

Generalized Linear Latent and Mixed Model:

method, bayesian estimation, advantages, and applications to educational data.

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Dedication

To Manuel, for being my friend and father.
To Margarita, Susan, and Marysu, for their relentless encouragement.
To Ana, for showing me the value of family, here in this moorland.
To both of you, as you are always in my mind.
And to all that knowingly or not, help me to get here.
I am lucky due to all of you.
I hope I make you all proud.

A Manuel, por ser mi amigo y mi padre.
A Margarita, Susan y Marysu, por su incansable aliento.
A Ana, por mostrarme el valor de la familia, aquí en este páramo.
A ustedes dos, que siempre las tengo en mente.
Y a todos los que sabiendolo o no, me ayudaron a llegar aquí.
Soy un suertudo gracias todos ustedes.
Espero llenarlos de orgullo.

Abstract

(work in progress)

Keywords:

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Abbreviations

CFA	Confirmatory Factor Analysis.
DDM	Dual Dependence Models.
EFA	Exploratory Factor Analysis.
GLLAMM	Generalized Linear Latent and Mixed Model.
GLM	Generalized Linear Model.
GLMM	Generalized Linear Mixed Model.
HMC	Hamiltonian Monte Carlo.
iHMC	Interleaved Hamiltonian Monte Carlo.
IRT	Item Response Theory models.
MCMC	Markov Chain Monte Carlo.
ML	Maximum Likelihood.
MSEM	Multilevel Structural Equation Model.
SEM	Structural Equation Model.
VI	Variational Inference.

Chapter 1

Introduction

1.1 Preliminar considerations

Local independence is one of the key assumptions of Item Response Theory (IRT) models, and it is comprised of two parts: (i) local item independence and (ii) local individual independence [3, 24]. In the former case, the assumption entails that the individual's response to an item does not affect the probability of endorsing another item, after conditioning on the individual's ability. While in the case of the latter, the assumption considers that an individual's response to an item is independent of another person's response to that same item [58].

The literature has shown that IRT models are not robust to the violation of local independence. The transgression of the assumption affects model parameter estimates, inflates measurement reliabilities and test information, and underestimates standard errors (see Yen [69], Chen and Thissen [9], and Jiao et al. [28]).

However, item response data arising from educational assessments often display several types of dependencies, e.g. testlets, where items are constructed around a common stimulus [67]; the measurement of multiple latent traits within individuals [58]; cluster effects, where correlation among individuals results from the sampling and measurement mechanism used to gather the data [57]; among others. A good motivating example, that will permeate this research, is the reading comprehension sub-test, from the Peruvian public teaching career national assessment. The test is designed to measure three hierarchically nested sub-dimensions of reading comprehension: literal, inferential, and reflective abilities. Furthermore, the items are bundled together in testlets related to a common text or passage. Finally, multiple cluster effects are present, e.g. at the region, and district level, just to mention a few.

Recent studies have proposed IRT Dual Dependency Models (DDM) to deal with the testlets and individual clustering dependencies observed in the data [16, 15, 14, 28, 12, 13, 58, 7]. The majority of these representations have been developed under the Bayesian framework, and they are similar in parametrization to multilevel models. On the other hand, an almost independent line of research, the Generalized Linear Latent and Mixed Models (GLLAMM) [51, 53, 62, 54], have extended the capabilities of hierarchical models on the estimation of multiple latent traits at different hierarchical levels. These developments have been motivated mostly under the frequentist framework, and they are similar in parametrization to a Multilevel Structural Equation Model (MSEM).

While the initial sense is that both developments are independent of each other, follow-

ing their literature, one can easily notice that they share more than a resemblance. Both follow a multilevel/hierarchical multidimensional approach to account for the clustering of persons within the samples and the item bundles (DDM), or the latent structures within the individuals (GLLMM). However, it is important to point out that in some cases the model parametrization between the two developments differs in a way, that some of them appear to be useful only under their specific contexts. Fortunately, their integration under the Bayesian framework is not only trivial but can be motivated under either type of model.

The benefits of the integration revolve around two facts: (i) the educational data often presents all of the aforementioned dependencies and more, as in the motivating example; and (ii) as it was hinted in the second paragraph, to reach appropriate conclusions from the parameter estimates, IRT models need to account for all of these dependencies. The latter is particularly important as, more often than not, a researcher is interested in producing inferences at the structural level of the model, i.e. how a different set of manifest variables explain the variability in the latent variables, or how the latent variables explain other manifest or latent variables, at different levels. As an example, one might be interested in finding evidence if the latent “abilities” of the teachers are explained by their initial educational conditions, i.e. if they were educated in an institute, university, or both. The main purpose of this would be to identify the type of teacher that might benefit more from the in-service training¹, offered by the national educational authorities, making the intervention cost-effective.

From the previous description, one can infer that the proposed IRT representation would be complex and highly dimensional. Moreover, as educational assessments are usually scored in a binary way (the individual either endorse or did not the item), and because not all individuals are assessed by all the items, the model will be trained on sparse data. From the modeling perspective, neither of the previous points presents a challenge for the bayesian framework. However, it has long been recognized that complex parametrizations, that allow this powerful modeling schemes, introduce pathologies that make Markov Chain Monte Carlo methods (MCMC) face performance challenges [17, 18, 44, 45, 5]. This is highly relevant because, in order to make inferences about the posterior distribution of the parameters, the chains need to achieve three requirements, highly related to the performance of the method: stationarity, convergence, and good mixing [38].

Throughout the bayesian IRT literature, one often finds that four solutions are offered to ensure the fulfillment of the previous requirements, and they can be classified into two broad groups: (i) solutions that involve changing the settings of the MCMC methods, and (ii) solutions that involve readjusting the Bayesian model.

In the first category, we find two proposals: (a) increasing the number of iterations per chain, with large burn-in and thinning processes, and (b) designing model-specific MCMC algorithms. The easiest to implement and more prevalent in the literature is the former, e.g. Fujimoto [15] used chains with 60,000 iterations, where 15,000 were discarded and the remaining were thinned in jumps of 3; while Fujimoto [14] used 225,000 iterations, with burn-in of 30,000 and thinning with jumps of 15. Among the drawbacks of this solution are the large computational times; the user involvement in deciding the specific setting for the process, which could be different for different parameters in the same model;

¹Intervention designed with the purpose of potentiating specific abilities in teachers that are currently part of the public teaching career.

and finally, the lack of confidence that larger chain iterations actually produce a proper posterior investigation. On the other hand, several authors have developed high-tech MCMC algorithms that aim to optimize their performance within a particular class of models [45]. In these cases, the developers re-evaluate not only the use of the programming language, with the purpose of speeding and improving performance (e.g. Fujimoto [15]); but also the inclusion of ad-hoc model assumptions, like the ones used in staple software developments like Mplus [41] or Stata [52]. It is clear from the previous that this solution is not accessible to all researchers, either because of the lack of programming skills, or the restrictive cost of access involved in acquiring the software. But more importantly, these solutions are not always applicable to a wider framework of similar models [45].

In the second category, we also find two proposed solutions: (a) re-write the model in an alternative parametrization, and (b) encode prior information through the prior distributions. On both solutions, the purpose is to ensure the identification of the parameters within the model, which helps to stabilize the MCMC procedure [19]. An example of the former is Fujimoto [15], which decomposed the items' discriminatory parameters into overall and specific item discriminations. For the latter, Fujimoto [16] used informative priors also for the items' discrimination parameters.

More often than not, researchers use two or more of the aforementioned solutions to reach an acceptable performance in the chains. However, as point out by Betancourt and Girolami [5], even the most simple hierarchical models present formidable pathologies, that no simple correction can be performed to visit the posterior distribution properly. This is true no matter the rotation/rescaling of the parameter, or the amount of data. In this context, several authors [17, 18, 44, 45, 5] showed that prior information can be included in the model, not only through the prior distributions but also by encoding it in the model itself, changing the posterior sampling geometries by removing the dependence of the parameters on other sampled parameters, therefore favoring the performance of MCMC chains.

Given all of the above, the present research will focus its attention on showing how easy is to account for all of the dependencies that educational data often display, under the GLLAMM framework. Furthermore, given that only the literature related to gaussian hierarchical models have shown the benefits of changing the posterior sampling geometries, through the use of the non-centered parameterization [17, 18, 44, 45, 5], it seems sensible to provide a similar assessment for nonlinear hierarchical models, and in particular, the ones with latent stochastic processes like IRT [45]. Finally, the research will apply the newfound knowledge to data coming from a large Teacher's standardized educational assessments from Peru.

1.2 Objectives

As mentioned in the previous paragraph, the present research has a three-fold purpose:

1. Motivate the Bayesian GLLAMM for binary outcomes [51, 53, 62, 54]. The representation will emphasize the modeling of multiple hierarchical latent structures and testlets. This, in turn, will effectively blur the division between the GLLAMM framework and IRT models.
2. Empirically evaluate the benefits of changing the posterior sampling geometry. The

emphasis here will be on comparing the centered and non-centered parametrizations [17, 18] in terms of performance of the chains, the parameters' recovery, and the ability of the model to produce appropriate inferences.

3. Apply the model and its parametrization to a real data setting. Here the emphasis will be to assess the conclusions arrived from the application of the model and what they could imply for the educational authorities.

Given the aforementioned goals, the researcher believes the master's thesis contributes to the literature in two aspects:

1. In a theoretical and methodological sense, as the research is focused on describing a model that effectively controls for the multiple dependencies usually observed in educational datasets; and
2. In a more practical sense, as the study will provide empirical evidence if changing the sampling posterior geometries could (could not) benefit the performance of MCMC methods and therefore the inferences, under IRT models.

Finally, it is important to mention, that the computational implementation of the method will be developed in **Stan** [65] and **R** [48, 64].

1.3 Organization

Chapter 2 will motivate the GLLAMM for dichotomous outcomes, and define its components. Chapter 3 will describe the bayesian framework, its benefits and shortcomings. Furthermore, it will outline the evidence behind the change in posterior sampling geometries, and the computational implementation of the model. Chapter 4 will show the results of an empirical simulation study designed to assess the benefits of the re-parametrization, proposed in the previous chapter. Chapter 5 will describe the instruments, the data collection process, and scales under analysis, for a large standardized educational assessment. In addition, the chapter will show the conclusions achieved by the application of the model in the said data. Finally, Chapter 6, will discuss the conclusion for the research, and it will outline the path of future research topics that can be derived from the present effort.

Chapter 2

The GLLAMM for dichotomous outcomes

The Generalized Linear Latent and Mixed Model (GLLAMM) is a framework that unifies a wide range of latent variable models. Developed by Rabe-Hesketh and colleagues [51, 53, 52, 62, 54], the method was motivated by the need of a Multilevel Structural Equation Model (MSEM) that accommodated for unbalanced data, noncontinuous responses and cross-level effects among latent variables. The authors focused its development mainly from the frequentist perspective, however, they offered a general guidance on implementing the model under the bayesian framework (see Skrondal and Rabe-Hesketh [62]).

2.1 Model motivation

Consider a large standardized assessment composed of three sub-test designed to evaluate the reading comprehension, mathematical reasoning, and pedagogical knowledge of teachers; where each sub-test has several dichotomously scored items.

Focusing on the first sub-test, the items were designed to measure only one of the three hierarchically nested sub-dimensions of reading comprehension: literal, inferential, and reflective abilities. Furthermore, it is assumed the three sub-dimensions are all that is needed to measure the reading comprehension ability, effectively making this scale, the highest level latent variable in the model, similar to a hierarchical Confirmatory Factor Analysis (CFA). Finally, the items were bundled in groups of five to a common text or passage, i.e. testlets, that provided the stimulus over which the individual is assessed. Figure 2.1 shows the path diagram of the hypothesized dimensional structure, for the hierarchical cross-classified IRT model corresponding with the instrument.

With the purpose of providing an easier motivation of the model, we will not consider yet the cluster effects; however, later in the presentation we will show how easy is to introduce them in the model. Just for future reference, under this example, one expects to observe clustering effects, because individuals from different regions did not have the same educational opportunities, effectively causing differences among them at a regional level.

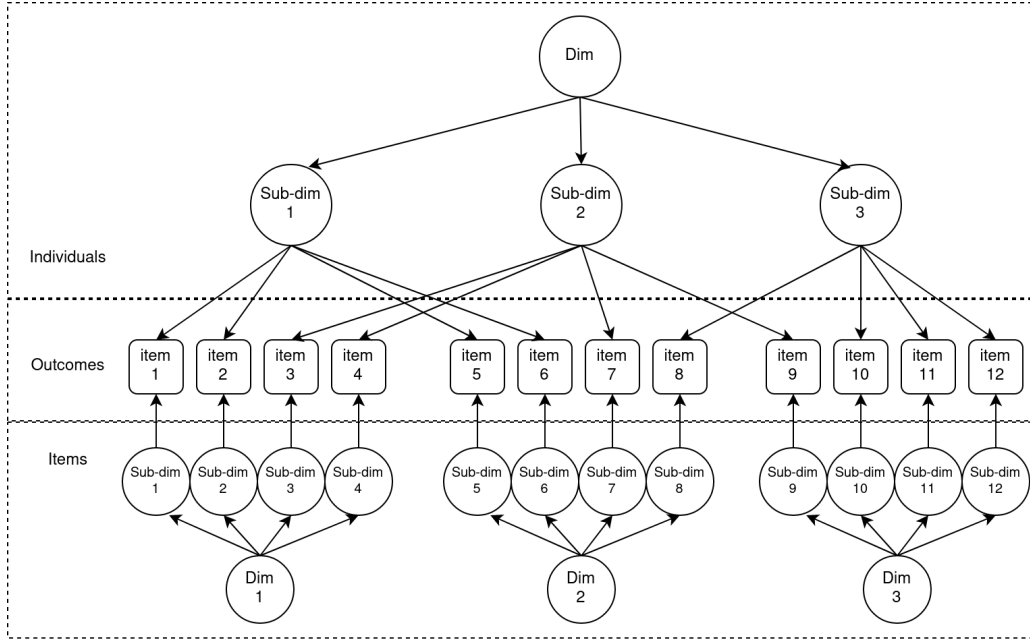


Figure 2.1: Path diagram of the dimensional structure for a hierarchical cross-classified IRT model. Squares represent dichotomous manifest variables, and circles represent latent variables. The figure is based on a reduced set of items, while the errors and scales of the latent variables are not represented. Different sub-dimensions at the individuals block represent the literal, inferential and reflective abilities, while at the items blocks represent the items' difficulties. The dimensions at the individuals block represent the reading comprehension ability, while at the items block represent the multiple testlets.

2.2 Model definition

Following Rabe-Hesketh et al. [51, 53], we continue defining the GLLAMM in two parts: (i) the response model, and (ii) the latent structure.

In case the reader is interested in outcomes different than the dichotomous case, refer to Appendix A.1.

2.2.1 Response model

Conditional to all parameters $\Omega = \{\beta, \Lambda, \Theta, \Psi, \Gamma\}$, including all the latent variables, and the “stacked” vector of covariates for the first level (\mathbf{X}) and in the structural part (\mathbf{W}); the response model can be represented by a Generalized Linear Model (GLM) [43, 37] with a distributional and a systematic part. The latter composed of a linear predictor and a link function.

For the distributional part, the dichotomous items y_{jkd} are modeled at the first level by a Bernoulli probability mass function $f(\cdot)$, in the following form:

$$f(y_{jkd} = 1 | \mathbf{X}, \mathbf{W}, \Omega) = \pi_{jkd}^n (1 - \pi_{jkd})^{1-n} \quad (2.1)$$

where n denotes the endorsement of the item in the Bernoulli trial. On the other hand, for the systematic part, the probability of endorsing the item π_{jkd} is linked to a linear

predictor v_{jkd} through an inverse-link function $h(\cdot)$, in the following form:

$$P(y_{jkd} = 1 \mid \mathbf{X}, \mathbf{W}, \boldsymbol{\Omega}) = \pi_{jkd} = h(\tau_k + v_{jkd}) \quad (2.2)$$

where τ_k is k 'th item threshold, assumed to be zero for the binary case [51], while the inverse-link function can be defined in three ways:

$$h(x) = \begin{cases} \exp(x)[1 + \exp(x)]^{-1} \\ \Phi(x) \\ \exp(-\exp(x)) \end{cases} \quad (2.3)$$

corresponding to the logistic, standard normal $\Phi(x)$, and Gumbel (extreme value type I) cumulative distributions, respectively. It is usual to report the last in terms of link functions $g(\cdot) = h^{-1}(\cdot)$. In that case, these corresponds to the well known logit, probit and complementary log-log, respectively. Finally, the linear predictor is defined by:

$$v_{jkd} = \sum_{p=1}^P x_{jp} \beta_p + \sum_{m=2}^{M+1} \sum_{k=1}^{K(m)} \eta_k^{(m)} \alpha_k^{(m)} + \sum_{l=2}^{L+1} \sum_{d=1}^{D(l)} \theta_{jd}^{(l)} \lambda_d^{(l)} \quad (2.4)$$

where individuals are indexed by $j = 1, \dots, J$, and J represents the total number of individuals in the sample. β_p denotes regression parameter for the x_{jp} explanatory variable with $p = 1, \dots, P$, and P denoting the total number of explanatory variables. $\eta_k^{(m)}$ is the k th item latent dimension at level m with loading $\alpha_k^{(m)}$, where $k = 1, \dots, K(m)$, $K(m)$ denotes the number of dimensions at level $m = 2, \dots, M + 1$, and M represents the number of levels in the items block. $\theta_{jd}^{(l)}$ denotes the individual's d th latent dimension at level l with loading $\lambda_d^{(l)}$, where $d = 1, \dots, D(l)$, $D(l)$ represents the number of dimensions at level $l = 2, \dots, L + 1$, and L denotes the number of levels in the individuals block.

Notice equation (2.4) can be re-written in matrix form in the following way:

$$v_{jkd} = \mathbf{X}_j \boldsymbol{\beta} + \sum_{m=2}^{M+1} \boldsymbol{\eta}^{(m)} \boldsymbol{\alpha}^{(m)} \mathbf{A}_j^{(m)} + \sum_{l=2}^{L+1} \boldsymbol{\theta}_j^{(l)} \boldsymbol{\lambda}^{(l)} \mathbf{B}_j^{(l)} \quad (2.5)$$

where \mathbf{X}_j represents the individual's design matrix of explanatory variables that maps the parameter vector $\boldsymbol{\beta}$ to the linear predictor; and $\mathbf{X} = [\mathbf{X}_1^T, \dots, \mathbf{X}_J^T]^T$ the "stacked" design matrix of \mathbf{X}_j . Moreover, $\boldsymbol{\eta}^{(m)} = [\eta_1^{(m)}, \dots, \eta_{K(m)}^{(m)}]^T$, and $\boldsymbol{\alpha}^{(m)} = [\alpha_1^{(m)}, \dots, \alpha_{K(m)}^{(m)}]^T$ are the vectors of the item's latent dimensions with corresponding loadings at level m , mapped by a block matrix $\mathbf{A}_j^{(m)}$. Similarly, $\boldsymbol{\theta}_j^{(l)} = [\theta_{j1}^{(l)}, \dots, \theta_{jD(l)}^{(l)}]^T$, and $\boldsymbol{\lambda}^{(l)} = [\lambda_1^{(l)}, \dots, \lambda_{D(l)}^{(l)}]^T$ are the vectors of the individual's latent dimensions with corresponding loadings at level l , mapped by a block matrix $\mathbf{B}_j^{(l)}$.

Finally, in order to have a more concise representation of the model, we can re-express equation (2.5) in the following way:

$$\begin{aligned} v_{jkd} &= \mathbf{X}_j \boldsymbol{\beta} + \boldsymbol{\eta} \boldsymbol{\alpha} \mathbf{A}_j + \boldsymbol{\theta} \boldsymbol{\lambda} \mathbf{B}_j \\ &= \mathbf{X}_j \boldsymbol{\beta} + \boldsymbol{\Theta} \boldsymbol{\Lambda} \mathbf{H}_j \end{aligned} \quad (2.6)$$

where $\boldsymbol{\alpha} = [\boldsymbol{\alpha}^{(2)T}, \dots, \boldsymbol{\alpha}^{(M+1)T}]^T$ and $\boldsymbol{\lambda} = [\boldsymbol{\lambda}^{(1)T}, \dots, \boldsymbol{\lambda}^{(L+1)T}]^T$ represent all the loadings corresponding to the items and individuals dimensions at all levels; whereas $\boldsymbol{\eta} =$

$[\boldsymbol{\eta}^{(2)T}, \dots, \boldsymbol{\eta}^{(M+1)T}]^T$ and $\boldsymbol{\theta} = [\boldsymbol{\theta}^{(2)T}, \dots, \boldsymbol{\theta}^{(L+1)T}]^T$ represent the latent dimensions and sub-dimensions of items and individuals at all levels, respectively. Consequently, \mathbf{A}_j and \mathbf{B}_j are their mapping block matrices. Furthermore, $\boldsymbol{\Lambda} = [\boldsymbol{\alpha}^T, \boldsymbol{\lambda}^T]^T$ and $\boldsymbol{\Theta} = [\boldsymbol{\eta}^T, \boldsymbol{\theta}^T]^T$ to represent the “stacked” vector of loadings, and dimensions, respectively; and \mathbf{H}_j its mapping block matrix.

Considering figure 2.1 as reference, we would have an empty level-1 covariates matrix \mathbf{X}_j , as we do not have explanatory variables ($P = 0$). Moreover, we have $M = 2$ levels at the items block, with $K_2 = 12$ and $K_3 = 3$. Consequently, $\boldsymbol{\eta}^{(2)} = [\eta_1^{(2)}, \dots, \eta_{12}^{(2)}]^T$ and $\boldsymbol{\eta}^{(3)} = [\eta_1^{(3)}, \eta_2^{(3)}, \eta_3^{(3)}]^T$ denotes the items’ difficulties and testlet effects, respectively. On the other hand, we have $L = 2$ levels in the individuals block, with $D_2 = 3$ and $D_3 = 1$. Therefore, $\boldsymbol{\theta}^{(2)} = [\theta_1^{(2)}, \theta_2^{(2)}, \theta_3^{(2)}]^T$ which denotes the literal, inferential and reflective abilities; whereas $\boldsymbol{\theta}^{(3)} = \theta_1^{(3)}$ represent the reading comprehension latent variable. Furthermore, since we are trying to express an IRT model, it makes sense to put some restrictions to the parameter set. In this case, we establish $\boldsymbol{\alpha}^{(2)} = -\boldsymbol{\lambda}^{(2)}$ with $\boldsymbol{\lambda}^{(2)} = [\lambda_1^{(2)}, \dots, \lambda_{12}^{(2)}]^T$ representing the item’s discriminatory parameter, where $\boldsymbol{\lambda}^{(2)} > \mathbf{0}$. This resemble to a multidimensional generalization of the linear predictor observed in the archetypical Rasch [56], or 2PL [33] models, i.e. $\lambda_d^{(2)}(\theta_{jd}^{(2)} - \eta_k^{(2)})$, where $|\lambda_d^{(2)}| = |\alpha_k^{(2)}|$ denotes the discriminatory power of item k , $\eta_k^{(2)}$ its difficulty, and $\theta_{jd}^{(2)}$ the ability of the individual at dimension d . In addition, $\boldsymbol{\lambda}^{(3)} = [\lambda_1^{(3)}, \lambda_2^{(3)}, \lambda_3^{(3)}]^T$ would represent the loadings from reading comprehension to their respective sub-dimensions; whereas $\boldsymbol{\alpha}^{(3)} = [\alpha_1^{(3)}, \alpha_2^{(3)}, \alpha_3^{(3)}]^T$ would represent the item-specific loadings from the testlets, usually set as $[1, 1, 1]^T$, indicating they explain directly the items difficulties at the lower level.

Finally, notice that trough the use of \mathbf{A}_j and \mathbf{B}_j design block matrices, and more generally with \mathbf{H}_j , the model departs from the traditional multivariate framework for formulating structural models, i.e. a wide data format; and adopts a univariate approach, i.e. a long data format. The former stores the subject’s repeated outcomes in a single row, with multiple response vectors and explanatory variables appended column-wise to the outcome data. The later stores the subject’s repeated outcomes in a single “stacked” response vector with as many rows as there are repeated measurements, and explanatory variables appended column-wise to the outcome data, distinguished from each other, by a design block matrix.

Cluster effects

Considering the previous, we can see that modeling clustering is as easier as to add more random effects to the linear predictor defined in equation (2.4), in the following form:

$$\begin{aligned} v_{jkdc} &= v_{jkd} + \sum_{c=1}^C \delta_c \\ &= v_{jkd} + \boldsymbol{\delta} \mathbf{Z}_j \end{aligned} \tag{2.7}$$

where $c = 1, \dots, C$, which denotes the number of clusters, v_{jkd} is defined as in equation (2.4), and \mathbf{Z}_j is a design block matrix.

2.2.2 Latent structure

The structural model for the latent variables is represented in the following form:

$$\mathbf{\Theta} = \underset{(S \times S)(S \times 1)}{\mathbf{\Psi}} \mathbf{\Theta} + \underset{(S \times Q)(Q \times 1)}{\mathbf{\Gamma}} \mathbf{W} + \underset{(S \times 1)}{\mathbf{\zeta}} \quad (2.8)$$

where $S = K + D$, $K = \sum_m K_m$, and $D = \sum_l D_l$. Furthermore, $\mathbf{\Psi}$ and $\mathbf{\Gamma}$ are parameter matrices that map the relationship between the latent variables $\mathbf{\Theta}$, and the “stacked” vector of covariates \mathbf{W} , respectively; while $\mathbf{\zeta}$ is a vector of errors or disturbances. It is important to indicate that \mathbf{W} considers a different set of covariates from \mathbf{X} , as we hypothesize they explain the variability in the latent variables at different levels.

Notice equation (2.8) is the generalization of a single-level Structural Equation Models (SEM) to a multilevel setting, however, the main difference in the GLLAMM representation is that the latent variables may vary at different levels.

Additionally, considering that $\mathbf{\Theta}$ has no feedback effects, is permuted, and sorted according to the levels of interest, then $\mathbf{\Psi}$ will be a strictly upper triangular matrix. In this regard, (i) the absence of feedback loops imply the method deals with non-recursive models, i.e. none of the latent variables are specified as both causes and effects of each other [31]; and (ii) the strictly upper triangular structure reveals the GLLAMM does not allow latent variables to be regressed on lower level latent or observed variables, implying the method deals with reflective measurement¹[4]. For a more detailed explanation on the topic see Edwards and Bagozzi [11].

However, notice that because in the IRT framework $\boldsymbol{\eta}$ and $\boldsymbol{\theta}$ should be orthogonal to each other by design, we can further decompose equation (2.8) in the following form:

$$\boldsymbol{\eta} = \underset{(K \times K)(K \times 1)}{\mathbf{\Psi}_\eta} \boldsymbol{\eta} + \underset{(K \times Q)(Q \times 1)}{\mathbf{\Gamma}_\eta} \mathbf{W}_\eta + \underset{(K \times 1)}{\mathbf{\zeta}_\eta} \quad (2.9)$$

$$\boldsymbol{\theta} = \underset{(D \times D)(D \times 1)}{\mathbf{\Psi}_\theta} \boldsymbol{\theta} + \underset{(D \times Q)(Q \times 1)}{\mathbf{\Gamma}_\theta} \mathbf{W}_\theta + \underset{(D \times 1)}{\mathbf{\zeta}_\theta} \quad (2.10)$$

where $\mathbf{\Psi}_\eta$, $\mathbf{\Psi}_\theta$, $\mathbf{\Gamma}_\eta$, and $\mathbf{\Gamma}_\theta$ are the dimension-specific parameter matrices that map the relationship between the corresponding latent variables $\boldsymbol{\eta}$ and $\boldsymbol{\theta}$; with $\mathbf{\zeta}_\eta$ and $\mathbf{\zeta}_\theta$ being the dimension-specific vector of disturbances. Finally, the matrices \mathbf{W}_η and \mathbf{W}_θ would be the dimension-specific covariates.

Considering figure 2.1 as reference, we did not specified any structural relationships $\mathbf{\Psi}$; nor declare any additional covariates \mathbf{W} . However, chapter 4 and 5 will show an implementation where we hypothesized a set of covariates explain the variability on some of the latent variables.

2.3 Model assumptions

Following Skrondal and Rabe-Hesketh [62], the framework has two main assumptions:

- (M1) **Complete latent space.** The latent space is considered complete if all the latent variables, that we hypothesize affect the outcomes, are considered in the model [23]. In the GLLAMM representation, these would be all latent variables $\mathbf{\Theta}$ at levels $l > 1$ and $m > 1$.

¹A latent variable is considered reflective when it is thought to be the cause of the lower level latent or manifest variables.

(M2) **Local Independence**, also known as conditional independence, is defined in the following form:

$$f(\mathbf{y} = \mathbf{1} \mid \mathbf{X}, \mathbf{W}, \boldsymbol{\Omega}) = \prod_{j=1}^J \prod_{d=1}^D \prod_{k=1}^K f(y_{jkd} = 1 \mid \mathbf{X}, \mathbf{W}, \boldsymbol{\Omega}) \quad (2.11)$$

where $f(\mathbf{y} = \mathbf{1} \mid \mathbf{X}, \mathbf{W}, \boldsymbol{\Omega})$ denotes the level-1 conditional likelihood, and \mathbf{y} the vector of all responses at the first level. It is important to mention that equation (2.11) results from the union of two parts [58, 3, 24]:

- (a) **Local item independence**, which entails the individual's response to an item does not affect the probability of endorsing another item, after conditioning on the individual's ability. This is expressed in the following mathematical form:

$$f(y_{j..} = 1 \mid \mathbf{X}, \mathbf{W}, \boldsymbol{\Omega}) = \prod_{d=1}^D \prod_{k=1}^K f(y_{jkd} = 1 \mid \mathbf{X}, \mathbf{W}, \boldsymbol{\Omega}) \quad (2.12)$$

where $y_{j..} = [y_{j11}, \dots, y_{jKD}]$ is the vector of all items for individual j and, as previously defined, $K = \sum_m K_m$ and $D = \sum_l D_l$.

- (b) **Local individual independence**, which entails that an individual's response to an item is independent of another person's response to that same item. The assumption is expressed in the following form:

$$f(y_{.kd} = 1 \mid \mathbf{X}, \mathbf{W}, \boldsymbol{\Omega}) = \prod_{j=1}^J f(y_{jkd} = 1 \mid \mathbf{X}, \mathbf{W}, \boldsymbol{\Omega}) \quad (2.13)$$

where $y_{.kd} = [y_{1kd}, \dots, y_{Jkd}]$ is the vector of all individuals endorsing item k from dimension d .

Chapter 3

Bayesian estimation

The practical use of the GLLAMM developed in chapter 2 requires the estimation of all of the items and individuals' dimensions, loadings, regression and structural parameters. These can be obtained within two frameworks: the Frequentist and Bayesian.

The current chapter centers its attention on describing the Bayesian estimation procedure, using the Markov Chain Monte Carlo method (MCMC). For a full development of GLLAMM under the Frequentist framework refer to Rabe-Hesketh and colleagues [51, 53, 62, 54].

3.1 Benefits and shortcomings

3.1.1 Why Bayesian?

The reasons why Bayesian statistics is attractive to perform the estimation of the parameters of any model, and especially for the GLLAMM developed in chapter 2, are:

1. It is built on a simulation-based estimation method, therefore, it can handle all kinds of priors and data-generating processes [13]. This is especially useful with highly complex and over-parameterized models, where other methods are unfeasible or work poorly [2, 30].
2. The likelihood functions are used to define the posterior sampling distributions, however, they can also be used in a generative way. The likelihood for the data, and priors for the parameters, form the basis to produce samples from the posterior distribution. However, they can also be used to simulate observations, allowing us to test the ability of the method/data to recover the parameters of interest [38].
3. The Bayesian are at least as good as the Frequentist estimates [2, 68, 27]. This is true when the method uses uninformative 'flat' priors. However, because the procedure allows us to integrate prior beliefs or knowledge about the parameters, beyond the observed responses, it can produce results even when the scenario raises issues of non-convergence or improper estimation under Maximum Likelihood methods (ML) [62, 13, 38]. Examples of such are:
 - (a) when we have small sample sizes.

- (b) when individuals have null scores or aberrant response patterns [24, 1]. The latter happens when examinees answered some relatively difficult and discriminating items correctly, while answering some of the easiest incorrectly.
- (c) when parameters need to be confined to a permitted space, e.g. the estimation of positive unique factors variances, where the opposite is known as ‘Heywood cases’ [36]
- (d) when we need to estimate parameters under sparse data, where the asymptotic theory is unlikely to hold [13];

3.1.2 Are you sure there’s nothing wrong?

Of course the Bayesian framework has shortcomings, among them:

1. It exposes the user to arbitrary decisions about the running of the chains, in order to ensure a proper performance, e.g. how many iterates does the chain need to achieve precise estimates?, what is the right size for the burn-in and warm-up phases?, how should the thinning procedure be performed, if any?, should we follow the same procedure for all parameters of interest?, among others [62].
2. The user has multiple options to evaluate the performance of the method, and most of them are visual, making it hard to assess if a proper posterior investigation have been made [20]. More specifically, the user has multiple options to assess if the chain achieves the three requirements for performance: stationarity, convergence, and good mixing [38].
3. The procedure makes it hard to discover parameters’ lack of identification [62]. Inadequate mixing of the chain could lead us to think unidentified parameters have been estimated with precision, when in fact what we have are ‘flat’ posteriors [29].
4. Oftentimes the posterior sampling geometry of the model makes it hard to find proper solutions for the parameter space, no matter the rotation/rescaling of the parameter, or the amount of data [5]. This is especially true in complex hierarchical models.
5. The greater the complexity of the model, the harder it is to communicate/share the implementation with other scientist. This is especially true, when researcher re-parameterize the model to solve the previous point [38].
6. The procedure usually requires more time to achieve a proper solution, compared to the classical methods. This is especially true in models with high complexity [66, 59].

Although some of the previous shortcomings have made the Bayesian procedure a “controversial” implementation, most of them already have acceptable solutions.

For the first point, a popular approach is to use a large number of iterates, or multiple chains with different initial states. This is mostly applicable under the Metropolis-Hastings and Gibbs sampling methods. However, recent solutions like the Hamiltonian Monte Carlo method (HMC) [5] is less reliant on these decisions, as it implements a different sampling mechanism (see section 3.4).

About the second point, it is well accepted that the visual assessment of stationarity and convergence is easier, and this procedure usually has additional support from statistics like **Rhat** [19]. On the contrary, a visual evaluation of ‘good’ mixing remains as a hard task. A recent approach to increase the possibility of a well mixed chain is to change the posterior sampling geometry of the model [44, 45, 5, 38] (see section 3.5).

On the third point, the most common solution is to use regularizing priors, i.e. priors that are more ‘skeptical’ of wider parameter spaces [38]. However, it is important to mention, there are scenarios where one achieves poor parameter estimates, even in the presence of ‘enough’ data and regularizing priors, but this shortcoming is also applicable to the classical estimation procedures, e.g. the estimation of the variance parameters in random effects models [62].

About the fourth point, as it was mentioned in previous paragraphs, a recent approach to solve this issue is to change the posterior sampling geometry of the model. This means to re-parameterize the model in a way that removes the dependence of the parameters on other sampled parameters, or even, produce a sample mechanism that is located in a continuous between a centered (CP) and non-centered parametrization (NCP), e.g. Interleaved HMC (iHMC), and Variational Inference (VI) [17, 18, 44, 45, 5, 22] (see section 3.5).

Finally, the fifth and sixth points can be considered the ‘price’ a scientist has to pay, to be able to fit models that conforms better with the observed data generating processes. Although, recent developments are striving to improve upon the last one.

3.2 Bayesian GLLAMM for dichotomous outcomes

3.2.1 Posterior distribution

Denoting \mathbf{Y} as the observed data and $\mathbf{\Omega} = \{\boldsymbol{\beta}, \boldsymbol{\Lambda}, \boldsymbol{\Theta}, \boldsymbol{\Psi}, \boldsymbol{\Gamma}\}$, i.e. all the parameters declared in section 2.2.1 and 2.2.2; the posterior distribution is obtained using the Bayes theorem, in the following way:

$$P(\mathbf{\Omega} | \mathbf{Y}) = \frac{P(\mathbf{Y} | \mathbf{\Omega}) P(\mathbf{\Omega})}{\int P(\mathbf{Y} | \mathbf{\Omega}) P(\mathbf{\Omega}) d\mathbf{\Omega}} \quad (3.1)$$

this is possible since the Bayesian approach makes no distinction between latent variables and parameters. All of them are considered random quantities [62]. Furthermore, since inference only requires representing the likelihood of the data $P(\mathbf{Y} | \mathbf{\Omega})$ and the prior distribution $P(\mathbf{\Omega})$; and because the denominator is just a (hard to calculate) constant, the posterior can be represented in the following form, without loss of generality:

$$P(\mathbf{\Omega} | \mathbf{Y}) \propto P(\mathbf{Y} | \mathbf{\Omega}) P(\mathbf{\Omega}) \quad (3.2)$$

3.2.2 Prior distributions

Similar to Patz and Junker [46], we use an independent distributional structure for the joint priors of the parameters at the highest level of the GLLAMM, in the following form:

$$\begin{aligned} P(\mathbf{\Omega}) &= P(\boldsymbol{\beta}, \boldsymbol{\Lambda}, \boldsymbol{\Theta}, \boldsymbol{\Psi}, \boldsymbol{\Gamma}) \\ &= P(\boldsymbol{\beta}) P(\boldsymbol{\Lambda}) P(\boldsymbol{\Theta}) P(\boldsymbol{\Psi}) P(\boldsymbol{\Gamma}) \\ &= P(\boldsymbol{\beta}) [P(\boldsymbol{\alpha}) P(\boldsymbol{\lambda})] [P(\boldsymbol{\eta}) P(\boldsymbol{\theta})] [P(\boldsymbol{\Psi}_\eta) P(\boldsymbol{\Psi}_\theta)] [P(\boldsymbol{\Gamma}_\eta) P(\boldsymbol{\Gamma}_\theta)] \end{aligned} \quad (3.3)$$

However, giving the hierarchical and cross-classified structure of the model, the lower level parameters' priors will also depend on further parameters, e.g. variances and covariances of the latent variables¹. These are known as *hyperparameters*, and their prior distributions as *hyperpriors*. Because of the previous, we are not going to detail their lower level representation, as they are highly dependent on the specifics of the model.

Finally, as recommended by several authors the priors will be mildly informative [38, 16, 66, 28, 1, 68], model-specific and determined by a prior predictive investigation. Chapter 4 and 5 will show the process of prior elicitation in the context of a simulated and real dataset, respectively.

3.2.3 Likelihood

Following Rabe-Hesketh et al. [51], the likelihood function is build in a recursive way. First, we replace the structural model (2.8) into the linear predictor (2.6):

$$v_{jkd} = \mathbf{X}_j \boldsymbol{\beta} + (\mathbf{I} - \boldsymbol{\Psi})^{-1} [\boldsymbol{\Gamma} \mathbf{W} + \boldsymbol{\zeta}] \boldsymbol{\Lambda} \mathbf{H}_j \quad (3.4)$$

Second, the linear predictor and inverse-link function (2.3) are used to construct the systematic part of the response (2.2), i.e. its expected value. Here we use a logit link for pedagogical purposes:

$$\pi_{jkd} = \frac{\exp(\tau_k + v_{jkd})}{1 + \exp(\tau_k + v_{jkd})} = \frac{\exp(v_{jkd})}{1 + \exp(v_{jkd})} \quad (3.5)$$

Third, the expected value is used in the distributional part (2.1), in the following form:

$$f(y_{jkd} = 1 | \mathbf{X}, \mathbf{W}, \boldsymbol{\Omega}) = \pi_{jkd}^n (1 - \pi_{jkd})^{1-n} \quad (3.6)$$

Fourth, considering assumptions (M1) and (M2) described in section 2.3, we produce the level-1 likelihood:

$$f(\mathbf{y} = \mathbf{1} | \mathbf{X}, \mathbf{W}, \boldsymbol{\Omega}) = \prod_{j=1}^J \prod_{d=1}^D \prod_{k=1}^K f(y_{jkd} = 1 | \mathbf{X}, \mathbf{W}, \boldsymbol{\Omega}) \quad (3.7)$$

Fifth, we define the marginal likelihood at levels l and m , conditional on the latent variables at levels $l + 1$ and $m + 1$, in the following form:

$$f_{(m)}^{(l)}(\mathbf{y} = \mathbf{1} | \mathbf{X}, \mathbf{W}, \boldsymbol{\Omega}) = \int \left[\prod f_{(m-1)}^{(l-1)}(\mathbf{y} = \mathbf{1} | \mathbf{X}, \mathbf{W}, \boldsymbol{\Omega}) \right] P(\boldsymbol{\Theta}_{(m)}^{(l)}) d\boldsymbol{\Theta}_{(m)}^{(l)} \quad (3.8)$$

where the product inside the brackets is over all units in level $(l - 1)$ and $(m - 1)$, the first level is defined in equation (3.7), and $P(\boldsymbol{\Theta}_{(m)}^{(l)})$ are the prior distributions for the latent variables at level l and m , with $\boldsymbol{\Theta}_{(m)}^{(l)} = [\boldsymbol{\eta}^{(m)}, \boldsymbol{\theta}^{(l)}]$. Finally, we define the likelihood as:

$$\mathcal{L}(\mathbf{X}, \mathbf{W}, \boldsymbol{\Omega}) = \prod_{m=2}^{M+1} \prod_{l=2}^{L+1} f_{(m)}^{(l)}(\mathbf{y} = \mathbf{1} | \mathbf{X}, \mathbf{W}, \boldsymbol{\Omega}) \quad (3.9)$$

and the log-likelihood as:

$$\ell(\mathbf{X}, \mathbf{W}, \boldsymbol{\Omega}) = \log \mathcal{L}(\mathbf{X}, \mathbf{W}, \boldsymbol{\Omega}) \quad (3.10)$$

¹Because of this sequential model specification, it is said the priors also have a “hierarchical” structure.

3.3 Model identification

As indicated by Rabe-Hesketh et al. [51], in order to fully specify the model and provide a scale for the latent variables, we have to make assumptions for either the distribution of the disturbances ζ , the distribution of one or more of the latent variables Θ , or as point out by Fujimoto [14] and several other authors, we could set restrictions for one or more of the loadings in Λ . The last is more prevalent in frequentist software packages like Winsteps [32].

Furthermore, as it is hinted by equation (3.9), it is assumed the latent variables at different levels are independent from each other, whereas latent variables at the same level may present dependency. In case of the latter, we presume the latent variables at the same level have a multivariate normal distribution with a mean and covariance structure determined by equations (2.9) and (2.10). In the case of the covariance matrices, these are determined by the covariance of the specific disturbances ζ .

3.4 Computational implementation

3.4.1 Hamiltonian Monte Carlo

For years the state-of-the-art platform for Bayesian statistical modeling have been the BUGS² project [35, 34], with its WinBUGS and OpenBUGS implementations. However, a more recent participant JAGS³ [47] has gain traction, due to its cross-platform capabilities. In any case, both platforms are not that different from each other. Both use two of the most popular and successful algorithms for performing MCMC: the Metropolis-Hastings [39, 25] and Gibbs Sampling [21] algorithms.

In general lines, the Metropolis algorithm follows a two-step procedure: (i) produce a new proposal for a parameter's value, and (ii) evaluate the proposal against the current, accepting the new value if it is more likely under the posterior distribution. On the other hand, the Gibbs sampling uses a similar procedure, but it gains efficiency by exploiting the knowledge behind the target distribution. The latter improvement catapulted the Gibbs sampler into the workhorse of high dimensional Bayesian computing.

However, both methods remain as highly random procedures, and because of it, they still have important limitations. The most important of them all is that, for several reasons, they do not yield independent and identically distributed samples (iid). This in turn means, the exploration of the posterior is made through a series of (sometimes highly dependent) values, causing the MCMC chain to converge to the target distribution only in the long run, i.e. when the number of iterations approach infinity ($t \rightarrow \infty$) [19].

In this setting two solutions have been proposed within these algorithms, and often-times the aforementioned software packages use them in conjunction. The first consist on improving the sampling mechanism by using a Hybrid MCMC method. A good example is the “Metropolis-within-Gibbs” algorithm [40]. On the other hand, the second consist on defining the number of iterates, burn-in and thinning processes in a way that it reduces the serial dependencies in the samples.

Nevertheless, the aforementioned solutions, while useful, do not solve all issues related

²Bayesian inference Using Gibbs Sampling

³Just Another Gibbs Sampling

with the convergence of the MCMC chains, as these can remain biased in subtle ways, that are more harder to identify [38]. Therefore, researcher have decided instead to propose new improved algorithms.

Is in this context were the Hamiltonian Monte Carlo or Hybrid Monte Carlo (HMC) was proposed by Duane et al. [10], using the theory of Hamiltonian Dynamics. While the full representation of method is out of the scope of this research, we can still make a high-level description of its process, with purpose of point out its benefits and shortcomings.

Assuming we have continuous distributions and the partial derivatives of the log-density function (the gradient) exists, the method iterates the updating of two vector spaces of a “friction-less particle” [42, 38]. First, it samples new values for the momentum vector of the particle, independent of the current values of its position vector, i.e. it gives the particle a random “flick”. In the second iteration, using Hamiltonian dynamics, a Metropolis update is performed to propose a new position vector for the particle. In this sense, one can say the HMC runs a small physics simulation, where the position of the particle denotes the current parameter values in the Markov chain, the momentum denotes the proposed path to a new set of values, and the log-posterior provides the surface over which the particle moves, where the gradient defines its curvature [38].

In principle, because HMC produce “more informed” proposals, it will accept everyone of them. In practice however, HMC uses a rejection criterion, that inform us when the method was not able to maintain the “balance” of the system, producing a bad numeric approximation (see section 3.5 for an example). For more on the background theory on Hamiltonian Dynamics and specifics about the HMC algorithm refer to Neal [42] and Betancourt and Girolami [5].

All of this just tells us that HMC is a highly complex algorithm. However, as McElreath [38] point out, the Gibbs strategy got its improvement over the Metropolis-Hastings by being less random, not more. And in that sense, HMC pushes this principle to a greater length, but manages to improve the efficiency of the MCMC procedure. This is especially true in cases where ordinary Metropolis or Gibbs sampling cannot make a proper exploration of the parameter space, e.g. with highly correlated parameters or with models with hundreds or thousands of parameters, like complex hierarchical models. Moreover, as HCM is more efficient, it requires less number of iterations to make a proper posterior investigation [38, 19]

Off course, this comes with a cost. The methods is more computationally intensive than the previous. However, because of the efficiency improvement and the need of less number of iterations, the method requires less computer time in total, even when each individual sample needs more.

3.4.2 Where can I find this magical software?

`Stan` [65] is the software package that will provide us with the machinery of HMC. Furthermore, the results produced from the software will be analyzed with `R` [48, 64], and its integration packages.

3.4.3 What about burn-in and thinning?

As previously mention, since HMC uses a different approach and produces more informative proposals, setting specific burn-in and thinning processes is no longer necessary.

However, the method does require to perform a warm-up procedure to adapt sampling, and to tune in two parameters of the algorithm: the number of steps, and the step size [65]. These parameters are used to make a discrete approximation of the momentum vector, i.e. the path of the particle.

Notice, this phase is similar to a procedure performed in JAGS, where the proposal distribution gets tuned up to improve the posterior investigation, but the similarities end there. The warm-up samples are not representative of the target posterior distribution, no matter how long this iterations continue [38]. Finally, after the warm-up is finished, and assuming the adaption was successful, the method will sample directly from the target distribution.

In the current research, we will use the default values set in the software, i.e. a total of 2000 iterations, where 1000 of them will be spend on warm-up. Notice this departs (by far) from most of the literature on Bayesian implementations of IRT models, e.g. Fujimoto [15] used chains with 60,000 iterations, where 15,000 were discarded and the remaining were thinned in jumps of 3; while Fujimoto [14] used 225,000 iterations, with burn-in of 30,000 and thinning with jumps of 15; just to mention a few.

3.4.4 Initial starts

As any of the previously simulation-based method requires, we need to set the starting values of the chains. This research decided to allow the software to sample the starting values from the priors set in the models.

3.5 To center or not to center

As it was point out by Betancourt and Girolami [5], even the most simple hierarchical models present formidable pathologies, that no simple correction can be performed to visit the posterior distribution properly. This is true no matter the rotation/rescaling of the parameter, or the amount of data.

A great example of this is what McElreath [38] dubbed the Devil’s funnel, where the author shows that you do not need complex model to start observing these issues. As an example, consider the following joint distribution:

$$\begin{aligned} v &\sim N(0, 3) \\ \theta &\sim N(0, \exp(v)) \end{aligned} \tag{3.11}$$

where v can be interpreted as the *hyperprior* of θ , and θ is dependent on the samples of v . The latter is what the literature dubbed as the Centered Parametrization (CP).

This joint distribution might seem familiar, as Bayesian hierarchical model practitioners often use it to ensure the standard deviation remains into the permitted parameter space ($\sigma \geq 0$). Similar to what is required for multiple parameters in an IRT setting. Moreover, it seems that any MCMC procedure would not have any issues exploring the posterior distribution of these parameters, as there are only two of them, but we would be wrong. One can see the `stan` code of the implementation in Appendix B.1.1.

Figure 3.1 shows the results of implementing the model on equation (3.11) in `stan`. For pedagogical purposes, the example was run without the use of data, however, its result easily extend to the case when the data is present.

As one can see from the figure, no proper exploration of the posterior distribution is performed. The chains show no sign of being “healthy”, i.e. they do not show stationarity or convergence (top panels), nor a good mixing (middle and bottom panels). This is further confirmed by the `Rhat` estimates and the effective sample sizes of the chains (`n_eff`) [19]. The `Rhat` were all above one (recommended threshold), and the effective sample sizes were 34 (v) and 293 (θ), respectively. Notice this imply the series of values remained highly correlated, even when one could expect the effective sample size was closer to the actual number of iterations 3000 (1000 samples for each of the 3 chains, after warm-up).

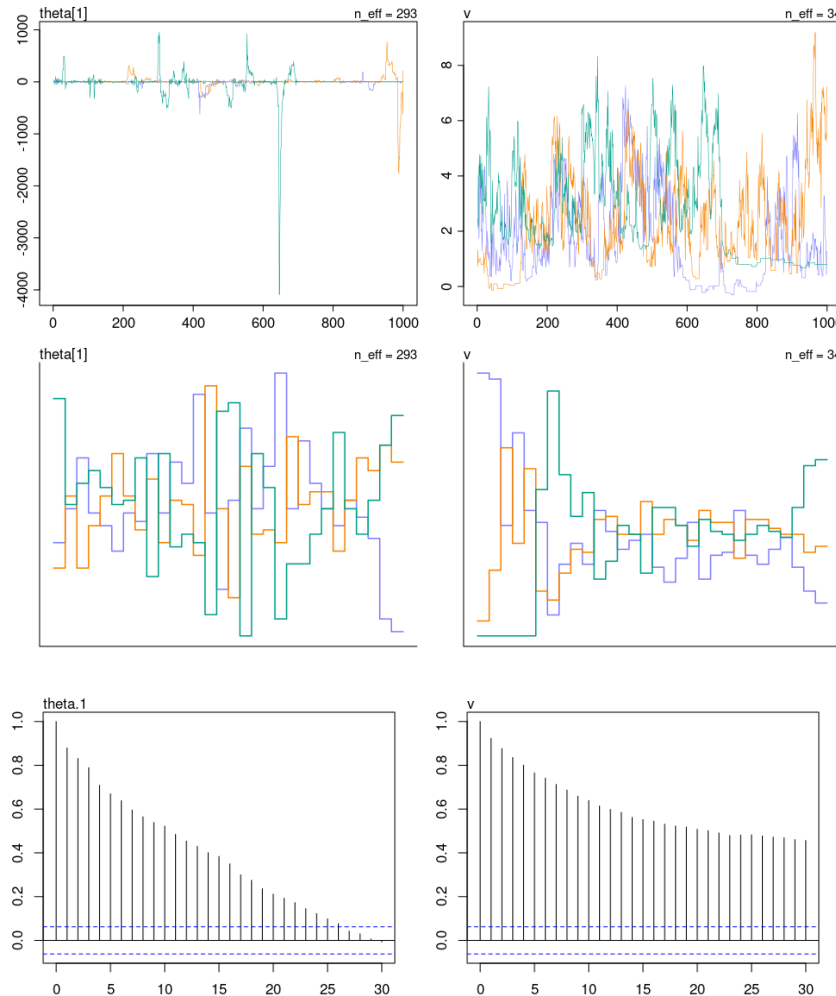


Figure 3.1: The Devil’s funnel. Centered Parametrization. (Top) It shows the traceplot for the iterations on three chains. (Middle) It shows the trunkplot for the same data. (Bottom) It shows the Auto-correlation Functions (ACF) of the iterations.

Wasn’t HMC the solution to this?

HMC is a powerful MCMC algorithm, and its benefits stand the test of other scenarios, as detailed by multiple authors [38, 19]. However, the issue with this example goes a little bit farther than what the algorithm can actually overcome, and this is true also for the

Metropolis and Gibbs sampler. Nevertheless, we will see the HMC still manages to be efficient within the constraints of the problem.

Figure 3.2 shows the posterior sampling geometry of the model in equation (3.11). The first thing we notice is the complexity of the posterior geometry, with a steep funnel shape as the values of v gets smaller and smaller. This makes sense, as the exponential of larger negative values, force the standard deviation of θ to be narrower and narrower around its mean (zero). The second thing we notice is that HMC does not “lose time” exploring the full parameter space of v or θ , something that could happen under the Metropolis-Hastings and Gibbs. In fact, HMC still manages to explore part of posterior distribution successfully, however, the exploration is not complete. Notice there are less accepted samples for $\theta > 0$. Moreover, the method to let us know which parts of the distribution did not explore appropriately, because of the complex geometry of the posterior (see red points indicating divergent transitions). The last is important, because HMC gives us the opportunity to identify where can we improve our parametrization, something that is not available on other algorithms.

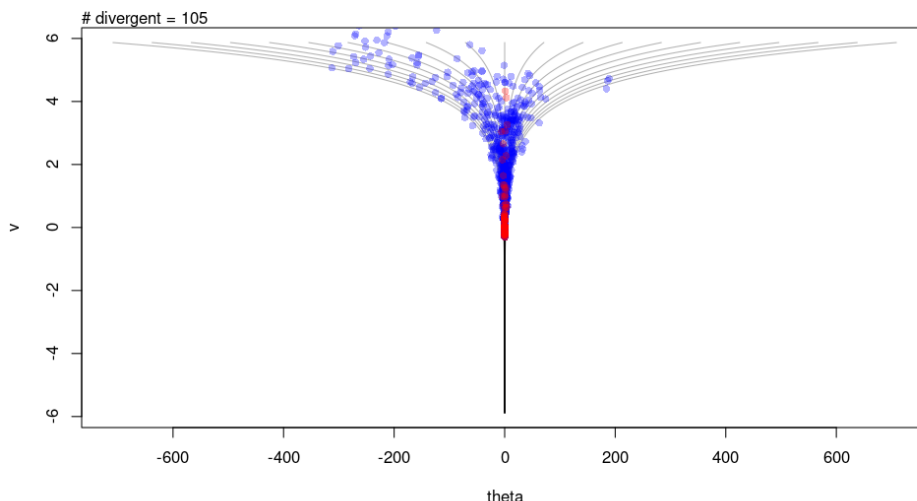


Figure 3.2: Posterior sampling geometry. Centered Parametrization. Blue points are accepted samples. Red points denote divergent transitions.

So, how can we solve it?

It turns out that the idea of encoding mildly informative priors, to stabilize the MCMC chains, has also a geometrical base. Consider the following change to equation (3.11):

$$\begin{aligned} v &\sim N(0, 1) \\ \theta &\sim N(0, \exp(v)) \end{aligned} \tag{3.12}$$

notice the only thing that we changed is the setting of a mildly informative prior for v . Figure 3.3 shows the posterior geometry for the joint distribution of equation (3.13).

The first thing to notice from the figure is that the geometry available for exploration is more broad, allowing HMC (or any other algorithm) to visit more parts of the distributions. On the other hand, it also stands out that the geometry shows less steep curvatures

around $\theta = 0$, although it is pretty steep still. Again, this favors the exploration of the posterior, and a proof of that is the reduction of the number of divergent transitions in the chains (although we still observe them in the steepest part of the geometry), and a mild improvement on the trace, tranks and ACF plots in figure 3.4.

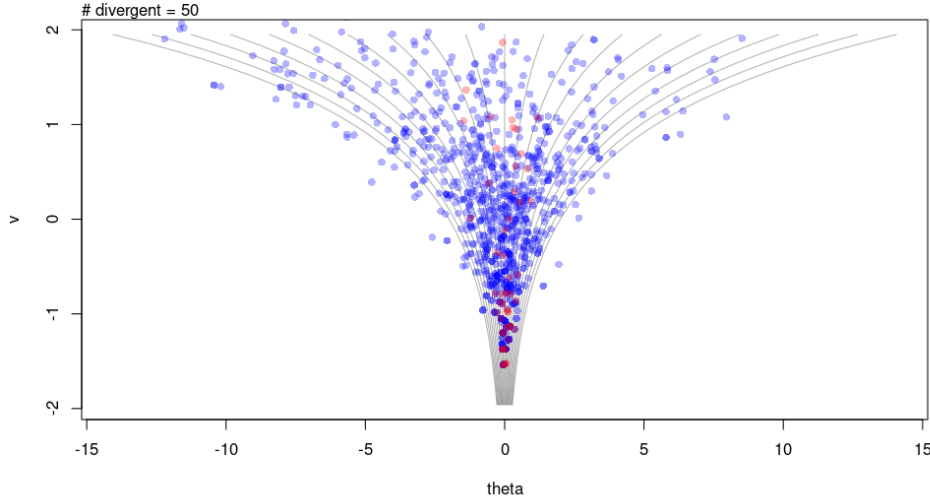


Figure 3.3: Posterior sampling geometry. Centered Parametrization with mildly informative priors. Blue points are accepted samples. Red points denote divergent transitions.

WORK IN PROGRESS

Although it seems that increasing the regularizing power of the priors is the answer to get rid of the sampling issues, raised by a complex posterior sampling geometry; there is a limit of information a prior can contain without imposing strong assumptions about the parameters in a model.

In this context, several authors [17, 18, 44, 45, 5] showed that prior information can be included in the model, not only through the prior distributions but also by encoding it in the model itself, changing the posterior sampling geometries by removing the dependence of the parameters on other sampled parameters, favoring the performance of MCMC chains. This is what the literature knows as the Non-Centered Parametrization (NCP). Consider the following modification to equation (3.11):

$$\begin{aligned} v &\sim N(0, 3) \\ z &\sim N(0, 1) \\ \theta &= \exp(v) * z \end{aligned} \tag{3.13}$$

notice we have break the dependence between θ and v . The idea comes from standardizing a variable, where $(\theta - \mu)/(\exp(v)) = z$, therefore $z \sim N(0, 1)$, then $\theta = \mu + \exp(v) * z = \exp(v) * z$ when $\mu = 0$ by design. More importantly, this can be extended to the multivariate case in a simple way, through the use of the Cholesky decomposition.

Figure 3.5 show the posterior sampling geometry of the model; while figure 3.6 shows the trace, trunk and acf plots for the non-centered parametrization of the model. Notice there are no divergent transitions, the exploration of the posterior distribution is

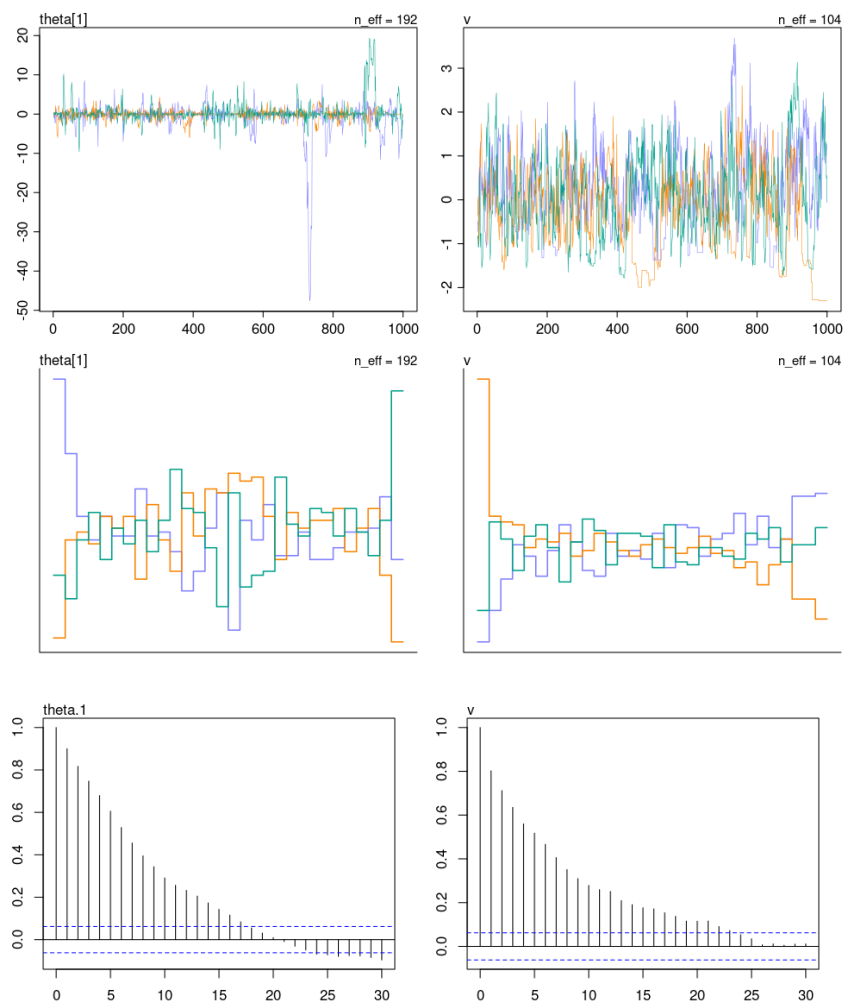


Figure 3.4: The Devil's funnel. Centered Parametrization with prior information. (Top) It shows the traceplot for the iterations on three chains. (Middle) It shows the trunkplot for the same data. (Bottom) It shows the Auto-correlation Functions (ACF) of the iterations.

done without any issues, and finally that get reflected in chains that clearly achieved stationarity, convergence and good mixing.

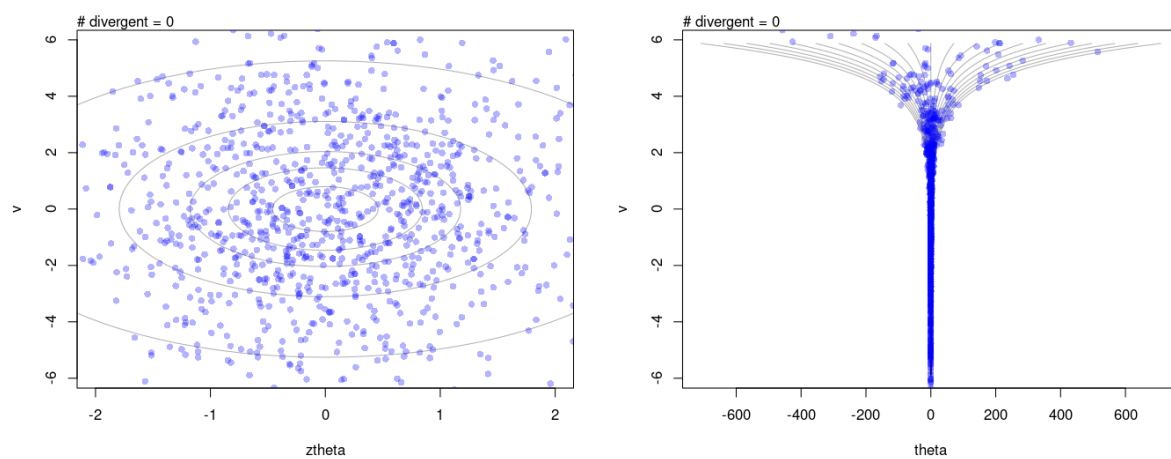


Figure 3.5: Posterior sampling geometry. Non-Centered Parametrization. (Left) Sampling geometry defined by the independent parameters v and z . (Right) Original sampling geometry defined by v and θ . Blue points are accepted samples. Red points denote divergent transitions.

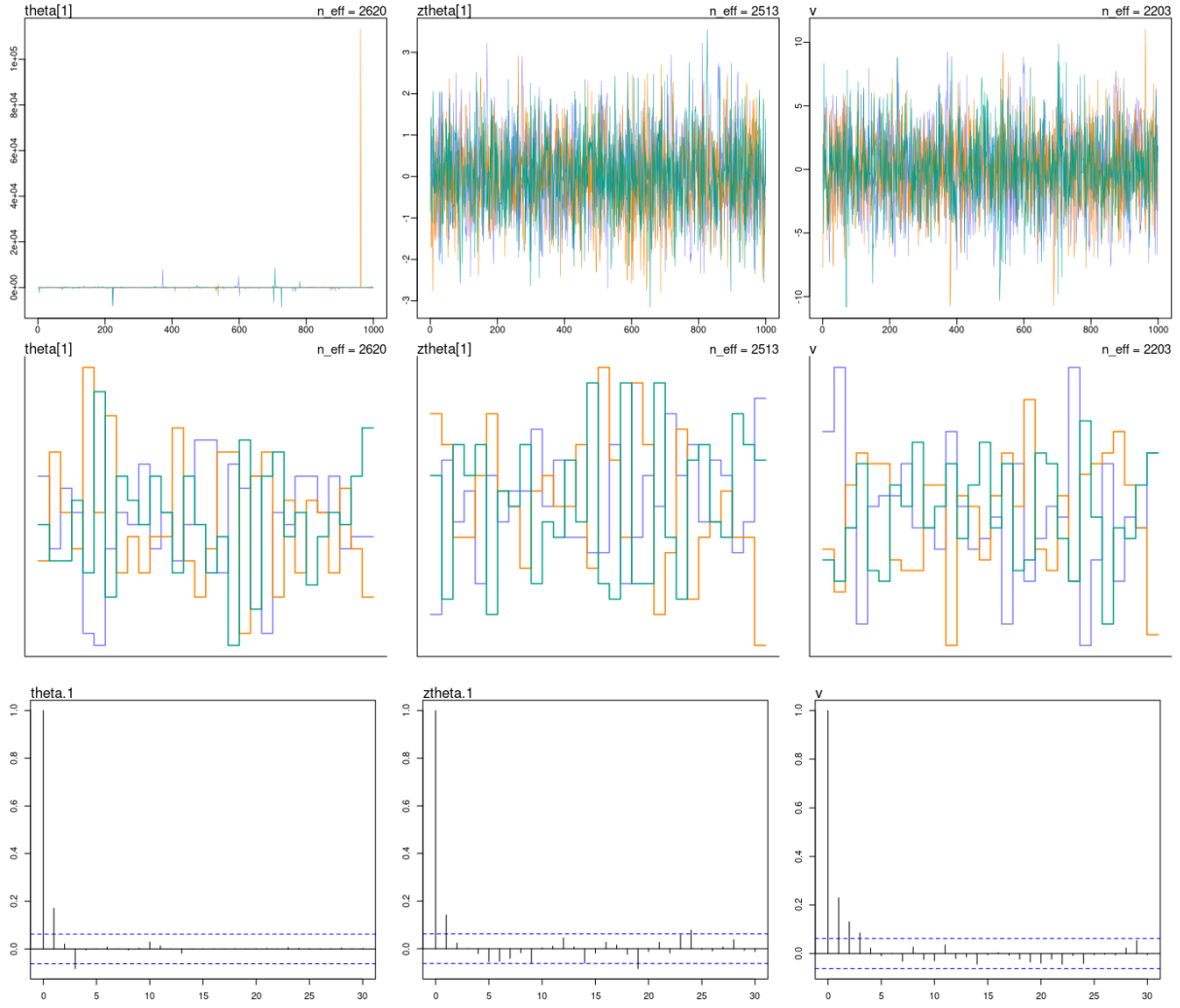


Figure 3.6: The Devil's funnel. Non-centered Parametrization. (Top) It shows the trace-plot for the iterations on three chains. (Middle) It shows the trunkplot for the same data. (Bottom) It shows the Auto-correlation Functions (ACF) of the iterations.

Chapter 4

Simulation Study

4.1 Simulated data

4.2 Models

4.3 Results

Chapter 5

Application

5.1 Instruments

5.2 Data

5.2.1 Collection

5.2.2 Sample scheme

5.3 Results

Chapter 6

Conclusion and Discussion

6.1 Discussion

6.2 Conclusions

6.3 Future development

Appendix A

Additional Theory

A.1 Other links and distributions

As stated in chapter 2, the GLLAMM is a unifying framework for a wide range of latent models. This is possible thanks to the flexibility in the modeling of the outcomes, coming from defining the response model as a GLM [37] (see section 2.2).

In the current section the author will try to briefly describe the most important link functions and outcomes distributions, that can be accommodated within the framework. For a more detailed approach on either of these, refer to Rabe-Hesketh et al. [51, 53, 52], Skrondal and Rabe-Hesketh [62], and Rabe-Hesketh et al. [54].

1. Continuous:

It results from selecting an identity link function for the scaled mean response,

$$\begin{aligned}\mu^* &= E[y^*|\mathbf{X}, \mathbf{Z}, \boldsymbol{\eta}] \\ &= v\end{aligned}\tag{A.1}$$

where $\mu^* = \mu\sigma^{-1}$, $y^* = y\sigma^{-1}$, and σ denotes the standard deviation of the errors.

On the other hand, the distributional part is defined by a Standard Normal distribution $\phi(x) = (2\pi)^{-1/2}\exp(-x^2/2)$,

$$\begin{aligned}f(y^*|\mathbf{X}, \mathbf{Z}, \boldsymbol{\eta}) &= \phi(\mu^*)\sigma^{-1} \\ &= \phi(v)\sigma^{-1}\end{aligned}\tag{A.2}$$

Notice that the same parametrization can be achieved considering $y^* = v + \epsilon^*$, and $\epsilon^* \sim N(0, 1)$. Additionally, the decision to standardize the response variables has been made with the purpose of making the estimation process easier, as such distribution is free of unknown parameters.

2. Polytomous:

It results from selecting a generalized logistic inverse-link function [6] for the expected value of the response, which in this case, describe the probability of endorsing

one of the S unordered available categories,

$$\begin{aligned}
 \mu_s &= E[y = y_s | \mathbf{X}, \mathbf{Z}, \boldsymbol{\eta}] \\
 &= P[y = y_s | \mathbf{X}, \mathbf{Z}, \boldsymbol{\eta}] \\
 &= \pi_s \\
 &= h(v_s)
 \end{aligned} \tag{A.3}$$

where v_s is the linear predictor for category s ($s = 1, \dots, S$), and $h(\cdot)$ is defined as:

$$h(x) = \exp(x) \cdot \left[\sum_{s=1}^S \exp(x) \right]^{-1} \tag{A.4}$$

It is important to note that, as in the dichotomous case, the same parametrization can be achieved using the concept of underlying continuous responses in the form $y_s^* = v_s + \epsilon_s$, where $y = s$ if $y_s^* > y_k^* \forall s, s \neq k$, ϵ_s have a Gumbel (extreme value type I) distribution, as the one defined in equation (2.3), and y_s denotes the random utility for the s category.

Finally, the distributional part is defined by a Multinomial distribution,

$$\begin{aligned}
 f[y = \{y_1, \dots, y_S\} | \mathbf{X}, \mathbf{Z}, \boldsymbol{\eta}] &= \frac{n!}{y_1! \dots y_S!} \prod_{s=1}^S \mu_s^{y_s} \\
 &= \frac{n!}{y_1! \dots y_S!} \prod_{s=1}^S \pi_s^{y_s}
 \end{aligned} \tag{A.5}$$

where y_s denotes the number of "successes" in category s .

3. Ordinal and discrete time duration:

For the ordinal case, the linear predictor is "linked" to the probability of endorsing category s , against all previous categories, in the following form:

$$\begin{aligned}
 \mu_s &= E[y = y_s | \mathbf{X}, \mathbf{Z}, \boldsymbol{\eta}] \\
 &= P[y \leq y_s | \mathbf{X}, \mathbf{Z}, \boldsymbol{\eta}] - P[y \leq y_{s-1} | \mathbf{X}, \mathbf{Z}, \boldsymbol{\eta}] \\
 &= h(\kappa_s - v_s) - h(\kappa_{s-1} - v_{s-1})
 \end{aligned} \tag{A.6}$$

where κ_s denotes the thresholds for category s . For discrete time duration, the linear predictor is "linked" to the probability of survival, in the s th time interval, as follows:

$$\begin{aligned}
 \mu_s &= E[t_{s-1} \leq T \leq t_s | \mathbf{X}, \mathbf{Z}, \boldsymbol{\eta}] \\
 &= P[T \leq t_s | \mathbf{X}, \mathbf{Z}, \boldsymbol{\eta}] - P[T \leq t_{s-1} | \mathbf{X}, \mathbf{Z}, \boldsymbol{\eta}] \\
 &= h(v_s + t_s) - h(v_{s-1} + t_{s-1})
 \end{aligned} \tag{A.7}$$

where T is the unobserved continuous time, and t_s its observed discrete realization. Additionally, for both type of responses, $h(\cdot)$ can be defined as the logistic, standard normal, and Gumbel (extreme value type I) *cumulative distributions*, as in equation (2.3).

Similar to the dichotomous and polytomous case, the same parametrization can be achieved using the concept of underlying latent variables with $y_s^* = v_s + \epsilon_s$, where $y = s$ if $\kappa_{s-1} < y_s^* \leq \kappa_s$, $\kappa_0 = -\infty$, $\kappa_1 = 0$, $\kappa_S = +\infty$, ϵ_s has one of the distributions in equation (2.3), and y_s denotes the random utility for the s category.

It is important to note, for discrete time duration responses, the logit link corresponds to a *Proportional-Odds model*, while the complementary log-log link to a *Discrete Time Hazards model* [55]. Other models for ordinal responses, such as the *Baseline Category Logit* or the *Adjacent Category Logit* models can be specified as special cases of the generalized logistic response function, defined in equation (A.4).

Finally, the distributional part is defined by a Multinomial distribution, as the one defined in equation (A.5).

4. Counts and continuous time duration:

It results from selecting an exponential inverse-link function (log link) for the expected value of the response,

$$\begin{aligned}\mu &= E[y|\mathbf{X}, \mathbf{Z}, \boldsymbol{\eta}] \\ &= \lambda \\ &= \exp(v)\end{aligned}\tag{A.8}$$

and a Poisson conditional distribution for the counts,

$$\begin{aligned}f[y|\mathbf{X}, \mathbf{Z}, \boldsymbol{\eta}] &= \exp(-\mu)\mu^y(y!)^{-1} \\ &= \exp(-\lambda)\lambda^y(y!)^{-1}\end{aligned}\tag{A.9}$$

It is important to mention that unlike the models for dichotomous, polytomous and ordinal responses, model for counts cannot be written under the random utility framework.

5. Rankings and pairwise comparisons:

Following Skrandal and Rabe-Hesketh [60], the parametrization for polytomous responses can serve as the building block for the conditional distribution of rankings. Selecting a "exploded logit" inverse-link function [8] for the expected value of the response, which describes the probability of the full rankings of category s ,

(work in progress)

$$\begin{aligned}\mu_s &= P[\mathbf{R}_s = \{r_s^1, \dots, r_s^1\}|\mathbf{X}, \mathbf{Z}, \boldsymbol{\eta}] \\ &= \pi_s \\ &= h(v_s)\end{aligned}\tag{A.10}$$

where v_s is the linear predictor for category s ($s = 1, \dots, S$), and $h(\cdot)$ is defined as:

$$h(x) = \prod_{s=1}^S \exp(x^s) \left[\sum_{s=1}^S \exp(x^s) \right]^{-1}\tag{A.11}$$

Again, as in specific previous cases, the same parametrization can be achieved using the concept of underlying latent variables.

Finally, the distributional part is defined by a Multinomial distribution,

$$\begin{aligned} f[y = \{y_1, \dots, y_S\} | \mathbf{X}, \mathbf{Z}, \boldsymbol{\eta}] &= \frac{n!}{y_1! \dots y_S!} \prod_{s=1}^S \mu_s^{y_s} \\ &= \frac{n!}{y_1! \dots y_S!} \prod_{s=1}^S \pi_s^{y_s} \end{aligned} \quad (\text{A.12})$$

where y_s denotes the number of "success cases" in category s .

6. Mixtures:

Given the previous definitions, the framework easily lends itself to model five additional settings:

- (a) **Different links and distributions for different latent variables.** This can be easily achieved by setting different links and distributions for each of the M_2 latent variables located at level 2.
- (b) **Left- or right-censored continuous responses.** Common in selection models (e.g. Heckman [26]), they can be achieved by specifying an identity link and Normal distribution for the uncensored scaled responses, as in equations (A.1) and (A.2); and a scaled probit link and Binomial distribution otherwise, as in equations (2.3) and (??).
- (c) **zero-inflated count responses.** where a log link and a Poisson distribution is set for the counts, as in equations (A.8) and (A.9); and a logit link and Binomial distribution is specified to model the zero center of mass, as in equations (??) and (??).
- (d) **Measurement error in covariates.** this setting occurs when standard models use variables, with measurement error, as covariates, e.g. a logistic regression with a continuous covariate that presents measurement error. For more details on this type of setting see Rabe-Hesketh, Skrondal and Pickles [50], Rabe-Hesketh, Pickles and Skrondal [49], and Skrondal and Rabe-Hesketh [61].
- (e) **Composite links.** Useful for specifying proportional odds models for right-censored responses, for handling missing categorical covariates and many other model types. For more details on this type of settings see Skrondal and Rabe-Hesketh [63].

Heteroscedasticity and over-dispersion in the response

Much like the Generalized Linear Mixed Model framework (GLMM), the GLLAMM allows to model heteroscedasticity, and over- or under-dispersion by adding random effects to the linear predictor, at level 1. The types of responses, in which such characteristics can be modeled, are the following:

1. Continuous:

We model **heteroscedasticity** in the following form:

$$\sigma = \exp(\boldsymbol{\alpha}^T \mathbf{Z}^{(1)}) \quad (\text{A.13})$$

Notice that the previous formula implies that equation (A.2) can be re-written in the following form:

$$f(y^*|\mathbf{X}, \mathbf{Z}, \boldsymbol{\eta}) = \phi(v + \boldsymbol{\alpha}^T \mathbf{Z}^{(1)}) \quad (\text{A.14})$$

where $\mathbf{Z}^{(1)}$ is the design matrix that maps the random effects $\boldsymbol{\alpha}$. Notice that equation (A.14) effectively corresponds to a model that includes random intercepts at level 1.

2. Ordinal, and discrete time duration:

Similar to the dichotomous case, by including random intercepts at level 1 in equation (A.6), we can model over- or under-dispersion:

$$\begin{aligned} \mu_s &= P[y \leq y_s | \mathbf{X}, \mathbf{Z}, \boldsymbol{\eta}] - P[y \leq y_{s-1} | \mathbf{X}, \mathbf{Z}, \boldsymbol{\eta}] \\ &= h(\kappa_s - v_s + \boldsymbol{\alpha}^T \mathbf{Z}^{(1)}) - h(\kappa_{s-1} - v_{s-1} + \boldsymbol{\alpha}^T \mathbf{Z}^{(1)}) \end{aligned} \quad (\text{A.15})$$

A similar parametrization can be used for discrete time duration.

3. Counts, and continuous time duration:

Finally, modifying equation (A.8) allow us to model over- or under-dispersion under a counts model:

$$\begin{aligned} \mu &= E[y | \mathbf{X}, \mathbf{Z}, \boldsymbol{\eta}] \\ &= \lambda \\ &= \exp(v + \boldsymbol{\alpha}^T \mathbf{Z}^{(1)}) \end{aligned} \quad (\text{A.16})$$

A.2 Sampling scheme

Appendix B

Code

B.1 Chapter 3: Bayesian estimation

B.1.1 To center or not to center

The devil's funnel, centered parametrization.

```
transformed data {  
    int<lower=0> J;  
    J = 1;  
}  
parameters {  
    real theta[J];  
    real v;  
}  
model {  
    v ~ normal(0, 3);  
    theta ~ normal(0, exp(v));  
}
```

The devil's funnel, centered parametrization with priors.

```
transformed data {  
    int<lower=0> J;  
    J = 1;  
}  
parameters {  
    real theta[J];  
    real v;  
}  
model {  
    v ~ normal(0, 1);  
    theta ~ normal(0, exp(v));  
}
```

The devil's funnel, non-centered parametrization.

```
transformed data {
```



```

        int<lower=0> J;
        J = 1;
    }
    parameters {
        real ztheta[J];
        real v;
    }
    transformed parameters{
        vector[J] theta;
        theta = exp(v) * to_vector( ztheta );
    }
    model {
        v ~ normal(0, 3);
        ztheta ~ normal(0, 1);
    }

```

B.2 Chapter 4: Simulation study

B.2.1 Simulated data

B.2.2 Models

FOLV

SOLV

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