



RprobitB: Bayes Estimation of Latent Class Mixed Multinomial Probit Models in R

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Abstract

RprobitB is an R package for Bayes estimation of multinomial probit models on discrete choice panel data. Its strength lies in modeling heterogeneous choices, because it is capable to approximate any underlying mixing distributions through a mixture of normal distributions. The number of latent classes do not need to be prespecified but can be updated within the algorithm on a weight-based strategy. Furthermore, the package provides great numerical stability since it does not require initialization nor approximation or maximization of any likelihood function. In this paper, we show how to estimate (mixed) probit models using **RprobitB** and make a comparison to other R packages that estimate probit models.

Keywords: Mixed multinomial probit models, Bayesian analysis, unobserved heterogeneity, R.

1. Introduction

Discrete choice models lie at the heart of many transportation models. This holds true for mode choice models as well as for models of vehicle purchase decisions, to name just a few applications. Traditionally, discrete choice models are interpreted as random utility models, including the multinomial logit (MNL) and the multinomial probit (MNP) model as the most prominent members. In their basic form, these models often fail to take into account heterogeneity of individual deciders, cf. [Train \(2009\)](#), Chapter 6, or [Train \(2016\)](#). A concrete example of heterogeneous preferences is constituted by the value of travel time, cf. [Cirillo and Axhausen \(2006\)](#). Modelling heterogeneity in preferences is indispensable in such cases and has been elaborated in both the MNL and the MNP model by imposing mixing distributions on the coefficients, cf. [Train \(2009\)](#) and [Bhat \(2011\)](#).

Specifying these mixing distributions is an important part of the model selection. In absence of alternatives, it has been common practice so far to try different types of standard parametric

distributions (including the normal, log-normal, uniform and tent distribution) and to perform a likelihood value-based model selection, cf. Train (2009), Chapter 6. Aiming to capture correlation patterns across parameters, Fountas, Anastasopoulos, and Abdel-Aty (2018) and Fountas, Pantangi, Hulme, and Anastasopoulos (2019) apply multivariate normal mixing distributions in their probit models, which however comes at the price of imposing the rather strong normality assumption on their parameters.

In order to alleviate these restrictions Train (2016) proposes a non-parametric approach based on grid methods. Building on the ideas of Train (2016) and Bhat and Lavieri (2018) recently Bauer, Büscher, and Batram (2019) introduced procedures for non-parametrically estimating latent class mixed multinomial probit models where the number of classes is chosen iteratively in the algorithm. These procedures have been demonstrated to be useful in reasonable sized cross-sectional data sets. However, for large panel data sets with a significant number of choice occasions per person, the approach is numerically extremely demanding in particular due to its non-parametric nature and has to deal with the curse of dimensionality.

In the Bayesian framework Scaccia and Marcucci (2010) presents the idea to estimate latent class logit models with a fixed prespecified number of Gaussian components. This approach does not require the maximization of the likelihood while at the same time it allows for approximation of the underlying mixing distribution. The same idea has also been applied to probit models, cf. Xiong and Mannering (2013) for an analysis of adolescent driver-injury data. In both cases however, the specification of the number of latent classes is based only on a trial-and-error strategy.

Extending Scaccia and Marcucci (2010) and Xiong and Mannering (2013), this paper presents a more flexible approach that combines the ideas of a Bayesian framework, approximating the mixing distribution through a mixture of normal distributions and updates on the number of latent classes within the algorithm analogously to Bauer *et al.* (2019).¹ As a consequence, the procedure unites the benefits of a reduced numerical complexity for the estimation compared to the non-parametric likelihood maximization approach and the ability to approximate any mixing distribution. Presenting simulation results on artificial test cases, it is shown that the approach is capable of approximating the underlying mixing distributions and thereby guiding the specification of mixing distributions for real-world applications.

The paper is organized as follows: Section ?? is dedicated to the model formulation. Section ?? defines the Bayesian framework and the updating scheme on the number of latent classes. Simulation results are presented in Section ?. Section ? concludes the paper.

2. The method

2.1. The latent class mixed multinomial probit model

Assume that we observe the choices of N decision makers which decide between J alternatives at each of T choice occasions². Specific to each decision maker, alternative and choice occasion, we furthermore observe $P_f + P_r$ choice attributes that we use to explain the choices.

¹This combination has been suggested at the ICMC talk presenting Bauer *et al.* (2019), which is gratefully acknowledged.

²For notational simplicity, we use a balanced panel where the number of choice occasions T is assumed to be the same for each decision maker. Differences however are straightforward to implement.

The first P_f attributes are connected to fixed coefficients, the other P_r attributes to random coefficients following a joint distribution mixed across decision makers. Person n 's utility \tilde{U}_{ntj} for alternative j at choice occasion t is modelled as

$$\tilde{U}_{ntj} = \tilde{W}_{ntj}'\alpha + \tilde{X}_{ntj}'\beta_n + \tilde{\varepsilon}_{ntj} \quad (1)$$

for $n = 1, \dots, N$, $t = 1, \dots, T$ and $j = 1, \dots, J$, where

- \tilde{W}_{ntj} is a vector of P_f characteristics of j as faced by n at t corresponding to the fixed coefficient vector $\alpha \in \mathbb{R}^{P_f}$,
- \tilde{X}_{ntj} is a vector of P_r characteristics of j as faced by n at t corresponding to the random, decision maker-specific coefficient vector $\beta_n \in \mathbb{R}^{P_r}$, where β_n is distributed according to some P_r -variate distribution g_{P_r} ,
- and $(\tilde{\varepsilon}_{nt:}) = (\tilde{\varepsilon}_{nt1}, \dots, \tilde{\varepsilon}_{ntJ})' \sim \text{MVN}_J(0, \tilde{\Sigma})$ is the models' error term vector for n at t , which in the probit model is assumed to be multivariate normally distributed with zero mean and covariance matrix $\tilde{\Sigma}$.

As is well known, any utility model needs to be normalized with respect to level and scale in order to be identified, cf. Train (2009), Section 5.2. Therefore, we consider the transformed model

$$U_{ntj} = W_{ntj}'\alpha + X_{ntj}'\beta_n + \varepsilon_{ntj}, \quad (2)$$

$n = 1, \dots, N$, $t = 1, \dots, T$ and $j = 1, \dots, J-1$, where (choosing J as the reference alternative) $U_{ntj} = \tilde{U}_{ntj} - \tilde{U}_{ntJ}$, $W_{ntj} = \tilde{W}_{ntj} - \tilde{W}_{ntJ}$, $X_{ntj} = \tilde{X}_{ntj} - \tilde{X}_{ntJ}$ and $\varepsilon_{ntj} = \tilde{\varepsilon}_{ntj} - \tilde{\varepsilon}_{ntJ}$, where $(\varepsilon_{nt:}) = (\varepsilon_{nt1}, \dots, \varepsilon_{nt(J-1)})' \sim \text{MVN}_{J-1}(0, \Sigma)$ and Σ denotes a covariance matrix with the top-left element restricted to one. Train (2009) provides an algorithm on how to transform $\tilde{\Sigma}$ to Σ . While taking utility differences in order to normalize the model with respect to level is a standard procedure, alternatives to fixing an error term variance in order to normalize with respect to scale exist, cf. Mori (2014).

Let $y_{nt} = j$ denote the event that decision maker n chooses alternative j at choice occasion t . Assuming utility maximizing behavior of the decision makers, the decisions are linked to the utilities via

$$y_{nt} = \sum_{j=1}^{J-1} j \cdot 1 \left(U_{ntj} = \max_i U_{nti} > 0 \right) + J \cdot 1 \left(U_{ntj} < 0 \text{ for all } j \right), \quad (3)$$

where $1(A)$ equals 1 if condition A is true and 0 else.

We approximate the mixing distribution g_{P_r} for the random coefficients³ $\beta = (\beta_n)_n$ by a mixture of P_r -variate normal densities ϕ_{P_r} with mean vectors $b = (b_c)_c$ and covariance matrices $\Omega = (\Omega_c)_c$ using C components, i.e.

$$\beta_n \mid b, \Omega \sim \sum_{c=1}^C s_c \phi_{P_r}(\cdot \mid b_c, \Omega_c), \quad (4)$$

³Here and below we use the abbreviation $(\beta_n)_n$ as a shortcut to $(\beta_n)_{n=1, \dots, N}$ the collection of vectors $\beta_n, n = 1, \dots, N$.

where $(s_c)_c$ are weights satisfying $0 < s_c \leq 1$ for $c = 1, \dots, C$ and $\sum_c s_c = 1$. One interpretation of the latent class model is obtained by introducing variables $z = (z_n)_n$ allocating each decision maker n to class c with probability s_c , i.e.

$$\text{Prob}(z_n = c) = s_c \quad \text{and} \quad \beta_n \mid z, b, \Omega \sim \phi_{P_r}(\cdot \mid b_{z_n}, \Omega_{z_n}). \quad (5)$$

The model defined by equations (2), (3) and (5) is what we call the latent class mixed multinomial probit model. We note that the model collapses to the (normally) mixed multinomial probit model if $P_r > 0$ and $C = 1$ and to the basic MNP model if $P_r = 0$.

2.2. The Bayesian framework

Our Bayesian analysis of the latent class mixed multinomial probit model builds upon the Bayesian framework of the MNP model, which has been developed by McCulloch and Rossi (1994), Nobile (1998), Allenby and Rossi (1998), and Imai and van Dyk (2005). Their work provides Markov chain Monte Carlo algorithms for numerically computing Bayes estimates of the posterior distribution of the MNP model parameters. A key ingredient is the concept of data augmentation, cf. Albert and Chib (1993), which treats the latent utilities as parameters themselves. Conditional on the latent utilities, the MNP model constitutes a standard Bayesian linear regression set-up, which renders drawing from the posterior distribution feasible without the need to evaluate any likelihood.

This section defines the Bayesian framework that we use in order to estimate the latent class mixed multinomial probit model. Section 2.3 outlines the choice of prior distributions. We apply an eight-component Gibbs sampler to approximate the models' joint posterior distribution, which is defined in Section 2.4. The number of latent classes is updated within the Gibbs sampler, which is discussed in Section 2.5.

2.3. Prior Settings

Bayesian analysis enables to impose prior beliefs on the model parameters. It is possible to either express strong a priori knowledge using informative prior distributions or to express vague knowledge using diffuse prior distributions. For our model, we apply the following conjugate priors:

- $(s_1, \dots, s_C) \sim D_C(\delta)$, where $D_C(\delta)$ denotes the C -dimensional Dirichlet distribution with concentration parameter vector $\delta = (\delta_1, \dots, \delta_C)$,
- $\alpha \sim \text{MVN}_{P_f}(\psi, \Psi)$,
- $b_c \sim \text{MVN}_{P_r}(\xi, \Xi)$, independent for all c ,
- $\Omega_c \sim W_{P_r}^{-1}(\nu, \Theta)$, independent for all c , where $W_{P_r}^{-1}(\nu, \Theta)$ denotes the P_r -dimensional inverse Wishart distribution with ν degrees of freedom and scale matrix Θ ,
- and $\Sigma \sim W_{J-1}^{-1}(\kappa, \Lambda)$.

The parameters of the prior distributions can be chosen based on estimation results of similar choice settings, resulting in informative priors. For the simulations in Section ??, we applied the diffuse prior approach, setting $\delta_1 = \dots = \delta_C = 1$; ψ and ξ equal to the zero vector; Ψ and

Ξ equal to the identity matrix with value 10 on the diagonal; ν and κ equal to $P_r + 2$ and $J + 1$, respectively (to obtain proper priors); Θ and Λ equal to the identity matrix.

2.4. The Gibbs Sampler

Sampling from the joint posterior distribution in the Gibbs sampler proceeds by iteratively drawing and updating each model parameter conditional on the other parameters.

Updating s . The class weights are drawn from the Dirichlet distribution

$$(s_1, \dots, s_C) \mid \delta, z \sim D_C(\delta_1 + m_1, \dots, \delta_C + m_C), \quad (6)$$

where for $c = 1, \dots, C$, $m_c = \#\{n : z_n = c\}$ denotes the current absolute class size. Mind that the model is invariant to permutations of the class labels $1, \dots, C$. For that reason, we accept an update only if the ordering $s_1 < \dots < s_C$ holds, thereby ensuring a unique labelling of the classes.

Updating z . Independently for all n , we update the allocation variables $(z_n)_n$ from their conditional distribution

$$\text{Prob}(z_n = c \mid s, \beta, b, \Omega) = \frac{s_c \phi_{P_r}(\beta_n \mid b_c, \Omega_c)}{\sum_c s_c \phi_{P_r}(\beta_n \mid b_c, \Omega_c)}. \quad (7)$$

Updating b . The class means $(b_c)_c$ are updated independently for all c via

$$b_c \mid \Xi, \Omega, \xi, z, \beta \sim \text{MVN}_{P_r}(\mu_{b_c}, \Sigma_{b_c}), \quad (8)$$

where $\mu_{b_c} = (\Xi^{-1} + m_c \Omega_c^{-1})^{-1}(\Xi^{-1}\xi + m_c \Omega_c^{-1}\bar{b}_c)$, $\Sigma_{b_c} = (\Xi^{-1} + m_c \Omega_c^{-1})^{-1}$, $\bar{b}_c = m_c^{-1} \sum_{n: z_n = c} \beta_n$.

Updating Ω . The class covariance matrices $(\Omega_c)_c$ are updated independently for all c via

$$\Omega_c \mid \nu, \Theta, z, \beta, b \sim W_{P_r}^{-1}(\mu_{\Omega_c}, \Sigma_{\Omega_c}), \quad (9)$$

where $\mu_{\Omega_c} = \nu + m_c$ and $\Sigma_{\Omega_c} = \Theta^{-1} + \sum_{n: z_n = c} (\beta_n - b_c)(\beta_n - b_c)'$.

Updating U . Independently for all n and t and conditionally on the other components, the utility vectors $(U_{nt:})$ follow a $J - 1$ -dimensional truncated multivariate normal distribution, where the truncation points are determined by the choices y_{nt} . To sample from a truncated multivariate normal distribution, we apply a sub-Gibbs sampler, following the approach of Geweke (1998):

$$U_{ntj} \mid U_{nt(-j)}, y_{nt}, \Sigma, W, \alpha, X, \beta \sim \mathcal{N}(\mu_{U_{ntj}}, \Sigma_{U_{ntj}}) \cdot \begin{cases} 1(U_{ntj} > \max(U_{nt(-j)}, 0)) & \text{if } y_{nt} = j \\ 1(U_{ntj} < \max(U_{nt(-j)}, 0)) & \text{if } y_{nt} \neq j \end{cases}, \quad (10)$$

where $U_{nt(-j)}$ denotes the vector $(U_{nt:})$ without the element U_{ntj} , \mathcal{N} denotes the univariate normal distribution, $\Sigma_{U_{ntj}} = 1/(\Sigma^{-1})_{jj}$ and

$$\mu_{U_{ntj}} = W'_{ntj}\alpha + X'_{ntj}\beta_n - \Sigma_{U_{ntj}}(\Sigma^{-1})_{j(-j)}(U_{nt(-j)} - W'_{nt(-j)}\alpha - X'_{nt(-j)}\beta_n), \quad (11)$$

where $(\Sigma^{-1})_{jj}$ denotes the (j, j) th element of Σ^{-1} , $(\Sigma^{-1})_{j(-j)}$ the j th row without the j th entry, $W_{nt(-j)}$ and $X_{nt(-j)}$ the coefficient matrices W_{nt} and X_{nt} , respectively, without the j th column.

Updating α . Updating the fixed coefficient vector α is achieved by applying the formula for Bayesian linear regression of the regressors W_{nt} on the regressands $(U_{nt:}) - X'_{nt}\beta_n$, i.e.

$$\alpha \mid \Psi, \psi, W, \Sigma, U, X, \beta \sim \text{MVN}_{P_f}(\mu_\alpha, \Sigma_\alpha), \quad (12)$$

where $\mu_\alpha = \Sigma_\alpha(\Psi^{-1}\psi + \sum_{n=1, t=1}^{N, T} W_{nt}\Sigma^{-1}((U_{nt:}) - X'_{nt}\beta_n))$ and $\Sigma_\alpha = (\Psi^{-1} + \sum_{n=1, t=1}^{N, T} W_{nt}\Sigma^{-1}W'_{nt})^{-1}$.

Updating β . Analogously to α , the random coefficients $(\beta_n)_n$ are updated independently via

$$\beta_n \mid \Omega, b, X, \Sigma, U, W, \alpha \sim \text{MVN}_{P_r}(\mu_{\beta_n}, \Sigma_{\beta_n}), \quad (13)$$

where $\mu_{\beta_n} = \Sigma_{\beta_n}(\Omega_{z_n}^{-1}b_{z_n} + \sum_{t=1}^T X_{nt}\Sigma^{-1}(U_{nt} - W'_{nt}\alpha))$ and $\Sigma_{\beta_n} = (\Omega_{z_n}^{-1} + \sum_{t=1}^T X_{nt}\Sigma^{-1}X'_{nt})^{-1}$.

Updating Σ . The error term covariance matrix Σ is updated by means of

$$\Sigma \mid \kappa, \Lambda, U, W, \alpha, X, \beta \sim W_{J-1}^{-1}(\kappa + NT, \Lambda + S), \quad (14)$$

where $S = \sum_{n=1, t=1}^{N, T} \varepsilon_{nt}\varepsilon'_{nt}$ and $\varepsilon_{nt} = (U_{nt:}) - W'_{nt}\alpha - X'_{nt}\beta_n$.

Since Σ is drawn from the unrestricted space of symmetric, positive-definite matrices, the samples still lack identification, cf. Section ???. Therefore, subsequent to the sampling, the normalization $\alpha^{(i)}/\sqrt{(\Sigma^{(i)})_{11}}$, $b_c^{(i)}/\sqrt{(\Sigma^{(i)})_{11}}$, $\Omega_c^{(i)}/(\Sigma^{(i)})_{11}$, $c = 1, \dots, C$ and $\Sigma^{(i)}/(\Sigma^{(i)})_{11}$ are required for the i th updates in each iterations i , cf. Imai and van Dyk (2005), where $(\Sigma^{(i)})_{11}$ denotes the top-left element of $\Sigma^{(i)}$. The draws for s do not need to be normalized. The remaining parameters could be normalized, if the results are of interest in the analysis.

The theory behind Gibbs sampling constitutes that the sequence of samples produced by the updating scheme can be considered as a Markov chain with stationary distribution equal to the desired joint posterior distribution. It takes a certain number of iterations for that stationary distribution to be approximated reasonably well. Therefore, it is common practise to discard the first B out of R samples (the so-called burn-in period). Furthermore, correlation between nearby samples should be expected. In order to obtain independent samples, we consider only every Q th sample when averaging values to compute parameter statistics like expectation and standard deviation. Adequate values for R , B and Q depend on the complexity of the considered Bayesian framework. In the simulations in Section ??, we performed $R = 100.000$ iterations, discarded the first $B = R/2$ samples and thinned the sequence by keeping every $Q = 200$ th sample, resulting in a size of $(R - B)/Q = 250$ samples for each parameter. The independence of the samples can be verified by computing the serial correlation. The convergence of the Gibbs sampler can be checked by considering trace plots and comparing the estimates for different sizes of the burn-in period.

2.5. Updating the Number of Latent Classes

Updating the number C of latent classes is done within the Gibbs sampler by executing the following weight-based updating scheme.

- We remove class c , if $s_c < \varepsilon_{\min}$, i.e. if the class weight s_c drops below some threshold ε_{\min} . This case indicates that class c has a negligible impact on the mixing distribution.

- We split class c into two classes c_1 and c_2 , if $s_c > \varepsilon_{\max}$. This case indicates that class c has a high influence on the mixing distribution whose approximation can potentially be improved by increasing the resolution in directions of high variance. Therefore, the class means b_{c_1} and b_{c_2} of the new classes c_1 and c_2 are shifted in opposite directions from the class mean b_c of the old class c in the direction of the highest variance.
- We join two classes c_1 and c_2 to one class c , if $\|b_{c_1} - b_{c_2}\| < \varepsilon_{\text{distmin}}$, i.e. if the euclidean distance between the class means b_{c_1} and b_{c_2} drops below some threshold $\varepsilon_{\text{distmin}}$. This case indicates location redundancy which should be repealed. The parameters of c are assigned by adding the values of s from c_1 and c_2 and averaging the values for b and Ω .

These rules contain choices on the values for ε_{\min} , ε_{\max} and $\varepsilon_{\text{distmin}}$. For the simulations in Section ??, we set $\varepsilon_{\min} = 0.01$ and $\varepsilon_{\max} = 0.7$. The adequate value for $\varepsilon_{\text{distmin}}$ depends on the scale of the parameters. In our case, we set $\varepsilon_{\text{distmin}} = 0.1$. We performed the strategy to start with a high number of 10 latent classes and executing the updating scheme discussed above within the second half of the burn-in period. The scheme is executed only every 50th iteration to allow for readjustments after each update.

3. Model specification in RprobitB

4. Illustrations

R> x = 1

5. Summary and discussion

This paper addressed the problem of specifying mixing distributions in the multinomial probit model with a panel data setting, constituting an important part of the model selection for which the literature does not provide much guidance so far. In the absence of alternatives, many applications of the mixed multinomial probit model rely on different types of standard parametric distributions for modeling heterogeneity in preferences in combination with a likelihood-value based model selection. This course of action is very restrictive and imposes strong assumptions on the distribution of the model parameters that could potentially lead to misspecification and biased estimates.

We proposed a new approach that improves the current specification strategies in several ways: First, our approach does not require any distributional assumption, since the latent class setting is flexible enough to approximate practically any distribution shape and allowing for any correlation pattern. Second, the weight-based updating scheme ensures that the number of latent classes does not need to be prespecified. Third, the imposed Bayesian estimation framework avoids many numerical problems that occur in the frequentist approach. Most notably, no likelihood function has to be evaluated nor approximated. Comparing the numerical estimation speed to the non-parametric frequentist approach of [Bauer *et al.* \(2019\)](#), we found that our implementation of the Bayesian approach is at least 10 times faster. The

improvement becomes more distinct for panel data settings with a high number of choice occasions. This is due to the fact that for given total sample size NT a large T is beneficial for the Bayesian approach as then the number of vectors β_n , $n = 1, \dots, N$ is comparatively small, while in the frequentist approach calculating the likelihood becomes more challenging for increasing the number T of choice situations faced by each of the N individuals. On the other hand, the grid based frequentist approach of Bauer *et al.* (2019) can potentially achieve a better approximation (especially of point masses) due to the relatively high number of latent classes. However, this approach requires that a suitable grid is set prior to the estimation with a specification of upper bounds for the coefficients. Additionally, the curse of dimensionality plays a crucial role, which is less of a burden in the Bayesian approach. Note that for a fully specified parametric structure these concerns do not play such a big role also for the frequentist approach.

Our simulation results verified that the proposed approach achieves good approximations of the mixing distribution in common choice modelling situations, where the underlying heterogeneity cannot be captured by standard parametric distributions. It would be interesting to apply the approach also to empirical data in the future. Additionally, further research on how to properly address sign-restricted coefficients is required.

Computational details

The results in this paper were obtained using R 4.1.0 with the **RprobitB** 0.1.0 package. R itself and all packages used are available from the Comprehensive R Archive Network (CRAN) at <https://CRAN.R-project.org/>.

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