quantities of interest. It can obtain the posterior distribution of output from prior probability distributions and likelihoods of inputs and parameters. Users are provided with probability intervals around forecasts which add value to model validation, scenario comparison and external review and comment procedures. However, this method could be extremely expensive computationally, as it requires several hundred runs of the model. The intermediate outputs must be known for intermediate validation.

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LIST OF TABLES AND FIGURES

Table 1: Parameters Used in Examples

Parameter	Description	Mean	SD	CoV	Distribution
x_1	The total number of population in zone O	2000	200	0.10	Lognormal
x_2	The trip production rate	2.303	0.2303	0.10	Lognormal
x_3	The base trip production	1000	100	0.10	Lognormal
x_4	The impedance parameter	-0.02*	0.002	0.10	Lognormal
${x_1}^{t_0}$	The total number of population in zone O at time t_0	1000	100	0.10	Lognormal
δ	Annual percentage increase in population	2%	0.2%	0.1	Lognormal

*To impose negativity, these parameters are drawn from a lognormal distribution and then given negative signs.

Table 2: Summary Statistics for Link-level Traffic Flows (n = 16)

	Mean (veh/day)	SD	CoV
Link 1	1006	58.83	0.0584
Link 2	1279	165.6	0.1294
Link 3	1569	21.87	0.0139
Link 4	1307	386.4	0.2957

Table 3: OLS Parameter Estimates for Traffic Flows on Links (n = 16 simulations)

Traffic Flow	v_1		v_2		v_3		v_4	
	Coefficients	t Stat	Coefficients	t Stat	Coefficients	t Stat	Coefficients	t Stat
Intercept	285.1	12.3	-775.5	-14.6	1290	37.3	-3815	-93.9
x_1	0.1796	31.5	0.5088	38.9	0.0608	7.14	1.199	120.0
x_2	0.0916	9.76	0.2507	11.7	0.0549	3.92	0.6049	36.8
x_3	156.5	31.5	443.3	38.9	52.95	7.14	1045	120.0
x_4	-2934	-6.25	-7267	-6.76	-493.8	-0.705	-3899	-4.74
Adjusted R^2	0.9925		0.9950		0.8789		0.9995	

Table 4: $\hat{\sigma}_i^2$ and ω_i over all *i* (n = 16)

i	$\hat{\sigma}_i^2$	ω_i	i	$\hat{\sigma}_i^2$	ω_i
1	5,832	0.0017	9	3,433	0.0052
2	6,336	0.0014	10	3,748	0.0042
3	6,032	0.1630	11	1,0140	0.0014
4	5,419	0.3250	12	9,270	0.0197
5	2,182	0.0226	13	1,947	0.2650
6	2,303	0.0163	14	1,862	0.1490
7	13,883	0.0045	15	20,352	0.0014
8	12,827	0.0058	16	19,022	0.0017

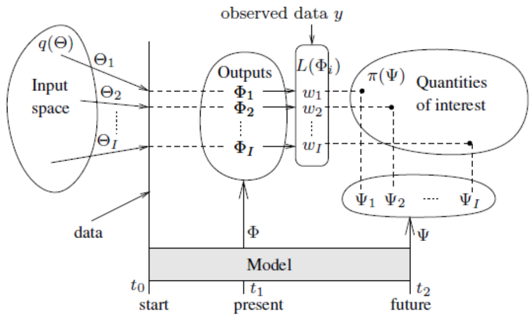

Figure 1: Illustration of the Bayesian Melding Method for Deterministic Models

The uncertain model inputs, $\varTheta$, refer to the starting time of the simulation, t_0, and the outputs, $\varPhi$ and the data relevant to the outputs, *y*, are observed at the ”present” time, t_1, while the quantities of interest, $\varPsi$, refer to the future, t_2. The quantities $\varTheta_i$, $\varPhi_i$ and $\varPsi_i$ refer to the *i*-th simulated values of inputs, outputs and quantities of interest, respectively.

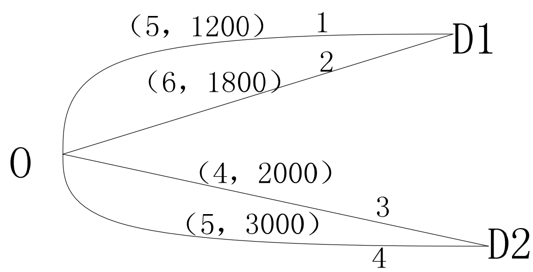

Figure 2: The Test Network

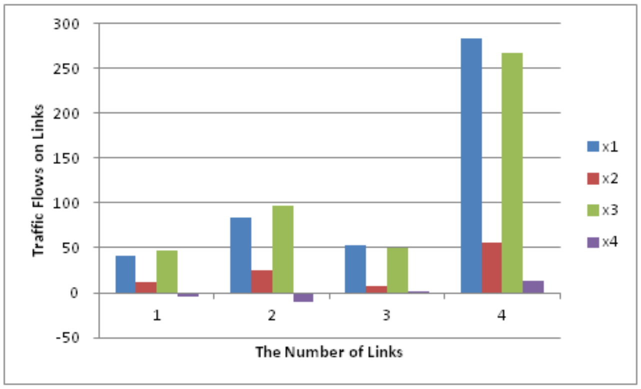

Fig. 3(a): First-order Indices

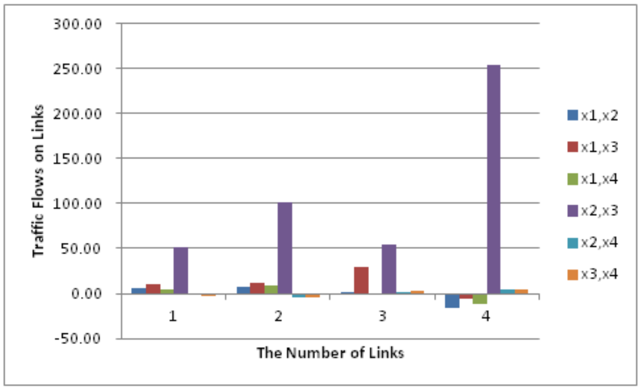

Fig. 3(b): Second-order Indices

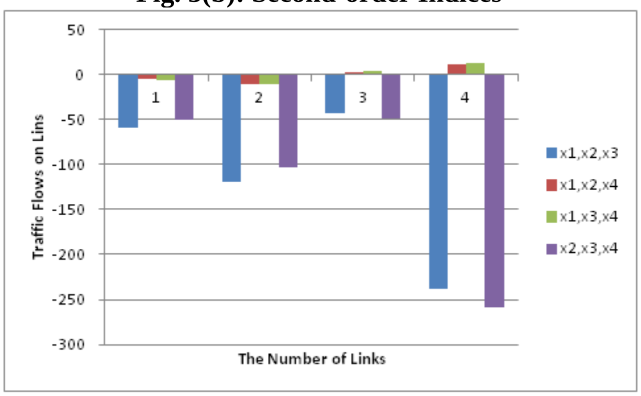

Fig. 3(c): Third-order Indices

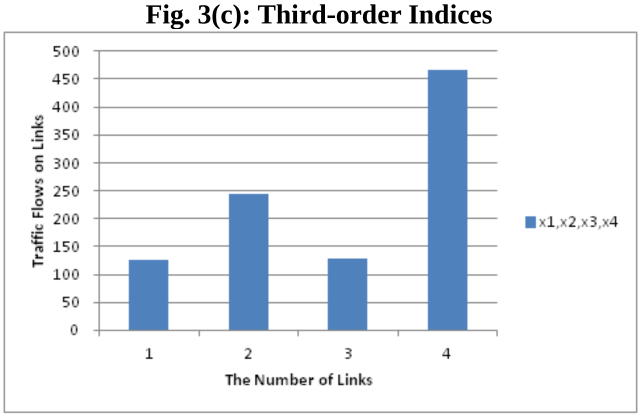

Fig. 3(d): Fourth-order Indices

Figure 3: The ith-order Indices Using LSAI

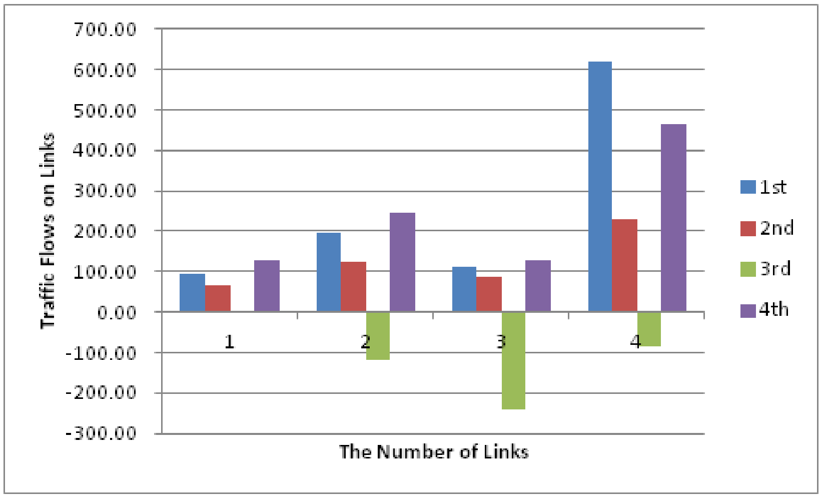

Fig. 4(a): Sums of ith-order Indices

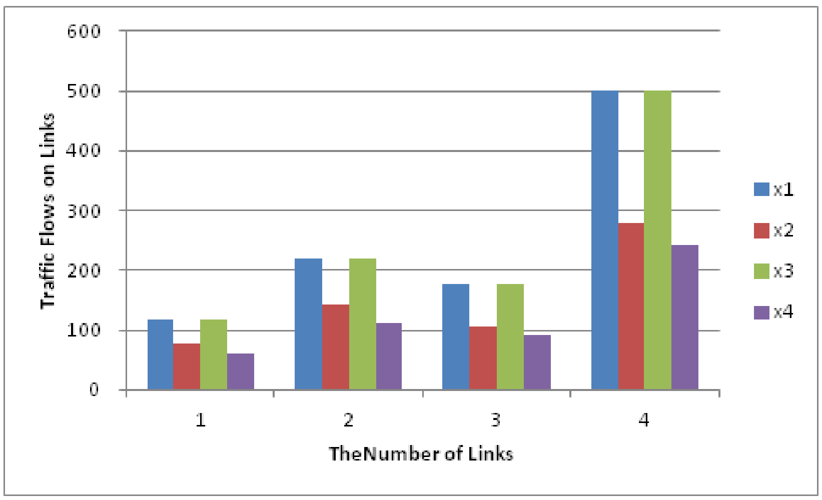

Fig. 4(b): Total-order Indices

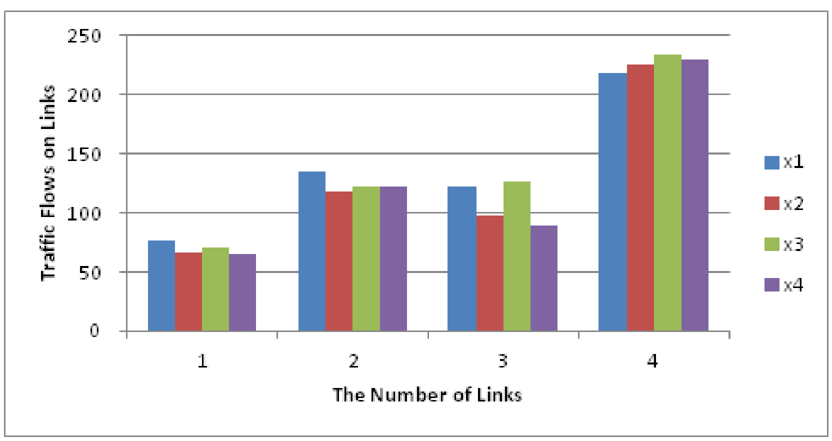

Fig 4(c): The Effect of Interactions Associated with Inputs

Figure 4: The Sums of ith-order Indices, Total-order Indices with the Effect of Interactions Associated with Inputs and Parameters Using LSAI

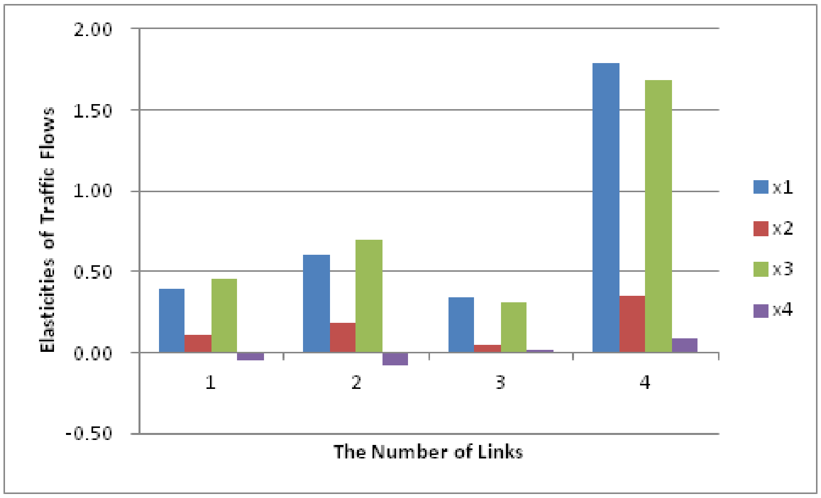

Fig. 5(a): First-order Index

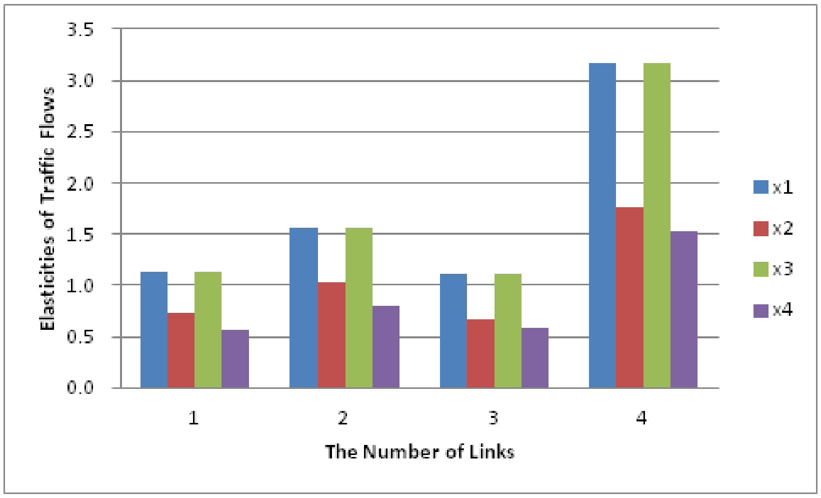

Fig. 5(b): Total-order Index

Figure 5: First-order and Total-order Indices of Link Flows Using LSAI