

# Bayesian Melding in Urban Simulations

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**Abstract:**

## 1 Introduction

- Simulation of processes in environmental disciplines often provide point results.
- The need of expressing uncertainty of such results widely recognized (Refsgaard and Henriksen (2004), van Asselt and Rotmans (2002)).
- Great deal of work in terms of uncertainty in hydrology and high risk areas (Beven and Binley (1992), Beven (2000), Christensen (2003), Neuman (2003), Korving et al. (2003)).
- Work on the whaling project (Raftery et al. (1995), Poole and Raftery (2000)).
- Application to UrbanSim (Waddell (2002), Waddell et al. (2003)).

## 2 UrbanSim

### 2.1 Description

UrbanSim is an urban simulation model operational in several urban areas in the United States (Waddell (2002), Waddell et al. (2003)). The system is implemented as a set of interacting models that represent the major actors and choices in the urban system, including household moving in a residential location, business choices of employment location and developer choices of locations and types of real estate development. It is taking an extremely disaggregated approach by modeling individual households, jobs, and real estate development and location choices using grid cells of  $150 \times 150$  meters in size. The model system microsimulates the annual evolution in locations of individual households and jobs, and the evolution of the real estate within each individual grid cell as the result of actions by real estate developers.

In this section, we give a brief description of the main components of the system. Our emphasis is less on the details of the algorithms of the individual models, but rather on the information on which models base their procedures. For details about the algorithms see Waddell et al. (2003).

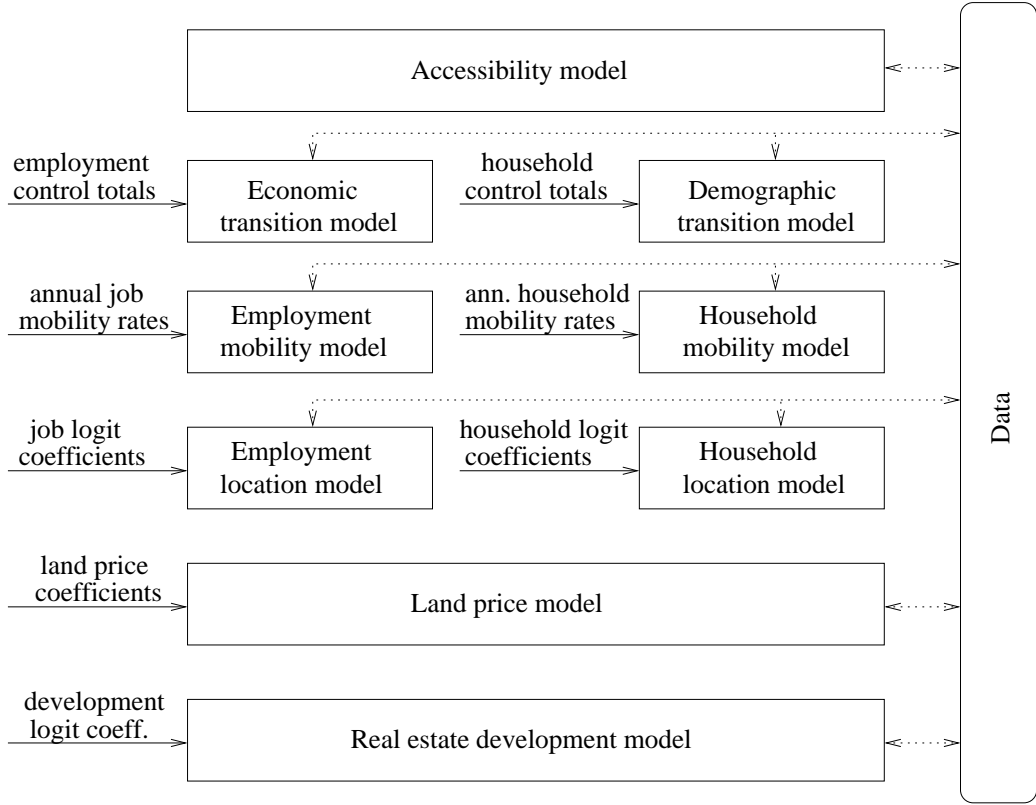


Figure 1: UrbanSim models in order of their runs (from top to bottom). The solid arrows show external input parameters, the dash arrows mark the data flow.

The core of UrbanSim consists of nine models that run in a certain order once per a simulated year. In Figure 1, the models are sorted from top to bottom according to their run order. Models that are placed on the same horizontal level are independent of each other.

A simulation is usually performed for a certain time period given in number of years. It is expected that at the beginning of the simulation, data reflect the true state in the starting year. We will call such data 'base year' data. Each model uses a certain partition of the data as an input and modifies a certain partition of the data according to the results of the run of this particular model. These relations are represented in Figure 1 by dashed arrows. Moreover, most of the models expect additional input parameters (see below) that are marked by solid arrows.

The simulation starts by running the **Accessibility model**. This model creates accessibility indices that summarize the accessibility from a given geographical unit to various activities. The indices are then used in Employment and Household location models where accessibilities are expected to influence household or business choice of location. The Accessibility model is loosely coupled with a Travel model (not included in the figure) that is for simplicity considered here as an external model.

The **Economic transition model** simulates job creation and loss. It uses aggregate employment forecasts (control totals) that are obtained from external sources (state economic forecasts, commercial or in-house sources). Analogously, the **Demographic transition model** simulates births and deaths in the population of households. Here again, control totals from aggregated forecasts obtained from external sources are used as an additional input.

The **Employment mobility model** determines which jobs will move from their current locations during the simulated year. It uses annual mobility rates directly observed over a recent period. They are computed from longitudinally linked business establishment files. Similarly, the **Household mobility model** simulates households deciding whether to move. The algorithm uses annual mobility rates estimated from the Census Current Population Survey.

The **Employment location choice model** is responsible for determining a location for each job that was either newly created or determined for moving. The **Household location choice model** chooses a location for each household that was either created or belongs to the mover set. Both models are based on a multinomial logit model calibrated to observed data. Thus, logit coefficients are required by the models as additional input parameters. These coefficients are usually estimated by external estimation procedures.

The **Land price model** simulates land prices of each grid cell as the characteristics of locations change over time. It is based on a hedonic regression (Waddell et al. 1993) using coefficients estimated externally from historical data.

The one year simulation is concluded by the **Real estate development model** that simulates developer choices about what kind of construction to undertake and where. It uses the multinomial logit model and here again, its coefficients are estimated externally using observed data.

## 2.2 Sources of uncertainty

In order to make a probabilistic analysis of any system, the first step is to identify all possible sources of uncertainty of this system (see e.g. Morgan and Henrion (1990), Dubus et al. (2003), Regan et al. (2003)). The goal of the analysis is then to quantify as much of the identified uncertainty as possible. This section reviews sources of uncertainty that are entering UrbanSim.

### 2.2.1 Measurement errors

As mentioned above, data that enter UrbanSim at the beginning of any simulation run (base year data) should reflect the true state of the world. The data are collected from different sources, such as census or commercial sources. Obviously, such data are subject to errors, moreover, they often contain missing values. For example, concerning parcel data, tax exempt properties like government-owned properties tend to have very incomplete data in the assessor files, since there is no compelling reason for assessors to collect these items. These data are massive in volume, and rely on individual property assessors to input data, and the resulting databases are often riddled with missing data and data errors. As a result, it is in user responsibility to deal with these limitations, for example by applying imputation procedures.

### **2.2.2 Systematic errors**

Systematic errors is a type of uncertainty that can bias the simulation results. It arises for example due to wrongly calibrated measurement tools or due to not completely random sampling procedures. An example of the latter case would be a situation where households belonging to a certain category, such as a certain race, are excluded from the sampling process when creating the household database from census sources. Both, the measurement errors and the systematic errors affect the quality of the base year data.

### **2.2.3 Uncertainty in model structure**

In this category, three types of uncertainty can be distinguished. First, the selection of variables that are entering the statistical models embedded in UrbanSim, such as the multinomial logit model or the hedonic regression. Second, the choice of the statistical model itself. For example, processes modelled by the multinomial logit could be modelled by other model of the discrete choice model family, such as the multinomial probit or mixed logit model (Train 2003). Third type of uncertainty in this category arises through the selection of the processes that are modelled by UrbanSim. It is obvious that the collection of UrbanSim models does not represent a complete set of processes that in real life influence the evolution in households and jobs locations. Therefore, since the UrbanSim system represent only an abstraction of all real life processes that affect the modelled quantities, it is subject to uncertainty.

### **2.2.4 Uncertainty in model input parameters**

As described in Section 2.1, there are several sets of input parameters that enter UrbanSim and all of them are estimated by external models or procedures. Since they are estimates of some true values, they can be used to make statistical inference and thus, can be included in the uncertainty analysis of the simulation results.

### **2.2.5 Stochasticity**

An important source of uncertainty arises by using random numbers within models. The fact that simulations with different seeds of the random number generator will produce different results, has to be taken into account in the uncertainty analysis. In UrbanSim, several models that use multinomial logit model use a sampling procedure for sampling choice alternatives. Additionally, both mobility models use sampling for determining movers according to given rates.

Table 1 summarizes for each model the information about the main component of the procedure, the estimation of the input parameters, and the fact if random numbers (RNs) are used by the model.

model	procedure	estimation of input param.	RNs
Accessibility	deterministic	–	no
Economic/Demographic transition	algorithmus based on joint prob. distr. of jobs/households	external sources	yes
Employment/Household mobility	random sampling	observed rates	yes
Employment/Household location choice	multinomial logit	multinomial logit	yes
Land price	hedonic regression	hedonic regression	no
Development	multinomial logit	multinomial logit	yes

Table 1: Procedure type, type of estimation of input parameters and random numbers (RNs) usage for each model.

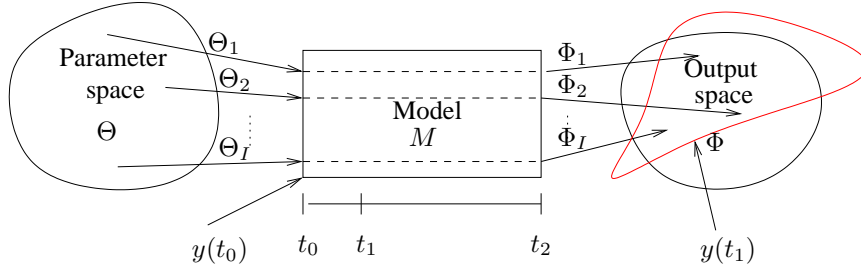


Figure 2:

### 3 Method

#### 3.1 Basic Notation

Let the  $D$ -dimensional space of all possible model input parameters be denoted by  $\Theta^D \subset \mathbb{R}^D$ . A model  $M$  expects  $\Theta_i^D \subset \Theta^D$  as its input and generates output  $\Phi_i^K \subset \Phi^K$ . Thus,  $\Phi^K \subset \mathbb{R}^K$  denotes the  $K$ -dimensional space of all possible model outputs. For simplicity, we omit the superscript and write  $\Theta$ ,  $\Theta_i$ ,  $\Phi$  and  $\Phi_i$ , respectively. Now, we can write  $\Phi_i = M(\Theta_i)$ , or more generally  $\Phi = M(\Theta)$ .

$M$  is considered as a simulator that starts at time  $t_0$  in a certain state and simulates given processes until time  $t_2$ . Thus,  $\Phi$  is related to a certain time point, here  $\Phi = \Phi(t_2)$ . The state at time  $t_0$  is usually based on observed data at  $t_0$ , denoted here by  $y(t_0)$  ( $y \subset \mathbb{R}^K$ ). If observed data are available for some  $t_1$  ( $t_0 < t_1 < t_2$ ), we can use  $y(t_1)$  to assess a more precise shape of the output space  $\Phi$ . The described scenario is shown in Figure 2.

### 3.2 Formulation

We define our quantities of interest  $\psi$  as a function of model outputs:

$$\psi = \Psi(\Phi) = \Psi(M(\Theta)).$$

Let  $q(\Theta)$  denote the prior distribution of  $\Theta$ . The likelihood of simulated outputs is

$$L(\Phi) = \text{prob}(y|\Phi). \quad (1)$$

Then the posterior distribution of inputs can be written as

$$p(\Theta) \propto q(\Theta)L(\Phi)$$

which can be translated into a posterior distribution of model outputs and quantities of interest.

### 3.3 Simulating posterior distribution

In Raftery et al. (1995) and Poole and Raftery (2000) a method called Bayesian melding has been proposed which puts analysis of simulation models on a solid statistical footing. It provided a purely deterministic model with a Bayesian framework in order to assess uncertainty about the natural rate of increase of bowhead whales.

The method is based on Monte Carlo simulation and can be described in a simplified way as follows:

1. Draw a sample  $\{\Theta_1, \dots, \Theta_I\}$  of values of the inputs from the prior distribution  $q(\Theta)$ .
2. Obtain  $\{\Phi, \dots, \Phi_I\}$  where  $\Phi_i = M(\Theta_i)$ .
3. Compute weights  $w_i = L(\Phi_i)$ . As a result, we get an approximate posterior distribution of inputs with values  $\{\Theta_1, \dots, \Theta_I\}$  and probabilities proportional to  $\{w_1, \dots, w_I\}$ .
4. The approximate posterior distribution of the quantities of interest has values  $\{\psi_1, \dots, \psi_I\}$  where  $\psi_i = \Psi(\Phi_i)$  and probabilities proportional to  $\{w_1, \dots, w_I\}$ .

The applications that we are dealing in this paper with are not deterministic. We consider here models that contain a stochastic component in terms of using random numbers. Runs with different seeds return different results. To include this source of uncertainty into the framework, we modify the above procedure as follows:

1. As above.
2. For each  $\Theta_i$ , run the model  $J$  times with different seeds to obtain  $\Phi_{ij}, j = 1, \dots, J$ .
3. Compute weights  $w_i = L(\bar{\Phi}_i)$  where  $\bar{\Phi}_i = \frac{1}{J} \sum_{j=1}^J \Phi_{ij}$ . Here again, we get an approximate posterior distribution of inputs with values  $\{\Theta_1, \dots, \Theta_I\}$  and probabilities proportional to  $\{w_1, \dots, w_I\}$ .
4.  $\psi$  now has a distribution given  $\Theta_i$ .

### 3.4 Likelihood

In order to compute the weights in Step 3 of Section 3.3, we need to define a likelihood function (Eq. 1). Specifically,

$$w_i \propto p(y|\Theta_i) = \prod_{k=1}^K p(y_k|\Theta_i). \quad (2)$$

Assessing  $p(y|\Theta_i)$  is based on the following model:

$$\Phi_{ijk} = \mu_{ik} + \delta_{ijk}, \text{ where } \delta_{ijk} \stackrel{iid}{\sim} N(0, \sigma_\delta^2) \quad (3)$$

$$(y_k|\Theta = \Theta_i) = \mu_{ik} + a + \epsilon_{ik}, \text{ where } \epsilon_{ik} \stackrel{iid}{\sim} N(0, \sigma_i^2) \quad (4)$$

Here,  $\mu_{ik}$  denotes the expected output for  $\Theta_i$  and  $k$ -th dimension of the output. Furthermore,  $\delta_{ijk}$  and  $\epsilon_{ik}$  denote model errors and  $a$  denotes the overall bias in the model.

Estimation of  $\mu_{ik}$ ,  $\sigma_\delta^2$ ,  $\sigma_i^2$ , and  $a$  can be done by approximate maximum likelihood (see Appendix A).

We denote these estimates by  $\hat{\mu}_{ik}$ ,  $\hat{\sigma}_\delta$ ,  $\hat{\sigma}_i^2$  and  $\hat{a}$ , respectively.

This yields a predictive distribution of our quantity of interest:

$$y_k|\Theta_i \sim N(\hat{a} + \hat{\mu}_{ik}, v_i) \quad \text{with } v_i = \hat{\sigma}_i^2 + \frac{\hat{\sigma}_\delta^2}{J}. \quad (5)$$

(see Appendix B for details).

We then have

$$w_i \propto p(y|\Theta_i) = \prod_{k=1}^K \frac{1}{\sqrt{2\pi v_i}} \exp \left[ -\frac{1/2(y_k - \hat{a} - \hat{\mu}_{ik})^2}{v_i} \right] \quad \text{and} \quad (6)$$

$$\log w_i \propto -\frac{K}{2} \log(2\pi v_i) - \frac{1}{2v_i} \sum_{k=1}^K (y_k - \hat{a} - \hat{\mu}_{ik})^2. \quad (7)$$

### 3.5 Posterior distribution of quantities of interest

Given that  $\hat{\sigma}_\delta$ ,  $\hat{\sigma}_i^2$  and  $\hat{a}$  were estimated at time point  $t_1$ , the marginal distributions of model outputs for the time point  $t_2$  are given by a mixture of normal distributions

$$p(\Phi_k) = \sum_{i=1}^I w_i N(\hat{a}b_a + \hat{\mu}_{ik}(t_2), (\hat{\sigma}_i^2 + \frac{\hat{\sigma}_\delta^2}{J})b_v), \quad k = 1, \dots, K \quad (8)$$

where  $b_a$  and  $b_v$  denote propagation factors (over the time period  $t_2 - t_1$ ) of the bias and the variance, respectively.

The resulting posterior distribution of the quantity of interest  $\psi$  is given by

$$p(\psi) = \sum_{i=1}^I w_i \left[ \prod_{k=1}^K \Psi(N(\hat{a}b_a + \hat{\mu}_{ik}(t_2), (\hat{\sigma}_i^2 + \frac{\hat{\sigma}_\delta^2}{J})b_v)) \right]. \quad (9)$$

## 4 Application

### 4.1 Model

In this section, we apply the described method to our test data. It consists of data from the area of Eugene-Springfield, OR, in 1980. Our goal is to make a prediction using UrbanSim for the year 2000. Specifically, our quantity of interest  $\psi$  is the spacial distribution of households in the considered area (on the traffic analysis zone (TAZ) level or its aggregation).

As model outputs  $\Phi$ , we are interested in number of households per TAZ. Thus, the number of traffic zones determines the dimension  $K$  of our output space, here  $K = 295$  (with possible reduction, see Section 4.2.2).

For computing the weights (Eqs. 6 and 7), we use observed number of households in each zone in 1994, denoted here as  $y_1, \dots, y_K$ .

#### 4.1.1 Prior on inputs

Input parameters that were derived by the multinomial logit procedure or by the hedonic regression (see Table 1) have known standard errors (SE) and covariance matrices (C). For these parameter sets we used the multivariate normal distribution  $\text{MVN}(\hat{\Theta}, C((\hat{\Theta})))$  where  $\hat{\Theta}$  is the parameter estimator of the true value  $\Theta$ . Note that the values of the covariance matrices were negligible (except of the diagonal) so that we used only diagonal matrices of  $\text{diag}(\text{SE}(\hat{\Theta})^2)$ .

For each mobility rate  $r$  in the employment and household mobility models we used the zero truncated normal distribution  $N(\hat{r}, (\frac{\hat{r}(1-\hat{r})}{n})^2)$  where  $\hat{r}$  is an estimation of the true rate  $r$  and  $n$  is the number of observations from which  $\hat{r}$  was obtained.

In terms of the control totals for the economic and demographic transition model, respectively, we obtained a predictions for the end year of the simulation and interpolate these values to the years prior to the end year. Additionally, we obtained several pairs of prediction and true observation values from the historical data, in order to estimate the standard error on these totals. Then we assigned each total  $c$  with the normal distribution  $N(c, \text{SE}(c))$ . *Should we say that our  $c$  is the true value from 2000?*

#### 4.1.2 Simulation

We run UrbanSim for 100 different inputs, each of them twice with different random seed. That is 200 runs in total, with  $I = 100$  and  $J = 2$ . Note that we confirmed our results on a simulation with  $I = 1000$  and  $J = 3$ . Since an UrbanSim simulation of this size is in practice not feasible due to the long run time, in this paper we refer to results of the smaller simulation but point to differences if any. The simulation was started in 1980 and run until 2000. Results  $\Phi_{ijk}(1994)$  and  $\Phi_{ijk}(2000)$  were saved for all  $i = 1, \dots, I$ ,  $j = 1, \dots, J$ ,  $k = 1, \dots, K$ .



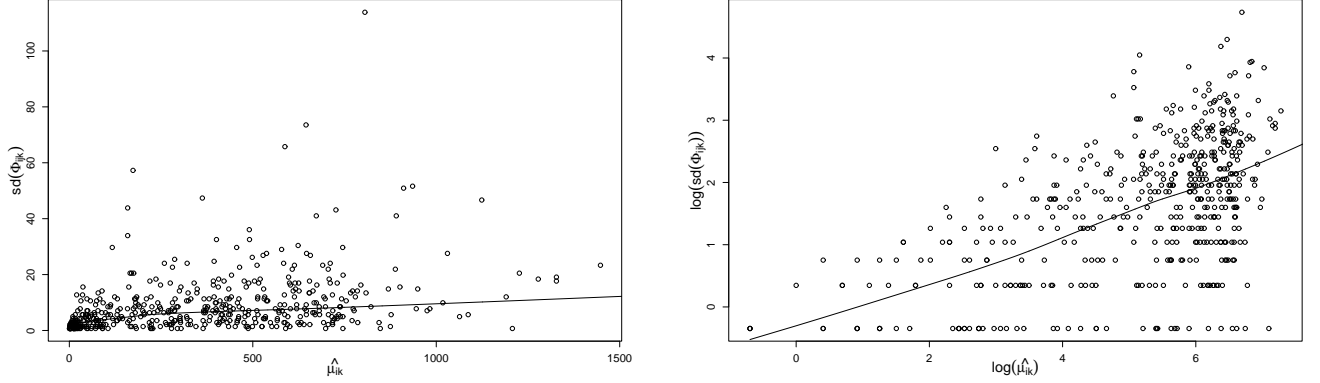


Figure 3: Scatter plot of  $\hat{\mu}_{ik}$  vs. standard deviation of  $\Phi_{ijk}$  for  $t = 1994$  and the corresponding lowess curve (raw data in the left panel, data on the log-log scale in the right panel). The plots contain 500 randomly selected points from  $I \cdot K = 29500$  points in total (excluding points where either  $\hat{\mu}_{ik}$  or  $\text{sd}(\Phi_{ijk})$  is equal zero). The lowess curve is based on all points.

## 4.2 Results

### 4.2.1 Transformation

In Equation 3 and 4, we are assuming that our model errors have constant variances  $\sigma_\delta^2$  over all  $i$  and  $k$ , and  $\sigma_1^2$  over all  $k$ .

In Figure 3 we examine the relationship between the estimate of  $\Phi_{ijk}(1994)$ , denoted by  $\hat{\mu}_{ik}$ , and its standard deviation,  $\text{sd}(\Phi_{ijk})$ . Obviously,  $\text{sd}(\Phi_{ijk})$  increases with increasing  $\hat{\mu}_{ik}$ . The relationship is approximately linear on the log-log scale, shown in the right panel of Figure 3.

A detailed analysis of the slope suggested to transform the data on the square root scale. Figure 4 shows the scatter plots from Figure 3 after the square root transformation. The relationship became weak, in particular the squared correlation coefficient is now  $R^2 = 0.03$ . Note that we excluded data from the analysis where either  $\hat{\mu}_{ik}$  or  $\text{sd}(\Phi_{ijk})$  is equal zero.

The relationship between the absolute error  $|y_k - \hat{\mu}_{ik}|$  and  $\text{sd}(\Phi_{ijk})$  after the transformation is shown in Figure 5. Here the squared correlation coefficient is  $R^2 = 0.01$ .

As a result, a square root transformation is applied to  $\Phi_{ijk}$  and  $y_k$  for all  $i, j, k$ , prior to any computation. Therefore, unless stated otherwise, results reported in the following sections refer to the transformed data.

### 4.2.2 Computing weights

From the results  $\Phi_{ijk}(1994)$  we estimated quantities necessary for computing the weights (Equations 6 and 7). They are summarized in Table 2. The table contains estimates for both, the small simulation ( $I = 100$ ) as well as the larger one ( $I = 1000$ ). It can be seen that the influence of the simulation size

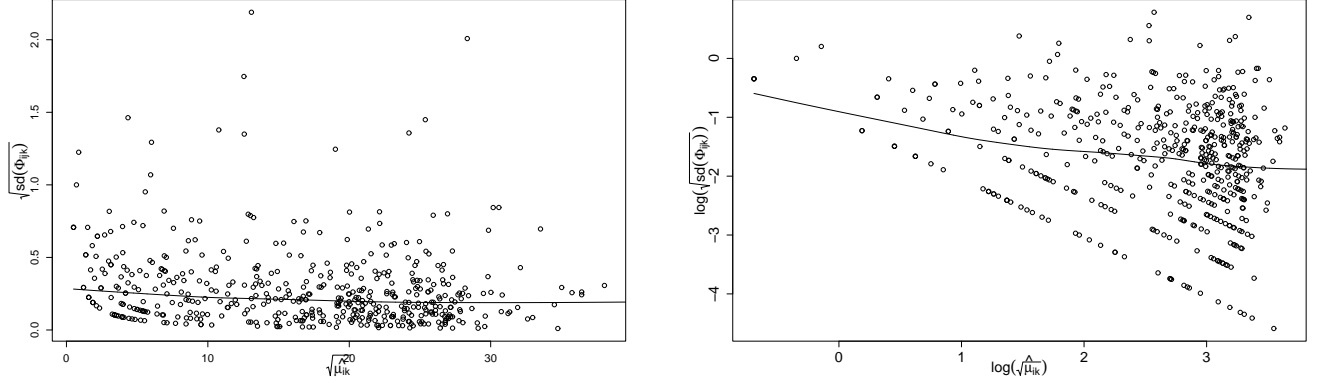


Figure 4: Data from Figure 3 on the square root scale.

estimate/sim. size	100 × 2	1000 × 3
$\hat{a}$	−0.156	−0.198
$\hat{\sigma}_\delta^2$	0.072	0.113
$\hat{\sigma}_i^2$	15.035(2.3)	14.992(1.8)
$v_i$	15.071(2.3)	15.015(1.8)

Table 2: Estimates required for computing the weights. Two simulation sizes  $I \times J$  are considered. Values for  $\hat{\sigma}_i^2$  and  $v_i$  denote the mean and standard deviation (in parentheses) computed over all  $i$ .

on the estimates is insignificant.

The values for  $\hat{\sigma}_i^2$  and  $v_i$  in the table denote the mean and standard deviation (in parentheses) computed over all  $i$ . Obviously,  $\hat{\sigma}_i^2$  is the dominant component in the variance  $v_i$ .

Note that for practical reasons, we excluded from the analysis zones where  $\hat{\mu}_1 = 0$ . These are mostly zones in which up to 1994 no residential units were placed. Thus, the dimension of the outputs was reduced to  $K = 265$ .

Table 3 shows the resulting seven highest weights and the minimum weight for the 100 simulation runs. Each weight evaluates results for 1994 of the particular simulation conditioned on the observed data in the same year. For example, simulation for  $i = 64$  which has the maximum weight provides results whose correlation coefficient with the observed data is  $R = 0.93$ . On the other hand, simulation for  $i = 33$  which has the minimum weight leads to  $R = 0.84$ .

#### 4.2.3 Posterior distribution

In order to compute the posterior distribution of our quantity of interest (Equations 8 and 9), we set the propagation factors  $b_a$  and  $b_v$  to 20/14. This results from the calculation  $\frac{2000-1980}{1994-1980}$ . Note that

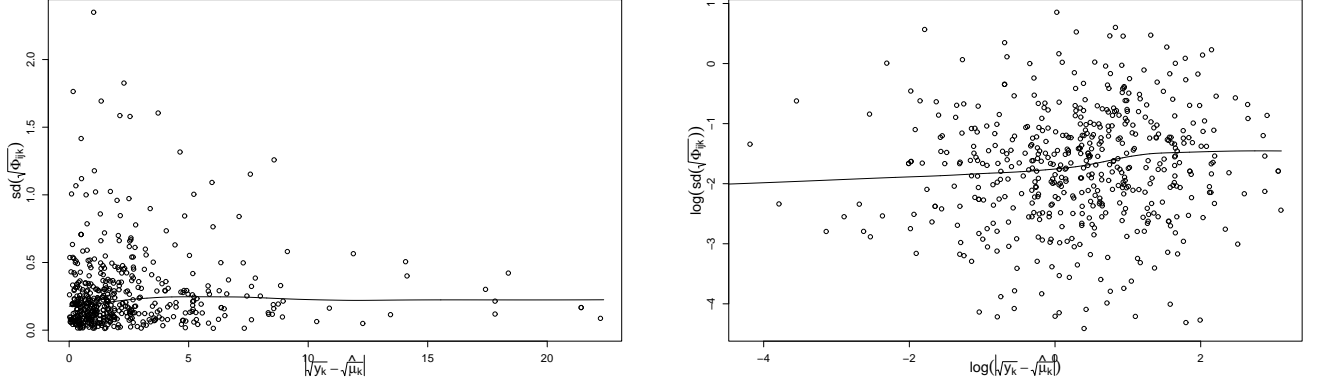


Figure 5: Absolute error of the transformed data,  $|\sqrt{y_k} - \sqrt{\hat{\mu}_{ik}}|$ , vs. standard deviation of  $\sqrt{\Phi_{ijk}}$  for  $t = 1994$  and the corresponding lowess curve (raw data in the left panel, data on the log-log scale in the right panel). As in Figure 3, the plots contain 500 randomly selected points, whereas the lowess curve is based on all points.

$i$	64	13	12	76	68	88	23	33(min)
$w_i$	0.8058	0.0883	0.0370	0.0217	0.0122	0.0116	0.0068	$4 \cdot 10^{-45}$

Table 3: 7 highest weights and the smallest weight for the  $100 \times 2$  simulation.

$t_2 = 2000$  and therefore the estimation of  $\mu_{ik}$  is based on  $\Phi_{ijk}(2000)$ .

An example of the resulting Bayesian melding distribution for one zone is shown in the left panel of Figure 6. The right panel shows a histogram of the results from the 200 UrbanSim runs without applying Bayesian melding. In both cases, the red line marks the true observation, the black vertical solid line marks the mean and the vertical dashed lines mark the 90% confidence interval. It can be seen that the Bayesian melding distribution is wider than the range provided by the simple multiple runs, and in fact the latter one misses the true observation far more often than the Bayesian melding procedure. This can be seen in Table 4 which show the number of missed cases and the coverage for both procedures. The exactly same results are obtained from the  $1000 \times 3$  simulation (*needs to be checked*).

method	missed cases	coverage
Bayesian melding	31	0.883
multiple runs	163	0.385

Table 4: Coverage of for the 90% confidence interval. Missed cases give the number of observations that fall outside of the confidence interval. The total number of observations is 265.

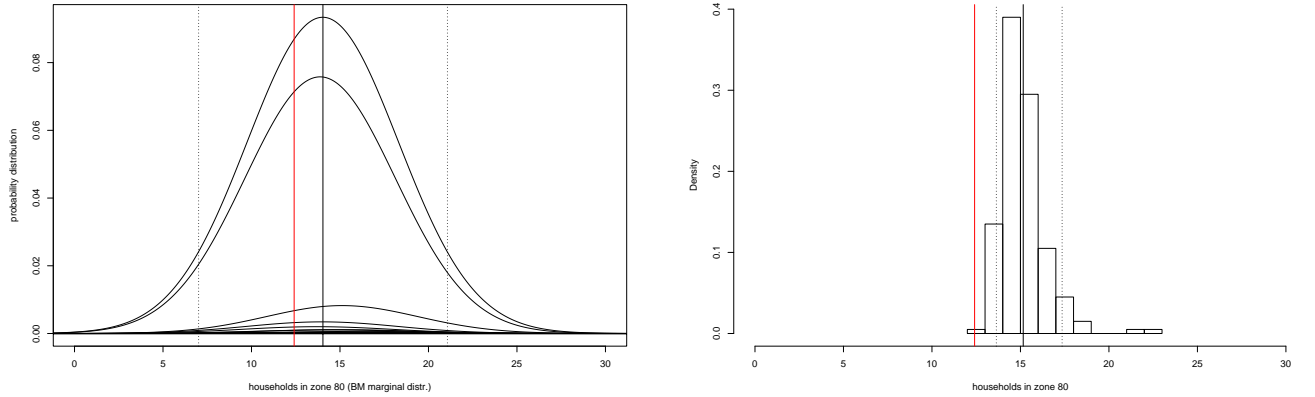


Figure 6: Results of zone 80. Left panel – Bayesian melding probability distribution. Right panel – histogram of multiple runs. The red line marks the true observation, the black vertical solid line marks the mean and the vertical dashed lines mark the 90% confidence interval. Both plots are made on a square root scale.

The table suggests that Bayesian melding is much better calibrated than a distribution provided by just simply taking results from multiple Monte Carlo runs.

We check the calibration by evaluating the corresponding verification rank histogram. A verification rank histogram can be used for checking a set of predictive distributions. It is a histogram of rankings of the data within values simulated from the distributions in question, in our case from  $p(\Phi_k)$ . If the ranking is uniformly distributed, there is a high evidence that the data come from the considered set of distributions.

We sample 99 values  $l$  with replacement from  $1, \dots, I$  with probabilities proportional to the weights  $w_i$ . For each  $l$  and each  $k$  we draw one normally distributed random number from the normal distribution given in the sum expression of Equation 8, where  $i$  is set to  $l$ . Since negative values do not make sense here, we consider a truncated normal distribution where we discard all values smaller than 0. The remaining values set to power of 2 build the posterior distribution of the model outputs. Each true observation is then ranked among values of the corresponding zone. The verification rank histogram is shown in the left panel of Figure 7. The right panel shows the empirical cumulative distribution function (CDF) for the rankings in the left panel. Figure 8 shows the same quantities for the multiple runs scenario. It is obvious that multiple runs provide a much less calibrated procedure than Bayesian melding.

#### 4.2.4 Aggregated results

Often, we are interested in spatial distribution on a higher aggregation level. This can be easily solved in the Bayesian melding framework by aggregation of the results obtained for smaller geographical units. Here we are dealing with aggregation of a mixture of truncated normal components which we solved by a simulation.

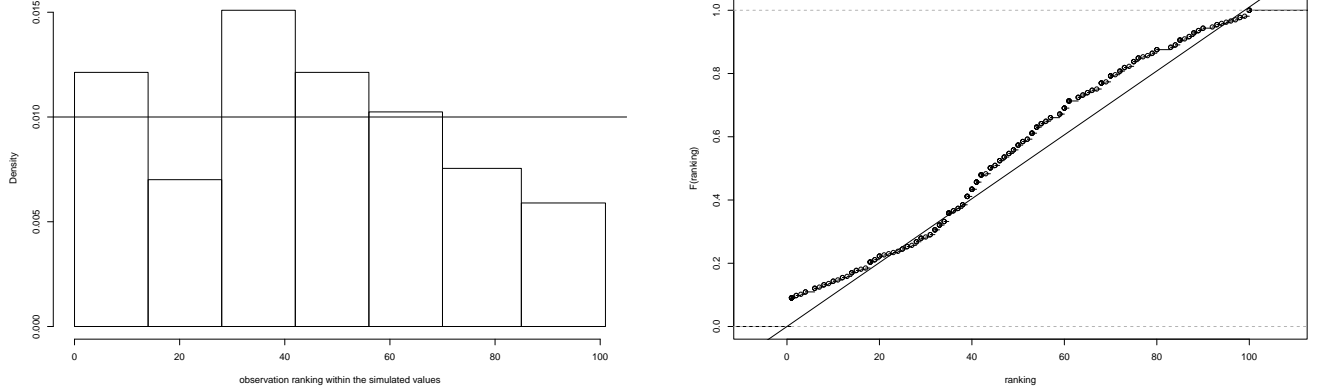


Figure 7: Verification rank histogram (left panel) and the corresponding CDF (right panel) for the Bayesian melding output.

Suppose we are interested in number of households that live in a certain radius around the central business district (cbd). Intuitively, we aggregate over zones that are located in that particular radius. Figure 9 shows histograms of results for four different radii, measured in time distance, each of them simulated by 1000 values. In all cases the true observation (marked by red line) falls very close to the mean value (black solid line) of the distribution. Each plot in Figure 9 shows the exact value for the true observation (obs), the mean and the 90% confidence interval (CI, marked by dashed lines), respectively.

## 5 Discussion

## Acknowledgement

## Appendix

### A Estimation

Let  $I$ ,  $J$ ,  $K$  denote the sample size of the input parameters (Step 1 of Section 3.3), the number of runs for the same input parameters (Step 2) and the dimension of the output space, respectively. Then, the quantities in Equations 3 and 4 can be estimated as follows:

- Estimation of  $\mu_{ik}$ :

$$\hat{\mu}_{ik} = \frac{1}{J} \sum_{j=1}^J \Phi_{ijk} \quad (10)$$

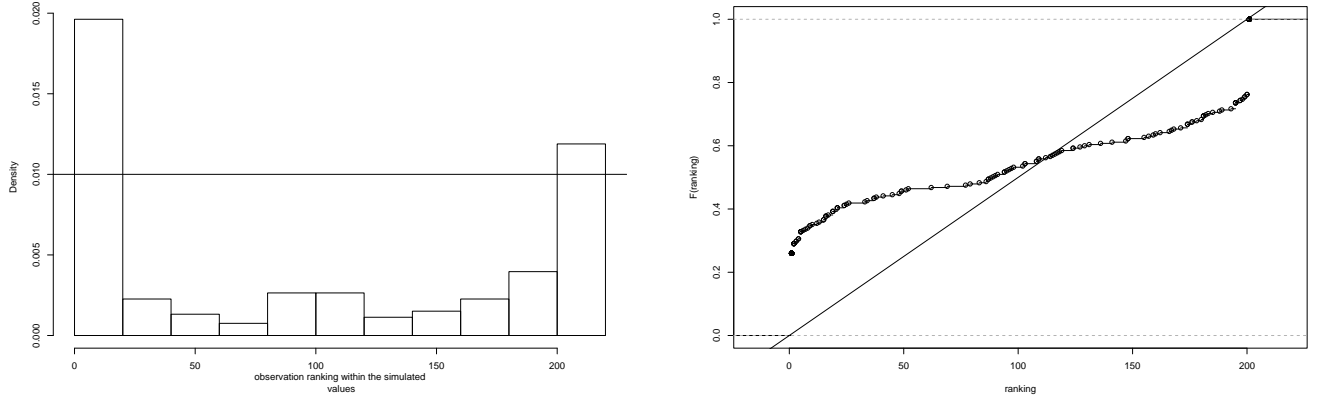


Figure 8: Verification rank histogram (left panel) and the corresponding CDF (right panel) for the output from multiple runs.

- Estimation of  $\sigma_\delta^2$ :

$$\hat{\sigma}_\delta^2 = \frac{1}{IJK} \sum_{ijk} (\Phi_{ijk} - \hat{\mu}_{ik})^2 \quad (11)$$

- Estimation of  $a$ :

$$\hat{a} = \frac{1}{IK} \sum_{i,k} (y_k - \hat{\mu}_{ik}) . \quad (12)$$

- Estimation of  $\sigma_i^2$ :

$$\hat{\sigma}_i^2 = \frac{1}{K} \sum_k (y_k - \hat{a} - \hat{\mu}_{ik})^2 . \quad (13)$$

## B Building posterior distribution

To build  $p(y_k|\Theta_i)$ , note that

$$(y_k - a - \hat{\mu}_{ik}) = (y_k - a - \mu_{ik}) - (\hat{\mu}_{ik} - \mu_{ik})$$

and therefore

$$E(y_k - a - \hat{\mu}_{ik}) = 0 \quad \text{and}$$

$$Var(y_k - a - \hat{\mu}_{ik}) = Var(y_k - a - \mu_{ik}) + Var(\hat{\mu}_{ik} - \mu_{ik}) = \sigma_i^2 + \frac{\sigma_\delta^2}{J}.$$

Then we get Equation (5).

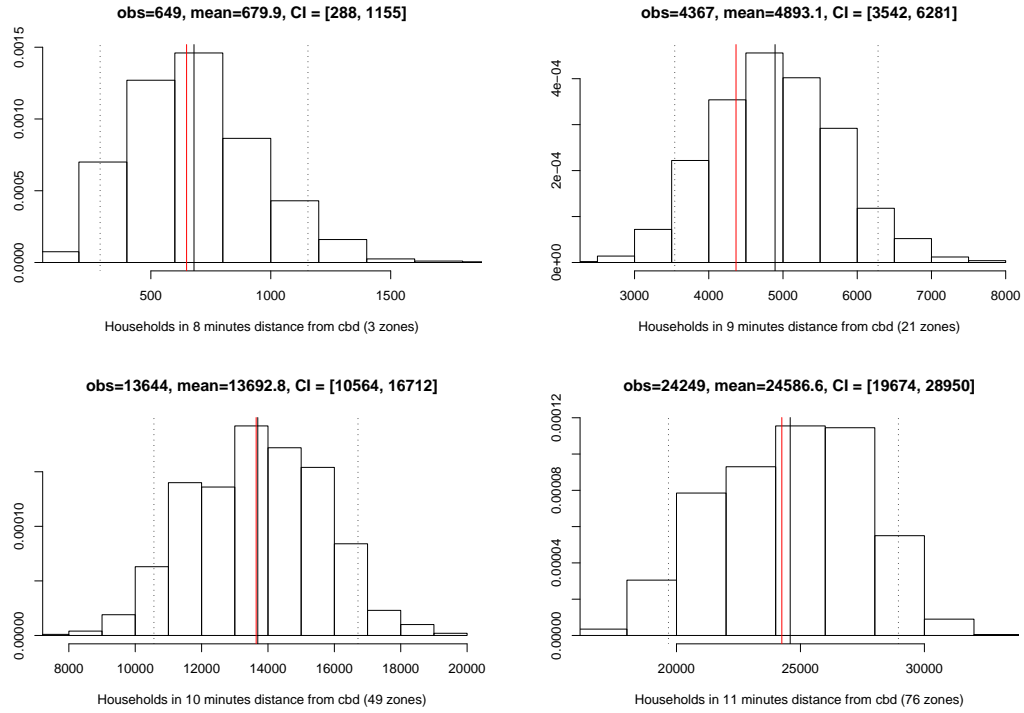


Figure 9: Histogram of simulated posterior distributions for aggregated quantity of interest – number of households living in 8,9,10, and 11 minutes distance from the central business district. Note that the simulated quantity is rescaled to the original scale.

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