An Early Stopping Bayesian Data Assimilation Approach for Mixed-Logit Estimation

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Abstract

The mixed-logit model is a flexible tool in transportation choice analysis, which provides valuable insights into inter and intra-individual behavioural heterogeneity. However, applications of mixed-logit models in practice are limited by the high computational and data requirements for model estimation. When estimating mixed-logit models on small samples, the *Bayesian* estimation approach becomes vulnerable to over and under-fitting. This is problematic for investigating the behaviour of specific population sub-groups or market segments, where a modeller may wish to estimate separate models for multiple similar contexts, each with low data availability. Similar challenges arise when adapting an existing model to a new location or time period, e.g., when estimating post-pandemic travel behaviour.

In order to address the data and transferability issues of the mixed-logit model, in this paper we propose a new Early Stopping Bayesian Data Assimilation (ESBDA) simulator for estimation of mixed-logit which combines a *Bayesian* statistical approach with Machine Learning (ML) model estimation methodologies. The ESBDA simulator is intended to improve the transferability of mixed-logit models and to enable the estimation of robust choice models with low data availability. This approach can therefore provide new insights into people's choice behaviour where the traditional estimation of full mixed-logit models was not previously possible due to low data availability, and open up new opportunities for investment and planning decisions support.

To assess the performance of the new approach, we benchmark the ESBDA estimator against the Direct Application approach and two reference simulators: (i) a basic hierarchical Bayes (HB) simulator with random starting parameter values; (ii) a Bayesian Data Assimilation (BDA) simulator without *early stopping*. Two case-studies are used to investigate the relative performance of the simulators in varied contexts.

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The experimental results show that the proposed ESBDA approach can effectively overcome under and over-fitting and non-convergence issues in simulation. The resulting models from ESBDA clearly outperform those of the reference simulators in terms of predictive accuracy. Furthermore, we find that models estimated with ESBDA tend to be more robust, with significant parameters with signs and values consistent with behavioural theory, even when estimated on small samples.

Keywords: Data Assimilation, Discrete Choice Models, Hierarchical Bayes, Machine Learning, Mixed-Logit, Model Transferability

1. Introduction

Discrete Choice Models (DCMs) based on random utility theory are a key research tool in behaviour analysis in areas such as transportation, economics, health, and many other disciplines where there is a focus on individual choice behaviour. Traditional DCMs, including the logit and Nested Logit (NL) models, make use of closed-form *utility specifications* with fixed parameters. This allows choice probabilities to be generated analytically without the need for simulation. Despite their computational convenience, the fixed parameters used in logit models do not account for the significant inter and intra-individual heterogeneity in individual decision-makers' behaviours.

Mixed-logit models accommodate heterogeneity in DCMs by treating model parameters as distributed over the population of interest (see Bhat, 2000; McFadden and Train, 2000; Train, 2003). Whilst they extend the behavioural capabilities of logit models, mixed-logit models have large data and computational requirements (Greene and Hensher, 2003). There are two predominant estimation techniques for mixed-logit models: the Maximum Simulated Likelihood (MSL) method and the *Bayes* approach. Both techniques can face issues with convergence and model fitting errors with low data availability (Bhat, 2001; Wang et al., 2006).

These issues can be problematic when investigating the behaviour of specific population sub-groups or market segments, where a modeller may want to estimate separate models for several similar contexts, each with low data availability. The same challenges arise when estimating a new model for a poorly sampled location or time period, where there may not be sufficient data to estimate a new model. In the meantime, empirical models are found to have low *transferability*; i.e. a model estimated in one context cannot accurately predict similar choices for a new context (Koppelman and Rose, 1985). This means that areas, population segments or new time periods with poor data availability cannot benefit substantially from existing models. There is therefore the need for an advanced simulation technique for mixed-logit estimation to address modelling anomalies caused by data shortage.

This study introduces and evaluates a new estimation approach for improving the predictive power and behavioural consistency of mixed-logit models for small sample modelling. The new approach, called Early Stopping Bayesian Data Assimilation (ESBDA), is developed to adapt a previously established model to a new population subgroup, location, or time period, with low data availability. This work builds on

existing concepts of model transferability (Ben-Akiva and Bolduc, 1987) and the Hierarchical Bayes simulation (Train, 2006). The configuration of ESBDA aims to address the recurrent issues of over-fitting and non-convergence in small sample modelling of mixed-logit models. The primary intended contribution of ESBDA is the improved transferability of mixed-logit models. This enables an inexpensive and practical way to estimate models for a new context.

In addition to tackling locational or demographic heterogeneity, the increased model transferability also enables existing models to be better adapted to future scenarios and/ or demographic changes. This is increasingly relevant, given the current rate of technological innovation, urban demographic changes and the pandemic shock. One potential application is the estimation of post-pandemic travel choice behaviour in a fast, inexpensive manner with relatively low data requirements.

2. Literature Review

2.1. Heterogeneity in Discrete Choice Models

There are many potential sources of heterogeneity in choice behaviour. Those identified in the literature include: difference in behavioural processes, knowledge (e.g., awareness, information) and points of view (e.g., perceptions, attitudes and cultural values) between individuals (Wood, 2000; Ajzen, 2001; Sparks et al., 2013); different circumstances between individual choices (Engel et al., 1968, 1982, 1995; Assael, 1995; Paulssen et al., 2014); and difference in the degree of familiarity, complexity, and perceived risks of the choice-set (Ajzen, 1987; Gärling et al., 1998; ?). Whilst the simplicity of logit models enables straightforward model estimation, the fixed parameters used in the utility specifications do not account for this heterogeneity.

There have been many proposed variants of the standard logit model to accommodate heterogeneity in choice behaviour. The predominant approach explored in the literature is to introduce flexibility in the model formulation by allowing individual parameters to be distributed across the modelled population. The parameter distributions can be discrete, as in the Latent Class Model (LCM) (Bhat, 1997; Greene and Hensher, 2003); or continuous, as in the Mixed-Logit Model (Cardell and Reddy, 1977; Ben-Akiva and Bolduc, 1996; McFadden and Train, 2000). There are also further extensions that integrate random parameters within individual latent classes (Bujosa et al., 2010; Greene and Hensher, 2013).

The LCM is developed under the assumption that individuals can be categorised into a set of homogeneous classes (Greene and Hensher, 2003). The classes are latent in that the analyst is unable to observe which individual belongs to which class (Greene and Hensher, 2013). The LCM accounts for heterogeneity through employing different utility specifications for each class. However, since the number of classes of a LCM is finite, it only allows a limited number of parameter variants. Additionally, it is difficult to determine an appropriate number of discrete classes in the dataset (Nylund et al., 2007). In contrast, the mixed-logit model has the merit of allowing individual's parameters to vary randomly over a continuous distribution through simulation (Greene and Hensher, 2003).

The mixed-logit model has been applied to capture a broad spectrum of heterogeneity sources. Examples of applications of mixed-logit models in the literature include addressing diverse choice preferences (e.g. Hess et al., 2005; Cirillo and Axhausen, 2006) and divergent willingness to pay (e.g. Bastin et al., 2010). The mixed-logit model is also widely used in dealing with correlations between alternatives (e.g. Brownstone et al., 2000) and across space (e.g. Bhat and Sener, 2009). In general, mixed-logit models do not have a closed-form expression of the integral formula. As such, estimation of these models relies on simulation to approximate the mixing integration.

2.2. Model Transferability

Despite the fact that the theory of the mixed-logit model is clear, the practice of model estimation is vulnerable to errors when the sample size is small and does not comply with the high data quality requirement of the mixed-logit model estimation (Greene and Hensher, 2003). *Model transfer* is a technique that can be used to remedy low data availability by developing a model for a new application context on the basis of a previously estimated model. It therefore allows existing models to be of use to helping understand relatively poorly sampled areas. The idea of *transferability* can be considered at various levels of generality. Four typical hierarchical layers of transferability are: (i) underlying theory of travel behaviour; (ii) model structure; (iii) empirical specification; and (iv) parameter values (Ben-Akiva and Bolduc, 1987; Hansen, 1981; Sikder et al., 2013). In this paper we focus on the *transferability* of parameter values.

Model transferability attracted intense research interest in the 1970s and 80s (e.g. Watson and Westin, 1975; Atherton and Ben-Akiva, 1976; Galbraith and Hensher, 1982; Ben-Akiva, 1979; Lerman, 1981; Louviere, 1981), including several practical applications (e.g. Barton-Aschman Associates, 1981, 1982; Schultz, 1983). In this period, researchers expected the parameters of travel behaviour models to remain stable in predicting travel behaviour in new contexts (Galbraith and Hensher, 1982). For example, Richards and Ben-Akiva (1975) argue that true behavioural models should be expected to be able to make predictions for different populations and locations without adjusting model coefficients.

Despite this optimism, later research identified that modelling in practice almost inevitably requires some adjustments to model coefficients before a model is transferred from one geographical area to another (Galbraith and Hensher, 1982; Koppelman and Rose, 1985). There have been few contributions in the literature focusing on model transferability since this period.

In the following sections, we present the mainstream model transfer methods identified by Karasmaa (2007). To compare these methods in clear mathematical language, we use a simplified utility function as an example — considering only the portion of utility that can be quantified by (i) a vector of observable attributes X and (ii) attributes' weights Γ_{in} . In the estimation context, the individual n's utility in the choice situation t takes the following form:

$$V_{in,1} = V(X_{in,1}, \Gamma_{in,1})$$
(1)

2.2.1. The Direct Application Approach

The simplest approach to model transfer is to apply the existing model directly with no change on its parameters. The utility in the application context takes the form

$$V_{in,2} = V(X_{in,2}, \Gamma_{in,1}) \tag{2}$$

We refer to this as the *Direct Application* approach.

2.2.2. The Transfer Scaling Approach

As discussed, modelling practice finds that *Direct Application* can lead to nonnegligible modelling errors. Nonetheless, it is shown that much of the *transfer bias* (i.e. the error from using the coefficients from the estimation context for a new application), can be addressed through adjusting model constants and scales (Algers et al., 1994; Badoe and Miller, 1995). This method represents the *Transfer Scaling* approach. It establishes that:

$$V_{in,2} = \mu_{i,2} * V(X_{in,2}, \Gamma_{in,1}) + \alpha_{i,2}$$
(3)

where $\mu_{i,2}$ represents the scale factor for alternative *i* and $\alpha_{i,2}$ is an alternative specific constant adjusted for the application context.

2.2.3. The Bayesian Approach

The third transfer method, the *Bayesian* approach, involves re-estimating model parameters. The transferred set of parameters is yielded through *Bayesian inference* (see function 8), instead of directly scaling the vector of parameters. The transferred model is adapted from a conjugate prior, i.e., an existing model estimated on rich data. Meanwhile, informative local data can be assimilated in the *Bayesian* process. In the basic *Bayesian* method, the information of the application context jointly enters the *Bayesian inference* as an estimated model. In advanced *Bayesian* methods, such as the *Joint Context Estimation* method, samples can be assimilated one by one through iterative use of *Bayesian inference*.

The computation of the *Bayesian* approach is more complicated than the direct or transfer scaling approaches. We omit the functions here, instead including a detailed introduction of *Bayesian inference* in Section 3.2.

2.2.4. Summary

It is a general consensus that more complex transfer approaches can better fit the application context than the *direct application* approach. A key question for the more advanced transfer methods is to what extent the difference between the coefficient values in estimation and application contexts is caused by the true behavioural differences, and how much is caused by the imprecision in parameter estimates (which is normally measured by model variance). The *transfer scaling* method uses the application context data only to correct the transfer bias, therefore the differences in sampling errors between the two datasets are not explicitly considered (Karasmaa, 2007). Meanwhile, it postulates that the ratios of coefficients remain the same after transferring. Therefore, it does not consider the difference in the weights of independent variables between the estimation population and the application population.

In contrast, the *Bayesian* approach can address the problem of different sampling errors by adjusting the random variation in the utility function of the different datasets to be equal. Furthermore, coefficients of independent variables are updated separately, therefore the transferred model can have a weighting system for the independent variables that is different to the existing model. For these merits, the paper investigates the *Bayesian* approach.

3. Theoretical Foundations

Here we establish the theoretical foundations of the ESBDA simulator. Firstly we provide a brief overview of the mixed-logit theory, to familiarise the reader with the notation and required background knowledge. Next, we provide a high-level overview of our approach, before covering the elements of the ESBDA approach in detail.

3.1. Overview of Mixed-logit

The mixed-logit model has the capability to approximate any random utility-based DCM to any degree of accuracy with appropriately specified distributions of the coefficients (McFadden and Train, 2000). For simplicity, the following analysis focuses on the linear utility specification and follows McFadden and Train (2000)'s notation:

In a choice situation, each alternative $i \in \{1, ..., J\}$ provides the decision-maker n some net benefit/utility. Utility Theory postulates that the decision-maker rationally chooses the option to maximise the utility. As the complete utility cannot fully be observed by the modeller, it is instead modelled as the sum of the observable portion of the utility and an unknown error term. The observable utility is a vector of observable attributes X_{in} weighted by the set of parameters Γ_{in} . The parameters represent the degree of importance/preference that each individual assigns to each attribute (Cherchi and Guevara, 2011). The standard DCM incorporates an independent and identically distributed (iid) Extreme-Value 1 type (EV1) error term ε to represent unobserved utility. Dividing the complete *utility* into the above assumptions leads to a logit model, where the *utility* of choice $i \in J$ is:

$$U_{in} = V(X_{in}, \Gamma_{in}) + \varepsilon_{in} \tag{4}$$

The corresponding probability is:

$$P(i|X_{in},\Gamma_{in}) = \frac{exp\{V(X_{in},\Gamma_{in})\}}{\sum_{j=1}^{J} exp\{V(X_{jn},\Gamma_{jn})\}},$$
(5)

In reality, the importance felt of each attribute Γ_{in} varies across population. To model the individual heterogeneity, we allow some of the importance (parameters/ coefficients) to take a random distribution. Usually, modellers are interested in the ratios of certain parameters rather than their absolute value. To ensure these ratios are identifiable, some coefficients can be kept as point values. Such specifications allow for a clear representation of the ratio between some coefficients, e.g., willingness-to-pay. As such, Γ_{in} can be partitioned into random parameters β'_n and fixed parameters α' . Analogously, X_{in} can be split into z_{in} and x_{in} pertaining to α' and β'_n respectively. Assume $\beta'_n \sim N(\zeta, \Omega)$ where ζ denotes a mean vector and Ω represents a covariance matrix. Accordingly, $V(X_{in}, \Gamma_{in})$ in equation 5 becomes:

$$V(X_{in}, \Gamma_{in}) = \alpha' z_{in} + \beta'_n x_{in} \tag{6}$$

The new *utility* function is function 7 and probability equation 5 can be updated correspondingly.

$$U_{in} = \alpha' z_{in} + \beta'_n x_{in} + \varepsilon_{in} \tag{7}$$

Without a closed-form expression, estimation of mixed-logit models heavily relies on simulation tools. The two dominant simulation means for mixed-logit models are Maximum Simulated Likelihood (MSL) and the *Bayesian* approach. The principle of MSL is to search for the parameter set with which under the assumed model structure the observed data is most probable. It is achieved by maximising a likelihood function in simulation. In contrast, the *Bayesian* approach incorporates an initial set of parameters and update the parameters over and over again using *Bayesian* inference until they maintain stable values across subsequent iterations. As the process of *Bayesian* inference naturally involves iterative updates of model parameters, it provides an ideal platform for performing model transfer.

3.2. Proposed Approach

In this paper, we establish a new simulator which takes an existing model and reestimates the parameters for a new context, exploiting both the previous parameter estimates and the new data. Typical new contexts that could be considered are: (i) a new geographical location; (ii) a different demographic population segment; or (iii) a different time period.

A key application of this approach is updating a model for future choice behaviour estimation (see Figure 1). Another potential area of application is model segmentation, where a hierarchical modelling structure can be established to investigate heterogeneous choice behaviour hierarchically — from a general level to specific detailed segments — through layers of ESBDA (see Figure 2). In each level of segmentation, the coefficients, i.e., the *posterior*, estimated for the upper-level model are input to the ESBDA as the *prior* to estimate this level *posterior* coefficients, which then serve as the *prior* of the next level.



Figure 1: Modelling structure for continuous update of the current model with newly available data

The new simulator, called Early Stopping Bayesian Data Assimilation (ESBDA), has two central theoretical elements: Bayesian Data Assimilation (BDA) and *Early Stopping*.

3.2.1. Bayesian Data Assimilation

Bayesian Data Assimilation (BDA) is a term coined for time-series modelling, which describes a time-related model calibration/refinement technique that improves forecasting accuracy through using new information as it becomes available (Jazwinski, 1970; Reich and Cotter, 2015). We extend this to a more general purpose definition as 'the technique of *data assimilation* through *Bayesian inference* for general transfer/update of a previously established model.'

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Figure 2: Hierarchical modelling structure for a systematic DCM model segmentation

Bayesian inference is the process of updating the posterior probability $K(\theta|Y)$ using two antecedents: a conjugate prior probability distribution $k(\theta)$ which reflects initial ideas about the probability, and a likelihood function $L(Y|\theta)$ which is derived from a statistical model for a set of the observed data $Y = y1, ..., y_N$. According to Bayes theorem, we have:

$$K(\theta|Y) = \frac{L(Y|\theta)k(\theta)}{L(Y)}$$
(8)

We identify *Bayesian inference* as a promising approach to improving the transferibility of mixed-logit models, because the process of updating the *posterior* is transferable to adapting existing parameters to a new context. In the context of model transfer, the previously estimated combination of parameters plays the role of the *conjugate prior* and the combination of parameters to be estimated for the new context is the *posterior* to be inferred. Through assimilating sample data of the modelling object, the *prior* can be transferred into a *posterior* combination of parameters which fits to the target context.

There are two layers of *Bayesian inference* applied in this study for distinct purposes. It is important to distinguish the concept of 'data assimilation', that describes the outer layer, with the idea of 'hierarchical Bayes (HB)', which is the process of the inner layer. In the outer layer, the *prior* and the *posterior* are two versions of mixed-logit combinations of parameters and the transfer is processed through the assimilation of sample data. We define the process of assimilation'. The data assimilation process itself involves iterative internal *Bayesian inferences*, where each parameter is updated in turn on the condition of the values of the remaining parameters, in an iterative process. The *prior* and the *posterior* in each iteration are single parameters (rather than the combination of all parameters). This iterative process is the prominent 'HB', a technique introduced to estimate mixed-logit by McCulloch and Rossi (1994) and Allenby (1997) with normal distribution of coefficients, and generalised to non-normally distributed coefficients by Train (2001). We will return to the detail procedures of HB when illustrating the algorithm in Section 3.3.

3.2.2. Early Stopping

In Machine Learning (ML), *early stopping* is a commonly used technique to terminate model training before convergence to regularise the model and prevent over-fitting (Precheit, 1998). It tracks the real-time modelling error(s) on an *out-of-sample* validation dataset (separate from the training data) and terminates the modelling when an *early stopping* criterion is met. This technique is not typically used in the conventional mixed-logit estimation as this model type rarely has a high dimensional parameter space and therefore has a relatively low risk of *over-fitting*.

Nevertheless, we identify that *early stopping* has potential benefits for mixed-logit models when working with a small sample size. Firstly, *early stopping* can prevent the resultant model from over-fitting to the insufficient sample data which may not be representative of the population to be modelled. In MSL estimation, the error (E) is automatically monitored in the form of likelihood during the MSL's modelling progress. This ensures that the output parameter estimates are those that result in the lowest error (E). By contrast, the training progress of traditional *Bayesian* model does not examine whether or not the output parameter estimates lead to the optimal predictive error. In this sense, while the HB procedure uses a sampling approach and the MSL solves an optimisation problem, ESBDA consolidates these two methods in a hybrid approach; the integration of the *early stopping* procedure essentially configures the core of MSL simulator into the *Bayesian* simulator, which provides a convenient way to compare the predictive error during the modelling.

Furthermore, the use of an *early stopping* procedure provides a good complement to the convergence sign of the mixed-logit model. Whilst the basic HB procedure typically terminates the simulation when the mixed-logit model converges, the model may never converge when sample size is small. Under the existing estimation approach, the decision of when to stop the modelling process is arbitrary (e.g. when a default absolute number of iterations is reached). Instead, our use of an *early stopping* procedure avoids such arbitrariness. Despite these potential benefits, to the best of the authors' knowledge, our effort to configure the *early stopping* procedure of ML into a mixed-logit simulator is the first.

Among the mainstream classes of *early stopping* criteria illustrated by Precheit (1998), the following criterion is the most commonly used one in ML: Let E(T) denote the out-of-sample modelling error at epoch T and the lowest error obtained in epochs until T, $E_{opt}(T)$, is defined as:

$$E_{opt}(T) = \min_{T' \le T} E(T') \tag{9}$$

It is often not the best time to halt the training immediately after the first sign of no further decrease of modelling error (*E*). The reason is that modelling performance may hover around a plateau of no improvement or even a temporary drop before a substantial improvement. This concern can be addressed by incorporating a delay to *early stopping* with regard to the acceptable number (*k*) of epochs with no performance improvement since the last minimum *E* occurs. In other words, *early stopping* is triggered after epoch *T*, iff $E(T) > E(T - j) \forall j \leq k$. It is noteworthy that the output estimation is derived at epoch T - k rather than at *T* to retrieve the optimised model estimation.

3.3. Estimation Approach of ESBDA

Our simulator is an extension to the HB procedure for obtaining mixed-logit models parameters, which was initially established by Rossi et al. (1996) and Allenby (1997). In this paper, we build on the algorithm introduced by Train (2006)¹. The key extensions of the proposed simulator from the standard HB procedure are on the two ends of the original algorithm: (i) the adoption of a *conjugate prior* combination of parameters in the beginning and (ii) the *early stopping* procedure to terminate modelling.

To present the key modelling steps more clearly, we illustrate the iterative *Bayes* modelling process of ESBDA with the *early stopping* trigger in Figure 3.



Figure 3: Illustration of the iterative Bayes modelling process of ESBDA with an early stopping trigger.

ESBDA approximates the posterior estimates by assimilating new data through a Markov Chain Monte Carlo (MCMC) process. The essence of MCMC is to approximate an otherwise difficult-to-compute posterior distribution by draws from a Markov chain whose stationary distribution makes up the posterior distribution of interest (for general treatment, see Robert and Casella, 2013).

To reserve space, we state the HB procedure succinctly using the easy-to-follow multivariate normal. For an in-detail demonstration of the HB procedure, we direct the reader to Chapter 9 and 12 of Train (2003).

For the parameters of function 7, the conditional posteriors in each layer of *Bayesian* inference are:

- 1. $K(\beta_n | \alpha, \zeta, \Omega) \propto L(y_n | \alpha, \beta_n) \phi(\beta_n | \zeta, \Omega)$
- 2. $K(\zeta|\Omega, \beta_n \forall n)$ is $N(\sum_n \beta_n / N, \Omega / N))$. Note α does not enter this layer directly. Its affect on posterior ζ is passed through the draws of β_n from the first layer.
- 3. $K(\Omega|\zeta, \beta_n \forall n)$ is $IW(K + N, (KI + N\bar{S})/(K + N))$ where $\bar{S} = \sum_n (\beta_n \zeta)(\beta_n \zeta)'/N$. Similarly, α does not involve directly.
- 4. $K(\alpha|\beta_n) \propto \prod_n L(y_n|\alpha,\beta_n)$. The Metropolis–Hastings Algorithm (M-H) may be used again when the *prior* on α is essentially flat.

¹The code is available online: https://eml.berkeley.edu/Software/abstracts/ train1006mxlhb.html

The method can be conveniently adapted to variants of normal distribution simply through transformation of the underlying distribution. We denote the weights of random *utility* terms in an individual *n*'s *utility* function as c_n , and $c_n = T(\beta'_n)$, where *T* refers to a distribution transformation which depends only on the latent distribution parameters and which is weakly monotonic (to maintain $\partial c_n^k / \partial c_n^{\beta'_n} \ge 0$ for elements in β_n or c_n). The distributed random parameter is drawn in the same manner in modelling but it enters the *utility* function in its transformed form:

$$U_{in} = \alpha' z_{in} + T(\beta'_n) x_{in} + \varepsilon_{in}$$
⁽¹⁰⁾

Whilst the derivation of the resulting posterior in each layer may change in other types of flexible distributions, the procedures are broadly similar.

3.3.1. Early Stopping Parameters

To supervise *early stopping*, we employ Cross-Entropy Loss (CEL) (function 11) which monitors real-time predictive performance of the estimates during modelling. The CEL is a normalised version of the log-likelihood, whose absolute value is independent on sample size.

$$G_{CEL} = -\frac{1}{N} G_{\text{log-likelihood}},$$

$$= -\frac{1}{N} \sum_{n=1}^{N} \ln P(i_n | x_n)$$
(11)

where i_n is the index of the choice made by individual n.

The threshold value of an *early stopping* criterion is usually selected in an interactive fashion to seek the lowest generalisation error or yield the best 'price-performance ratio' (Precheit, 1998). To guarantee model termination, the stopping criterion is complemented by a rule that terminates modelling after a set number of epochs. The total number of epochs and the number of draws for simulating the distributed parameters are set on an ad-hoc basis. To relieve serial correlation of M-H, draws of *posterior* distribution of α , β_n are retained at regular intervals instead of consecutively (every T_1 epochs). CEL is tracked and plotted every T_2 epochs. We will demonstrate the chosen hyperparameter values in Section 4.4.

4. Experimental Methodology

Modelling experiments are carried out to benchmark the proposed ESBDA simulator against three reference approaches. This section presents the set-up of the experimentation.

4.1. Benchmarks

The first reference approach is the Direct Application approach, i.e., the exact *prior* model. The other reference approaches make use of Bayesian simulation. The *Nonconjugate prior Bayesian* Simulator is adapted from the HB procedure of Train (2006). The parameter estimates are initiated using purely random starting values. The estimation

Simulator	Prior-based Bayesi	an BDA simulators	Nonconjugate prior	Direct Application
	ESBDA Simulator BDA Simulator		Bayesian Simulator	Approach
Simulation mechanism	Bayesian modelling	Bayesian modelling	Bayesian modelling	No simulation
conjugate prior	Previously estimated parameters	Previously estimated parameters	No-prior	N/A
Early stopping procedures	Yes	No	No	N/A

Table 1: The ESBDA simulator and the benchmark simulators

is therefore based solely on the limited sample data of the modelling target. The BDA simulator initiates Bayesian estimation using the parameter values from the previously estimated model as the prior. It therefore exploits the potential of the *conjugate prior* in *Bayesian inference* and develops the new model from an informative *prior* model. The ESBDA simulator then adds *early stopping* to the BDA simulator, monitoring the model performance on an out-of-sample validation set.

4.2. Performance Measures

Three dimensions are investigated to assess the alternative simulators: (i) statistics of estimates, (ii) behavioural consistency of the resultant model and (iii) steadiness of the modelling process. The monitored statistics include the statistical significance of individual parameter estimates and predictive performance of the resultant model. In addition to CEL, which monitors the real-time predictive performance in model training (see Section 3.3), the other performance metric is Geometric Mean Probability of Correct Assignment (GMPCA) (Hillel, 2019). The GMPCA has a clear physical interpretation, the geometric average correctness of the output model, whilst CEL is difficult to interpret. It is established as

$$G_{\text{GMPCA}} = \left(\prod_{n=1}^{N} P\left(i_n | x_n\right)\right)^{\frac{1}{N}}$$
(12)

The data for each experiment is divided into three sets. The training set is used to train the mixed-logit model, and the validation set is held to determine *early stopping*. As the validation set is used to determine the optimal parameter estimates when the out-of-sample performance is highest, it is no longer an unbiased estimate of the model's predictive power. As such, a separate testing set is used with the final model to test the models' out-of-sample true predictive performance on previously unseen data.

We would like the simulator to output behaviourally-rich mixed-logit models, which are highly interpretable and thus informative to choice behaviour studies. Behavioural consistency of the output models is examined to eliminate estimations that are statistically significant but behaviourally meaningless. As such, we screen sign-errors and problematic relative ratios of the output parameters.

Finally, the simulation progress of each modelling experiment is monitored to assess how steadily the CEL progresses throughout a complete modelling; whether the estimation results truly converge; and when *early stopping* occurs.

4.3. Case-Studies

The ESBDA and benchmark simulators are compared on 2 case-studies: one covering vehicle purchase choice in California, and the other covering travel mode-choice in London. For each case-study, multiple modelling scenarios, or 'levels' are considered, each using different subsamples of the data. In each modelling scenario, the *conjugate prior* for the ESBDA and the BDA simulators comes from the optimal estimates at one higher level, whilst no *prior* is fed to the *Nonconjugate prior Bayesian* simulator. The Direct Transfer approach then evaluates the performance of the unmodified *prior* model on the new data. All models are trained and evaluated on the same sample data.

A model is first estimated for the full dataset (Level-0) using Bayesian estimation. Each subsequent level then represents the transfer of a model from the previous level to a smaller sample or sub-group of the population, e.g. in the Level-1 scenario, the trained model from Level-0 is transferred to a smaller sample. For these levels' labels, a higher number indicates a smaller sample, with less data available for model training (see Table in 3 and Table in 5). The process of deriving lower level models through ESBDA from the Level-0 model is illustrated in Figure 2.

4.3.1. Vehicle Purchase Choice Model in California

The first case-study models customers' willingness-to-purchase of all-electric and gas-electric vehicles using a stated preference survey conducted in California, USA. The baseline model for this case study is a mixed-logit model inherited from the demonstrative model of Train & Garrett's simulator (2006). The model is eminently suitable for testing the alternative simulators. The data and the *utility* function specification have undergone a thorough inspection in the previous experiment (see Train & Sonnier, 2004).

Variable	Symbol	Coefficient	Distribution
Purchase price (*10,000)	p_{in}	$\beta_{\text{price},n}$	lognormal
Operating cost (\$/month)	o_{in}	$\hat{\beta}_{\text{operate},n}$	lognormal
Range in hundreds of miles (0 if not electric)	r_{in}	$\beta_{\mathrm{range},n}$	lognormal
Electric (boolean)	e_{in}	$\beta_{\text{electric},n}$	normal
Hybrid (boolean)	h_{in}	$\beta_{\mathrm{hybrid},n}$	normal
High performance (boolean)	s_{in}	$lpha_{ m high}$	fixed
Medium or high performance (boolean)	m_{in}	$lpha_{ m midhigh}$	fixed

Table 2: Variables and coefficients of the California vehicle purchase choice model, and their distribution types

In this case-study, each respondent faces 15 rounds of choices, with three options given in each choice. The sample data contain respondents' stated choices and characteristics of the alternative vehicles, such as engine type (i.e., electric, hybrid or gasoline), purchase price, etc. As we do not have socio-economic details for survey respondents, the samples for Levels 1 and 2 are randomly selected from the full dataset. This means that the expected values of the true model parameters do not change for different modelling levels. As such, this case-study investigates the potential for overfitting on small training sample sizes for each simulator.

The model incorporates uniform weights for the same variables across the alternative choices. The uniform *utility* function of alternative i is as follows. The explanatory

Size level	Modelling object	Sample size					
		Training	Validation	Test			
Level-0	Full dataset (100 respondents).	1484	-	-			
Level-1	Randomly selected sample: 20 individuals per set	300	300	300			
Level-2	Randomly selected sample: 5 individuals per set	75	75	75			

Table 3: Levels of sample size of the California vehicle purchase choice model *Note.* The sample size of the full dataset is not 1500 because some choice records are missing.

variables and the coefficients of the model are presented in Table 2.

$$U_{in} = (\mu_{\text{price}} + \sigma_{\text{price}}\zeta_{\text{price},n})p_{in} + (\mu_{\text{operate}} + \sigma_{\text{operate}}\zeta_{\text{operate},n})o_{in} + (\mu_{\text{range}} + \sigma_{\text{range}}\zeta_{\text{range},n})r_{in} + (\mu_{\text{electric}} + \sigma_{\text{electric}}\zeta_{\text{electric},n})e_{in} + (\mu_{\text{hybrid}} + \sigma_{\text{hybrid}}\zeta_{\text{hybrid},n})h_{in} + \alpha_{\text{high}}s_{in} + \alpha_{\text{midhigh}}m_{in} + \varepsilon_{in}$$
(13)

4.3.2. Travel Mode Choice Model in London

The second case-study considers passenger mode-choice using revealed preference data collected in London, UK. The dataset, available online, is adapted from a closely tailored London travel dataset² which recreates the travel mode choice-set that are faced by the respondent at the time of travel (Hillel et al., 2018).

The ratio of parameters for time and cost, known as the *Value of Time*, is of particular interest in transport modelling. To ensure this ratio is well defined, we assign a normal distribution to the coefficient for cost and maintain all other coefficients/constants as fixed-values. People's perception and valuation of time vary when travelling in different modes. To reflect this, we set alternative-specific parameters for the *utility* functions of the four modes, i.e., driving $(U_{driving,n})$, public transit $(U_{public,n})$, cycling $(U_{cycling,n})$, and walking $(U_{walking,n})$. The *utility* functions are as follows (functions 14–17)³.

$$U_{\text{driving},n} = (\mu_{\text{cost}} + \sigma_{\text{cost}}\zeta_{\text{cost},n})c_{n_d} + \alpha_{\text{driving-time}}t_{d,n} + \alpha_{\text{var}}\nu_{d,n} + \varepsilon_{\text{driving},n}$$
(14)
$$U_{\text{public},n} = (\mu_{\text{cost}} + \sigma_{\text{cost}}\zeta_{\text{cost},n})c_{p,n} + \alpha_{\text{access-time}}t_{a,n} + \alpha_{\text{bus-time}}t_{b,n} +$$

$$\alpha_{\text{rail-time}} t_{r,n} + \alpha_{\text{change-walking-time}} t_{\text{change1},n} + \alpha_{\text{change-waiting-time}} t_{\text{change2},n} + (15)$$

$$C_{\text{public}} + \varepsilon_{\text{public},n}$$

$$U_{\text{cycling},n} = \alpha_{\text{cycling-time}} t_{c,n} + C_{\text{cycling}} + \varepsilon_{\text{cycling},n}$$
(16)

$$U_{\text{walking},n} = \alpha_{\text{walking-time}} t_{w,n} + C_{\text{walking}} \varepsilon_{\text{walking},n} \tag{17}$$

For the London model, we have detailed socioeconomic information for each individual in the dataset. This provides a platform to illustrate model transfer for hierarchical segmentation (as Figure 2 illustrates). Levels 1 to 3 represent data for specific population segments taken from the original sample. Since each modelling level represents a different demographic group, each modelling level represents a true transfer

²available on https://www.icevirtuallibrary.com/doi/suppl/10.1680/jsmic. 17.00018.

³To conserve space, we use $\beta_{\text{cost},n}$ to denote $(\mu_{\text{cost}} + \sigma_{\text{cost}}\zeta_{\text{cost},n})$ in the rest of this paper.

to a new application. As such, the expected values of the true model parameters are different for each modelling level. This case-study therefore investigates the ability of each simulator to transfer a model to a new application.

Following the recommendations in a systematic review of classification methodologies (Hillel et al., 2020), the validation and test folds are sampled grouped by household to ensure that trips of the same household are not classified into different folds. At each level, the training, validation and test datesets are allocated the same number of households. Therefore, the selected the number of households in each fold is fixed while the number of trips may vary.

Variable/Constant	Symbol	Coefficient	Distribution
Driving cost Public transport cost Driving time	$c_{d,n} \ c_{p,n} \ t_{d,n}$	$eta_{ ext{cost},n}\ eta_{ ext{cost},n}\ lpha_{ ext{cost},n}\ lpha_{ ext{driving-time}}$	normal normal fixed
Access time In-vehicle time on bus In-vehicle time on rail	$t_{a,n}$ $t_{b,n}$ $t_{r,n}$	$lpha_{ m access-time} \ lpha_{ m bus-time} \ lpha_{ m rail-time}$	fixed fixed fixed
Interchange walking time Interchange waiting time Cycling time	$t_{ ext{change1},n} \ t_{ ext{change2},n} \ t_{c,n}$	$lpha_{ m change-walking-time} \ lpha_{ m change-waiting-time} \ lpha_{ m cycling-time}$	fixed fixed fixed
Walking time Traffic variability Constant of the Public transit mode	$t_{w,n}$ $ u_{d,n}$	$lpha_{ ext{walking-time}} lpha_{ ext{traffic}} \ C_{ ext{public}}$	fixed fixed fixed
Constant of the Cycling mode Constant of the Walking mode	-	$C_{ m cycling} \ C_{ m walking}$	fixed fixed

Table 4: Variables and Coefficients of the London Travel Mode Choice Model, and the distributions of the coefficients

Sample size	Modelling object	Sample size Training	Validation	Test
Level-0	All journeys, regardless of travel purpose time period of travelling or the traveller's attributes, income, age, etc.	8331	-	-
Level-1	General home-office journeys, regardless of time period of travelling or the trav- eller's attributes, income, age, etc.	613	735	643
Level-2	Home-office journeys during morning peak-time, regardless of the traveller's at-tributes, income, age, etc.	266	264	325
Level-3	Home-office journeys during morning peak-time; the 26-35-year-old people whose household income is between £25,000-£49,999.	26	27	36

Table 5: Levels of sample size of the London travel mode choice model, and the corresponding modelling objective at each level

4.4. Chosen Hyperparameter Values

We set $T_1 = 10$ as the interval between checkpoints for tracking CEL and $T_2 = 20$ for plotting CEL draws. For *early stopping*, the maximum number of epochs that

Note. While the training, validation and test datesets are allocated the same number of households at each level, the number of trips varies among individuals. As such, the number of trips in each fold varies.

we allow no performance improvement is k = 200. As a complementary criterion, the modelling would be terminated after an absolute value of 10,000 epochs if *early stopping* does not occur.

5. Results

In this section, we investigate the experimental results with a particular focus on the small-sample properties of the alternative simulators.

5.1. Interpreting the Results

Performance of alternative simulators is compared on the grounds of (i) statistics of the output parameters combination, (ii) behavioural consistency of the output mixed-logit models to an empirical model (see Table 6 to 12); and (iii) the steadiness of the simulators' modelling progress (Figure 4 to 8).

In the tables, we highlight statistical insignificance, sign-errors as well as parameter estimates which may be statistically significant but are highly inconsistent with empirical modelling results. The investigation of behavioural consistency is mainly based on the judgement of the ratios of other parameters against the coefficient for cost (which we call monetary ratio in the paper). We highlight in the tables where the monetary ratio deviates over two orders of magnitude from the highest performing model from the level above. In the London example, the travel time-cost ratios (i.e. Value of Time) are of our particular research interest.

For each modelling level, the convergence progresses of alternative simulators are plotted on a graph (e.g. Figure 4). The difference between the ESBDA and BDA simulators lies only in *early stopping* and therefore they have the same CEL curve until *early stopping* occurs. They are both noted as prior-based BDA simulators and are represented by the same (red and yellow) lines in the plots. Epoch (T - k) when ESBDA outputs its estimation is marked by a red vertical dashed line. The CEL of each simulator is tracked for 10000 epochs. Whilst the training of ESBDA is terminated at epoch T if *early stopping* occurs, the CELs curves of BDA after ESBDA's *early stopping* illustrates how CELs would change if *early stopping* did not occur.

5.2. Illustrating the Results

The change of the alternative simulators' performance from Level-0 to lower level modelling scenarios follows the same trend in two case studies when the sample size reduces. To avoid repetitive analysis, we present the experimental results in order of levels rather than by case studies.

5.2.1. Level-0

As explained in Section 4.3, the primary purpose of the Level-0 modelling is to derive a 'mother model' to feed *conjugate prior* parameters to the lower level modelling, rather than to benchmark alternative estimation approaches. No prior model is used in the highest level (Level-0) experiment and *early stopping* does not occur, given the large training samples. As such, the three *Bayesian* simulators output identical parameter estimates. Therefore, to reserve space, Level-0 plots are omitted, and the identical

Simulator	Bayesian Si	mulators	Direct Appli	ication Approach
	(including]	ESBDA, BDA &		**
	Nonconjuga	te-prior Bayesian		
	Simulator)			
	1	Random coeffici	ent	
Latent				
	Mean	StDv	Mean	StDv
$\mu_{\rm price}$	-0.9166***	0.1851	-0.9056	0.1850
$\sigma_{\rm price}$	1.6340***	0.3027	1.5539***	0.4392
μ_{operate}	-5.2851***	0.4734	-5.2620***	0.5464
$\sigma_{\rm operate}$	3.1558***	0.9111	3.5568	1.4296
μ_{range}	-1.6768***	0.4531	-1.7435**	0.6222
$\sigma_{\rm range}$	1.7364**	0.5399	1.5896	0.8609
μ_{electric}	-1.3494***	0.2456	-1.4121***	0.3131
$\sigma_{ m electric}$	1.8121***	0.4348	2.0655**	0.7320
μ_{hybrid}	0.7314***	0.2200	0.6801***	0.2059
$\sigma_{\rm hybrid}$	1.9992***	0.3606	1.8305**	0.5583
Simulated				
$\beta_{\text{price},n}$	-0.8663	1.3747	-0.8215	1.3838
$\beta_{\text{operate},n}$	-0.0244	0.0844	-0.0296	0.0822
$\beta_{\mathrm{range},n}$	0.4988	0.9310	0.4137	0.8507
$\beta_{\text{electric},n}$	-1.2958	1.3916	-1.4304	1.4424
$\beta_{\mathrm{hybrid},n}$	0.7978	1.4029	0.6838	1.4024
		Fixed coefficies	nt	
$lpha_{ m high}$	0.1025	0.0980	0.1058	0.1005
$\alpha_{\rm midhigh}$	0.5729***	0.1021	0.5763***	0.1033

Table 6: Modelling Estimates (the California model, Level-0)

Note. The three *Bayesian* simulators, the *Nonconjugate-prior Bayesian*, BDA and ESBDA output identical estimates as there is no conjugate-prior model input to BDA or ESBDA at Level-0 and *early stopping* does not occur to ESBDA. * p < 0.05; ** p < 0.01; *** p < 0.001

Simulator	Bayesian Simula	tors						
	(including ESBDA, BDA & Nonconjugate-							
	prior Bayesian Simulator)							
	Random coeffici	ient						
Latent								
	Mean	StDv						
$\mu_{\rm cost}$	-0.1571***	0.0317						
$\sigma_{\rm cost}$	0.0174	0.0251						
Simulated								
$\beta_{\text{cost},n}$	-0.1605*	0.0116						
	Fixed coefficie	nt						
$\alpha_{ m driving-time}$	-3.4996**	1.4951						
$\alpha_{\text{access-time}}$	-3.4173***	0.7521						
$\alpha_{\text{bus-time}}$	-2.2110*	1.0712						
$\alpha_{\text{rail-time}}$	-2.3821**	0.6132						
$\alpha_{\text{change-walking-time}}$	-1.9474**	0.5913						
$\alpha_{\text{change-waiting-time}}$	-2.6313***	0.4553						
$\alpha_{\text{cycling-time}}$	-4.6405***	1.0172						
$\alpha_{\text{walking-time}}$	-6.2339***	0.6315						
α_{traffic}	-5.1859***	1.0467						
C _{public}	1.7403	1.4935						
C_{cycling}	0.2730	0.1501						
$C_{ m walking}$	3.5505***	0.4235						

Table 7: Modelling estimates (the London model, Level-0)

Note. As there is no prior model in the Level-0 experiment and early stopping does not occur to ESBDA, the three *Bayesian* simulators generate identical estimation.

The Direct Application approach is not applicable since there is no empirical model readily usable to the London model. * p < 0.05; ** p < 0.01; *** p < 0.001; Behavioural inconsistent parameter/price ratio: ': 2 orders of magnitude deviation from the prior model; '': 3 orders of magnitude deviation. estimates of the three *Bayesian* simulators are presented by a single column in Table 6 and 7.

Whilst there is no empirical model readily usable to the Level-0 London experiment, the Direct Application approach is applicable to the Level-0 California Model as we use exactly the same *utility* function and dataset with Train & Garrett's demonstrative modelling. In Table 6, we compare the estimation of the *Bayesian* simulators to that of the Direct Application approach, which applies the original algorithm of Train & Garrett's. As the table shows, the *Bayesian* simulators' output parameters are highly consistent to Train & Garrett's estimation. The significant consistency to the literature results demonstrates that the *Bayesian* simulators developed by us are at least functional estimators for mixed-logit models.

5.2.2. Level-1

For Level-1, the training sample of the California model is reduced to 300 choices made by 20 individuals. For every simulator based on each dataset, the CEL reaches a relatively stable asymptote. There is only a slight difference in the stable training set CEL levels between the *conjugate-prior* and the *nonconjugate-prior* simulators. While the training set CEL curves are relatively smooth (Figure 4), there are noticeable fluctuations in the validation set CEL. Specifically, the validation set CEL value can quickly jump by 2% within merely 20 epochs. Under the fluctuation, ESBDA is terminated by *early stopping* after 540 epochs and the optimal modelling results are outputs at the 340th epoch. As Table 8 shows, the model with the best predictive statistics as well as the best behavioural consistency is estimated by the ESBDA simulator. In contrast, the monetary ratios of a few parameter estimates by the two reference simulators diverge far from the ratios of the prior model to an extent that the estimation results are considered questionable from a behavioural perspective.



Figure 4: Comparison of Cross-Entropy Loss (CEL) of the *conjugate-prior*-based BDA and the *nonconjugate-prior Bayesian* Simulator (the California model, Level-1) The vertical red dashed line marks epoch (T - k) when ESBDA's estimation is output.

The training of Level-1 London model uses 613 samples. As shown in Figure 5, CELs of all the alternative simulators still progress steadily. They all outperform the direct application approach in terms of predictive error. *Early stopping* does not occur to ESBDA. The *nonconjugate-prior* simulator unsurprisingly converges much more

Simulator	(at the 340 th	Simulator epoch)	BDA Simulator			Nonconjugate-prior Bayesian Simulator		Application
		1 /	Randon	n coefficient	2			
Latent								
	Mean	StDv	Mean	StDv	Mean	StDv	Mean	StDv
$\mu_{\rm price}$	-1.5132***	0.3949	-1.8227*	0.7519	-1.7633**	0.6631	-0.9166	0.1851
$\sigma_{\rm price}$	1.8336**	0.6433	3.0558	2.7459	2.7880	2.1482	0.7751	0.3027
μ_{operate}	-5.8014***	0.7751	-7.0237***	1.9313	-10.9885**	3.4405	-5.2851	0.4734
$\sigma_{\rm operate}$	3.1118**	0.9784	3.5396	3.1166	5.3340	7.1342	3.1558	0.9111
μ_{range}	-2.4011**	0.7858	-10.2657*	5.0484	-4.5737	2.2737	-1.6768	0.4531
$\sigma_{\rm range}$	2.1558*	0.8384	4.0078	4.4142	2.3872	1.7787	1.7364	0.5399
μ_{electric}	-1.5876***	0.3424	-1.4709**	0.5043	-1.4075**	0.5076	-1.3494	0.2456
$\sigma_{\rm electric}$	1.4239*	0.5577	2.0086	1.3521	2.0442	1.2034	1.8121	0.4348
$\mu_{ m hybrid}$	0.5282	04048	0.4076	0.4216	0.5020	0.3756	0.7314	0.2200
$\sigma_{\rm hybrid}$	1.2361*	0.5409	1.4418	0.7715	1.4423	0.7541	1.9992	0.3606
Simulated								
$\beta_{\text{price},n}$	-0.5221	0.8996	-0.6549	1.6718	-0.6193	1.4678	-0.8663	1.3747
$\beta_{\text{operate},n}$	-0.0138	0.0513	-0.0049	0.0215	-0.0002!!	0.0014	-0.0244	0.0844
$\beta_{\mathrm{range},n}$	0.2797	0.6189	0.0002!	0.0007	0.0349	0.0667	0.4988	0.9310
$\beta_{\text{electric},n}$	-1.5761	1.2672	-1.4330	1.4882	-1.3701	1.5028	-1.2958	1.3916
$\beta_{\text{hybrid},n}$	0.5383	1.1049	0.4356	1.2176	0.5344	1.2181	0.7978	1.4029
				coefficient				
$\alpha_{ m high}$	0.0958	0.1783	0.0866	0.1965	0.0883	0.2016	0.1025	0.0980
$\alpha_{ m midhigh}$	0.8014***	0.1928	0.8682^{***}	0.2178	0.8588^{***}	0.2201	0.5729	0.1021
				lling error				
	CEL	GMPCA	CEL	GMPCA	CEL	GMPCA	CEL	GMPCA
Validation set	0.8695	0.4192	0.8788	0.4153	0.8906	0.4104	0.9124	0.4015
Test set	1.1683	0.3109	1.2283	0.2928	1.2294	0.2925	1.2475	0.2972

Note. * p < 0.05; ** p < 0.01; *** p < 0.001; Behavioural inconsistent parameter/price ratio: !: 2 orders of magnitude deviation from the prior model; !!: 3 orders of magnitude deviation.

Table 8: Modelling estimates (the California model, Level-1)

Simulator	ESBDA S	imulator	BDA Simula	ntor	Nonconjuga		Direct Application		
	(no early sto	pping)			Bayesian Simulator		Approach		
			Random	coefficient					
Latent									
	Mean	StDv	Mean	StDv	Mean	StDv	Mean	StDv	
$\mu_{\rm cost}$	-0.1531***	0.0409	-0.1531***	0.0409	-0.1706***	0.0144	-0.5171	0.0317	
$\sigma_{ m cost}$	0.0149	0.0275	0.0149	0.0275	0.0147	0.0076	0.0174	0.0251	
Simulated									
$\beta_{\text{cost},n}$	-0.1641	0.2182	-0.1641	0.2182	-0.1816	-0.1202	-0.1605	0.0116	
				coefficient					
$\alpha_{\rm driving-time}$	-4.2537**	1.5895	-4.2537**	1.5895	-0.6409	0.8530	-3.4996	1.4951	
$\alpha_{\text{access-time}}$	-5.7911***	1.2652	-5.7911***	1.2652	-4.1264*	1.8979	-3.4173	0.7521	
$\alpha_{\text{bus-time}}$	-3.4614**	1.0902	-3.4614**	1.0902	-1.6666	0.9127	-2.2110	1.0712	
$\alpha_{\text{rail-time}}$	-4.2861*	1.6784	-4.2861*	1.6784	-0.4644	1.2405	-2.3821	0.6132	
$\alpha_{\text{change-walking-time}}$	-4.8911*	2.4391	-4.8911*	2.4391	-0.2100	0.6514	-1.9474	0.5913	
$\alpha_{\text{change-waiting-time}}$	-4.0699**	1.3559	-4.0699**	1.3559	-2.6317	2.1184	-2.6313	0.4553	
$\alpha_{\text{cycling-time}}$	-6.3078***	1.1257	-6.3078***	1.1257	-3.9240**	1.2912	-4.6405	1.0172	
$\alpha_{\text{walking-time}}$	-6.8432***	0.6762	-6.8432***	0.6762	-5.6200***	1.2597	-6.2339	0.6315	
α_{traffic}	-6.6577**	2.2360	-6.6577**	2.2360	-4.0050***	1.1174	-5.1859	1.0467	
C _{public}	2.4519***	0.5393	2.4519***	0.5393	3.2286***	0.9637	1.7403	1.4935	
C _{cycling}	0.6759	0.5050	0.6759	0.5050	1.6873*	0.8123	0.2730	0.1501	
Cwalking	4.0373***	0.5302	4.0373***	0.5302	4.7248***	1.2336	3.5505	0.4235	
U I				ling error					
	CEL	GMPCA	CEL	GMPCA	CEL	GMPCA	CEL	GMPCA	
Validation set	0.5765	0.5619	0.5765	0.5619	0.5664	0.5676	0.5857	0.5567	
Test set	0.5834	0.5580	0.5834	0.5580	0.5916	0.5534	0.6042	0.5465	

Table 9: Modelling estimates (the London model, Level-1)

Note. * p < 0.05; ** p < 0.01; *** p < 0.001; Behavioural inconsistent parameter/price ratio: !: 2 orders of magnitude deviation from the prior model; !!: 3 orders of magnitude deviation.



Figure 5: Comparison of Cross-Entropy Loss (CEL) of the *conjugate-prior*-based BDA simulators and the *Nonconjugate-prior Bayesian* Simulator (the London model, Level-1)

slowly, not reaching an asymptote until around 1000 epochs. Most parameters are statistically significant and their signs are consistent with behavioural expectations. Meanwhile, the GMPCA values for the output models are fairly evenly matched, with the two *prior*-based BDA simulators slightly outperforming with the test data.

Despite fine statistics, the monetary ratio of the output $\alpha_{change-walking-time}$ from the *nonconjugate-prior* simulator has deviated markedly (12.34 v.s. 1.16) from the corresponding Level-0 London model value. Several other time-cost ratios also have deviated by up to 80% of the previous values. Though the divergence is not as significant as the Level-1 California model's, the output mixed-logit model in this case may result in incorrect behaviour interpretations and mislead policy-decisions. In contrast, the estimated parameters combinations of other two *prior-based* simulators indicate a stable behavioural representation of the model.

5.2.3. Level-2

The benchmark simulators both show increased CEL fluctuations in modelling at Level 2 (Figure 6 & Figure 7). With a handful of 75 choice training samples, the California model undergoes intense volatility, and ESBDA therefore encounters *early stopping* at the 2110th epoch.

Difference between the simulators' modelling errors becomes marginal as the simulation continues, as shown by Figure 6. In the validation set and the out-of-sample test of the California model, however, the advantage of ESBDA's output model is clear in GMPCA. For all simulators, there is a large difference between the training and validation/test performances (as indicated by the CEL and GMPCA scores). This is due to the high relative sampling noise in the small sample sizes for the validation and test sets. For the BDA and *Nonconjugate prior Bayesian* simulators, this sampling noise results in model overfitting during estimation, with resulting parameter values inconsistent with behavioural theory. The monetary ratios of some parameters' vary by over 3 orders of magnitude from the Level-1 model, BDA's parameter $\beta_{n_electric}$, additionally has an incorrect sign. This is despite the model being applied to the same context as the Level-1 model and the training data randomly drawn from the Level-1 data.

This shows a clear limit of both the nonconjugate-prior and BDA simulators in

Simulator	ESBDA Sin (at the	nulator 2110 th	BDA Simula	tor		Nonconjugate-prior Bayesian Simulator		Direct Application Approach		
	epoch)						11			
Random coefficient										
Latent										
	Mean	StDv	Mean	StDv	Mean	StDv	Mean	StDv		
$\mu_{\rm price}$	-0.1974	0.9121	-0.2090	1.4562	-0.2539	1.5939	-1.5132	0.3949		
$\sigma_{\rm price}$	2.6323	2.2431	8.2019	13.0608	9.2272	16.7234	1.8336	0.6433		
μ_{operate}	-2.4376***	0.3761	-7.6778	4.2876	-5.1315	2.8804	-5.8014	0.7751		
$\sigma_{\mathrm{operate}}$	3.5423	2.8795	33.9150	82.7603	20.4377	57.7694	3.1118	0.9784		
μ_{range}	-0.9645	0.8876	-8.9406	6.4381	-7.7546	5.7963	-2.4011	0.7858		
$\sigma_{\rm range}$	2.6502	1.7987	41.5634	100.0234	28.3021	141.887	2.1558	0.8384		
μ_{electric}	-1.5067	1.5765	-0.0101	2.1043	-0.1724	1.9302	-1.5876	0.3424		
$\sigma_{\rm electric}$	2.6780^{**}	0.9251	17.3402	51.3003	12.6582	24.0391	1.4239	0.5577		
$\mu_{ m hybrid}$	1.0523	1.5755	-0.0819	2.3232	-0.2299	1.7389	0.5282	04048		
$\sigma_{ m hybrid}$	4.4210	3.9012	20.1810	72.1741	11.0272	30.1289	1.2361	0.5409		
Simulated										
$\beta_{\text{price},n}$	-4.1604	8.7820	-24.8885	157.8406	-34.3783	245.7799	-0.5221	0.8996		
$\beta_{\text{operate},n}$	-0.1070	0.2083	-131.2370 [!]	2692.2057	-29.4556!	452.4227	-0.0138	0.0513		
$\beta_{\text{range},n}$	1.5674	3.1203	730.7354!!	19697.7659	32.1690	693.3362	0.2797	0.6189		
$\beta_{\text{electric},n}$	-1.0674	1.7843	0.1453 ^e	4.1886	-0.2052!	3.6437	-1.5761	1.2672		
$\beta_{\mathrm{hybrid},n}$	1.0965	2.0724	0.0759!	4.5287	-0.2407	3.4049	0.5383	1.1049		
•			Fixe	d coefficient	•					
$\alpha_{ m high}$	0.7528^{*}	0.3271	0.5807	0.5610	0.6476	0.5601	0.0958	0.1783		
$\alpha_{\rm midhigh}$	0.6046	0.3906	0.0517!	0.5007	0.0274!	0.5095	0.8014	0.1928		
			Mo	delling error						
	CEL	GMPCA	CEL	GMPCA	CEL	GMPCA	CEL	GMPCA		
Validation set	1.1391	0.3201	1.1872	0.3050	1.1903	0.3041	1.1992	0.3014		
Test set	1.4465	0.2354	1.5120	0.2205	1.9494	0.1424	1.9754	0.1387		

Table 10: Modelling estimates (the California Model, Level-2)

Note. * p < 0.05; ** p < 0.01; *** p < 0.001;

Behavioural inconsistent parameter/price ratio: 1: 2 orders of magnitude deviation from the prior model; 11: 3 orders of magnitude deviation.



Figure 6: Comparison of Cross-Entropy Loss (CEL) of the *conjugate-prior*-based BDA simulators and the *Nonconjugate-prior Bayesian* Simulator (the California model, Level-2). *Note:* there is a big gap between training and validation sets in performance, even at epoch 0 for the prior-based BDA - this is a result of sampling noise in the very small test and validation samples.

Simulator			BDA Simulat	or	Nonconjuga	te-prior	Direct	Application
	(at the 80 th e	epoch)			Bayesian Simulator		Approach	
			Random	coefficient				
Latent								
	Mean	StDv	Mean	StDv	Mean	StDv	Mean	StDv
$\mu_{\rm cost}$	-0.1613***	0.0030	-0.1515***	0.0200	-0.1567***	0.0116	-0.1531	0.0409
$\sigma_{\rm cost}$	0.0040^{***}	0.0002	0.0241	0.0126	0.01930^{*}	0.0077	0.0149	0.0275
Simulated								
$\beta_{\text{cost},n}$	-0.1670	0.0627	-0.1656	0.1535	-0.1693	0.1376	-0.1641	0.2182
·			Fixed co	pefficient				
$\alpha_{\text{driving-time}}$	-2.9900***	0.1950	-1.0078	2.3048^{*}	-5.2698	2.1117	-4.2537	1.5895
$\alpha_{\text{access-time}}$	-3.8152***	0.3183	-3.9098*	1.5454	-2.4823	2.3405	-5.7911	1.2652
$\alpha_{\text{bus-time}}$	-2.5568***	0.6217	-1.2926	0.9609	-1.8107	1.7206	-3.4614	1.0902
$\alpha_{\text{rail-time}}$	-2.3364***	0.1017	-0.3130	1.8523	-0.8199	2.9039	-4.2861	1.6784
$\alpha_{\text{change-walking-time}}$	-2.3003***	0.1561	-0.7313	1.6394	-0.0641	1.0505	-4.8911	2.4391
$\alpha_{\text{change-waiting-time}}$	-2.5137***	0.1764	-3.3472	1.8070	-2.6195	2.6344	-4.0699	1.3559
$\alpha_{\text{cycling-time}}$	-5.0906***	0.2034	-4.5897***	1.0737	-5.0841	2.8613	-6.3078	1.1257
$\alpha_{\text{walking-time}}$	-6.7379***	0.2872	-8.5262***	1.2530	-7.5704*	2.1896	-6.8432	0.6762
α_{traffic}	-5.3766**	0.3347	-10.1548***	2.8023	-9.4864**	3.4395	-6.6577	2.2360
C_{public}	1.7731***	0.1849	1.8745*	0.7839	1.6103	0.9444	2.4519	0.5393
Ccycling	0.4090^{***}	0.1131	0.8278	0.6686	0.8456	0.8890	0.6759	0.5050
Cwalking	3.6822***	0.2830	5.0738***	0.7619	4.4023***	1.2089	4.0373	0.5302
·				ing error				
	CEL	GMPCA	CEL	GMPCA	CEL	GMPCA	CEL	GMPCA
Validation set	0.5368	0.5845	0.5517	0.5760	0.5489	0.5776	0.5493	0.5773
Test set	0.6164	0.5398	0.8928	0.4095	1.1476	0.3174	0.8732	0.4176

Table 11: Modelling estimates (the London model, Level-2)

Note. * p < 0.05; ** p < 0.01; *** p < 0.001; ^e sign-error; Behavioural inconsistent parameter/price ratio: !: 2 orders of magnitude deviation from the prior model; !!: 3 orders of magnitude deviation.



Figure 7: Comparison of Cross-Entropy Loss (CEL) of the *conjugate-prior*-based BDA simulators and the *Nonconjugate-prior Bayesian* Simulator (the London model, Level-2)

terms of sample size required. Hence the corresponding benchmark models are considered as invalid behavioural models. For the ESBDA simulator, *early stopping* prevents the model from overfitting during model training, and the final model parameters are consistent with the Level-1 estimates and behavioural expectations.

Unlike the California model, given a total of 266 training samples, the Level-2 London model has much steadier modelling progress and much less time-cost ratio deviation. Yet the training and validation model's prediction performances do not differ much, ESBDA shows a clear advantage in its out-of-sample prediction, GMPCAs being 0.5398 v.s. 0.4095 v.s. 0.3174 v.s. 0.4176.

5.2.4. Level-3

The sample size for the Level-2 California modelling is already very small (merely 5 individuals' data for training), which does not support subdivision for Level-3 experimentation. As such, Level-3 modelling is carried out for the London case-study only.

As with the Level-2 scenario for the California case-study, the sampling noise from the very small sample size for the Level-3 London model results in large discrepancies in train and test performance for the nonconjugate-prior estimator as well as the BDA without *early stopping*. This indicates that overfitting occurs during model estimation. Once again, the *early stopping* procedure in the ESBDA simulator prevents this overfitting, and results in a final model with substantially higher test performance. Moreover, the overfit BDA and noncojugate-prior models have substantial sign and scale errors in the parameters resulting from the overfitting, whilst the ESBDA maintains full consistency with behavioural expectations.

Simulator		4		Nonconjugate-prior Bayesian Simulator		Direct Application Approach		
			Random	coefficient				
Latent								
	Mean	StDv	Mean	StDv	Mean	StDv	Mean	StDv
$\mu_{\rm cost}$	-0.2219**	0.0706	-0.3780	0.6723	-0.6685	0.6493	-0.1613	0.0030
$\sigma_{\rm cost}$	0.0770***	0.0056	0.8515	1.0724	1.1269	1.5951	0.0040	0.0002
Simulated								
$\beta_{\text{cost},n}$	-0.2470	0.2746	-0.4616	0.9136	-0.7647	1.0510	-0.1670	0.0627
			Fixed co	oefficient				
$\alpha_{\rm driving-time}$	-3.4202***	0.1423	2.1181 ^e	2.7649	-5.7653	2.7036	-2.9900	0.1950
$\alpha_{\text{access-time}}$	-3.3099***	0.2615	3.6504 ^e	3.1918	3.9425 ^e	2.1141	-3.8152	0.3183
$\alpha_{\text{bus-time}}$	-2.5795***	0.1886	3.0410 ^e	3.0798	7.1499 ^e	3.8681	-2.5568	0.6217
$\alpha_{\text{rail-time}}$	-2.2033***	0.2303	-1.2485	3.1867	12.5610 ^e	6.4642	-2.3364	0.1017
$\alpha_{\text{change-walking-time}}$	-0.8872	0.6649	-1.8847	4.8146	-1.2363	2.4461	-2.3003	0.1561
$\alpha_{\text{change-waiting-time}}$	-2.4913***	0.3341	5.0345 ^e	5.8134	5.5778 ^{*e}	2.2320	-2.5137	0.1764
$\alpha_{\text{cycling-time}}$	-5.2001***	0.5262	-5.2188*	1.7910	2.7879 [*] e	2.4994	-5.0906	0.2034
$\alpha_{\text{walking-time}}$	-6.2652***	0.2117	-13.9090*	4.7416	-5.5405	3.1127	-6.7379	0.2872
α_{traffic}	-5.2321***	0.3069	-14.5173*	4.7514	-4.7229*	1.7556	-5.3766	0.3347
C_{public}	1.6822***	0.2160	4.8957**	1.4114	-0.4629 ^e	2.1898	1.7731	0.1849
C _{cycling}	0.8333	0.4028	5.3572*	1.9971	-1.4617	1.8743	0.4090	0.1131
Cwalking	3.5707***	0.4112	11.0504*	3.8048	1.9144	1.1669	3.6822	0.2830
<u> </u>			Modell	ing error				
	CEL	GMPCA	CEL	GMPCA	CEL	GMPCA	CEL	GMPCA
Validation set	0.5869	0.5561	1.1364	0.3209	0.9305	0.3944	0.6089	0.5439
Test set	0.6635	0.5150	1.2883	0.2757	1.0905	0.3360	0.6971	0.4980

Table 12: Modelling estimates (the London model, Level-3)

Note. * p < 0.05; ** p < 0.01; *** p < 0.001; e sign-error; Behavioural inconsistent parameter/price ratio: !: 2 orders of magnitude deviation from the prior model; !!: 3 orders of magnitude deviation.



Figure 8: Comparison of Cross-Entropy Loss (CEL) of the *conjugate-prior*-based BDA and the *Nonconjugate-prior Bayesian* Simulator (the London model, Level-3)

Overall, ESBDA shows clear advantage over the benchmark simulators in quality of estimates, steadiness of the modelling process, the generally higher GMPCA and a major merit in deriving behavioural interpretative and insightful mixed-logit models. These advantages are gradually manifested as sample size reduces.

Modelling results clearly demonstrate the value of the early-stopping procedure when dealing with very small sample sizes. Note that each modelling level represents a certain demographic group in the London study-case. As such, the estimated models represent true transferred models from the corresponding prior models. Robust performance of the ESBDA in the London study-case therefore demonstrates the ability of the BDA and ESBDA to achieve better model transfers, and the ability of the ESBDA to prevent overfitting with very small training samples. Therefore, these results illustrate the potential of ESBDA in model transfer.

6. Conclusions and Further Work

This study advances the basic *Bayesian* simulator of Train & Garrett (2006) to enable new contexts with lower data availability to establish their models by transferring from an existing mixed-logit model of another context with rich data. Through the combination of *Bayesian* modelling and Machine Learning (ML) techniques, the modelling of the proposed Early Stopping Bayesian Data Assimilation (ESBDA) simulator incorporates a previously established parameters combination as an informative *conjugate-prior* and assimilates collected data through iterative *Bayesian inference*. Data assimilation helps the resultant model avoid the under-fitting problem caused by naive application of any empirical model that is not tailored to the new context. The *early stopping* procedure, on the other hand, prevents the modelling from over-fitting or non-convergence, which are two recurrent problems in small sample modelling. Meanwhile, through the *early stopping* procedure, a lightweight Maximum Simulated Likelihood (MSL) analogue is equipped to complement the *Bayes procedure*. ESBDA has therefore consolidated the merits of these two most prominent mixed-logit simulators. **ESBDA** is benchmarked against the direct application approach and two reference simulators — a *non-conjugate* simulator and a Bayesian Data Assimilation (BDA) which has no *early stopping* trigger. The modelling study consists of experiments of two mixed-logit models and at multiple levels of sample size. Comparisons are made on (i) estimation statistics, i.e., statistical significance, in-sample and out-of-sample prediction errors; (ii) behavioural consistency of the estimated mixed-logit models; and (iii) steadiness of modelling process.

The output model of ESBDA outperforms its counterparts of the benchmark simulators in each of the three above dimensions in every experiment. The results also indicate the high behavioural consistency and strong explanatory power of the output models from ESBDA compared with the benchmark operators. Another advantage of *prior-based Bayesian* approaches (including BDA and ESBDA) is that they can avoid unreasonable variation in model estimates arising from random initial parameter estimates. Overall, the results in this paper indicate the ESBDA simulator could be used as a practical, economical and relatively time-saving tool to assist in analysing choice behaviour, particularly for modelling specific population groups and for future estimation with lower data availability.

The ESBDA simulator in its current state has several limitations that direct future studies to fulfilling its full potential. Firstly, we would like to explore technical updates which may reinforce the simulator, e.g., the *Cross-Validation* and *Hamiltonian Monte Carlo* techniques. Another direction for future study is to expand the adaptation of the ESBDA simulator to e.g., (i) mixed-logit models with a flexible mixing distribution, (ii) other types of classic Discrete Choice Models (DCMs) and (iii) extended DCMs (Walker, 2001), such as integrated framework, flexible error structures, and latent variables.

An important future work is to expand the applications of the ESBDA simulator. It is of our particular interest to develop (i) transferred models for sub-populations from the full population model, which helps to investigate heterogeneous choice behaviour between demographic groups and (ii) a *Bayesian* framework that continuously updates the future travel behaviour estimation model as new data becomes available, which accommodates the need to investigate post-pandemic travel behaviour.

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