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Abstract

Ordinal predictors are commonly used in regression models. Yet, they are often incorrectly 11 treated as either nominal or metric thus under- or overestimating the contained information. 12 This is understandable insofar as generally applicable solutions or corresponding statistical 13 software are still underdeveloped. We propose a new way of parameterizing regression coefficients of ordinal predictors, which we call monotonic effects. The reparameterization is 15 done in terms of a scale parameter b taking care of the direction and size of the effect and a 16 simplex parameter ζ modeling the normalized differences between categories. This ensures 17 that predictions are monotonotically increasing or decreasing, while changes between 18 adjacent categories may vary across categories. This formulation nicely generalizes to both 19 interaction terms as well as multilevel structures. Monotonic effects may not only be applied to ordinal predictors, but also to other discrete variables for which a monotonic relationship 21 is plausible. This includes variables representing count data or discrete points in time. Fitting motonotonic effects in a fully Bayesian framework is straightforward with the R package brms, which also allows to incorporate prior information and to check the assumption of monotonicity. 25

Keywords: Regression, Isotonic, Ordinal variables, Bayesian statistics, brms, Stan, R

Monotonic Effects: A Principled Approach for Including Ordinal Predictors in Regression

Models

1 Introduction

Over the last few decades, much statistical research has been devoted to handling 30 ordinal response variables in regression models starting with the seminal paper of McCullagh 31 (1980; see also Agresti, 2010; Bürkner and Vuorre, 2018; Liu & Agresti, 2005; Tutz, 2011 for 32 an overview). In Psychology, for instance, this kind of data is omnipresent in the form of 33 Likert scale items, which are often treated as being continuous for convenience without ever testing this assumption (Liddell & Kruschke, 2017). With researchers realizing the 35 importance of correctly modeling ordinal responses, the related models – often simply called ordinal models – are now increasingly applied in scientific practice. In the statistical language 37 R (R Core Team, 2018), for instance, several packages are available to fit ordinal models, 38 among others "ordinal" (Christensen, 2018), "VGAM" (Yee, Stoklosa, Huggins, & others, 39 2015), or "brms" (Bürkner, 2017b, 2017a) to name the perhaps most general ones. 40 Ordinal predictors seem to have received less attention in statistical research. There 41 are only two lines of research known to the authors of the present paper. One is a penalized 42 regression approach specifically designed for ordinal predictors (Gertheiss, 2014; Gertheiss et 43 al., 2011b; Gertheiss & Tutz, 2009) and the other are categorical types of isotonic regression (Barlow, Bremner, Brunk, & Bartholomew, 1972; Robertson, Wright, & Dykstra, 1988). 45 We begin by explaining the former approach. The main idea of the method of 46 Gertheiss and Tutz (2009) is to penalize large differences between adjacent categories. This reflects the expectation that if a variable is ordinal, changes may happen somewhat smoothly and larger differences should thus be unlikely. This approach allows for a very flexible handling of ordinal predictors in a way closely related to regression splines (Gertheiss & Tutz, 2009). The direction of the changes remains unspecified and may vary across the range 51 of the ordinal variable. Depending on the research question and variables under study, this 52 assumption might be somewhat too flexible. More specifically, we do often expect the

changes between adjacent categories to be *monotonic*, that is consistently negative or positive across the full range of the ordinal variable. At the same time, the size of the changes may still vary across categories by a substantial amount as ordinality does not necessarily contain information about distance between categories.

The research on *isotonic regression* deals with regression models subject to order 58 contraints (Barlow et al., 1972; Robertson et al., 1988). For instance, the effect of a drug is 59 assumed to be monotonically increasing with an increasing dose – an assumption that we 60 often want to "hard-code" into our models. Depending on the research question and nature 61 of the variable on which we want to impose a monotonicity constraint, different techniques may be favorable. If the variable is essentially continuous, such as the dose of a drug, we can 63 use parametric functions which are known to be monotonic (e.g., the log or logistic functions in simple cases) or use semi-parameteric approaches such as monotonic splines (Kelly & Rice, 1990; Lee, 1996; Leitenstorfer & Tutz, 2007; Pya & Wood, 2015). If the variable under study is categorical, the monotonicity assumption reduces to an ordering constraint on the group means with respective to the response variable. From the perspective of classical frequentist statistics, the latter case has been studied extensively in Barlow et al. (1972) and Robertson et al. (1988; see also Best and Chakravarti, 1990; Dykstra & Robertson, 1982; Lee, 1981; 70 Wu, Woodroofe, & Mentz, 2001). For the purpose of studying ordinal predictors, we are primarily interested in the categorical type of isotonic regression. 72

The idea and scope of the two approaches discuseed above is somewhat different.
While isotonic regression only restricts the *direction* of the changes, the penalized regression
method restricts the *size* of the changes leaving the direction untouched (although we may
also introduce order constraints in the latter according to Gertheiss et al., 2011b). None of
these two approaches is more reasonable per se and we should not necessarily think of them
as competing in how ordinal predictors should ideally be modeled. Rather, they make use of

¹ The term "isotonic" is mostly used synonymously to "monotonic" in the mathematical-statistical literature. We prefer the latter as we believe it to be understandable by a wider audience outside of mathematics.

different sets of assumptions which both reflect important aspects of ordinal variables. As we will see later on, we may even combine them naturally within the same framework.

In the present paper, we will introduce a monotonicity imposing parameterization of ordinal predictors, which we call *monotonic effects*. They represent a way to generalize the assumption of linearity to ordinal predictors. As explained in detail in the next section, the estimated parameters have an intuitive meaning and are thus easy to interprete and communicate. In simple cases, they also turn out to be equivalent to the results of categorical isotonic regression.

The structure of this paper is a follows. In Section 2, we will introduce monotonic
effects as well as their mathematical foundation in detail. We continue by explaining a
software implementation of monotonic effects in the R package "brms" (Bürkner, 2017b,
2017a), which supports a wide and growing range of Bayesian regression models. In Section
4, a case study dealing with measures of chronic widespread pain (Cieza et al., 2004;
Gertheiss et al., 2011a) will be discussed, in which we make extensive use of monotonic
effects. We end with a conclusion in Section 5. Some short mathematical proofs about the
properties of monotonic effects are presented in the Appendix.

2 Monotonic Effects

A predictor which we want to model as monotonic must be integer valued. The
integers may represent, for instance, count data, discrete points in time, or categories of an
ordinal variable. Since the latter is possibly the most relevant use case in psychology and
related disciplines, we speak of predictor categories in the following to refer to the values of a
monotonic predictor. As opposed to a continuous predictor, predictor categories are not
assumend to be equidistant with respect to their effect on the response variable. Instead, the
distance between adjacent predictor categories is estimated from the data and may vary
across categories. This is realized by parameterizing as follows: One parameter, b, takes care
of the direction and size of the effect similar to an ordinary regression parameter, while an

additional parameter vector, $\boldsymbol{\zeta}$, estimates the normalized distances between consecutive predictor categories. For a single monotonic predictor, \boldsymbol{x} , the corresponding predictor term η_n of observation n looks as follows:

$$\eta_n = b \sum_{i=1}^{x_n} \zeta_i \tag{1}$$

For notational convenience, we define $\sum_{i=1}^{0} \zeta_i = 0$. The parameter b can take on any 108 real value, while ζ is a simplex, which means that is it satisfies $\zeta_i \in [0,1]$ and $\sum_{i=1}^C \zeta_i = 1$ 109 with C being the number of categories (highest possible integer). If the monotonic effect is 110 used in a linear model and the lowest category of x is 0, b can be interpreted as the expected 111 difference between the highest and the lowest category of x, while ζ_i describes the expected 112 difference between the categories i and i-1 in the form of a proportion of the overall 113 difference b. Thus, the above parameterization emits an intuitive interpretation while 114 guaranteeing the monotonicity of the effect (see Appendix A for a formal proof). For 115 notational convenience we define $mo(x, \zeta) = \sum_{i=1}^{x} \zeta_i$ and call mo() the monotonic transform. 116 As visualized in Figure 1, we can understand monotonic effects as implying a piecewise linear 117 curve of which all components have the same sign. In a simple linear model, monotonic 118 effects are equivalent to categorical isotonic regression (see Appendix A). 119

Interaction terms including a monotonic predictor \boldsymbol{x} can be canonically written as

$$\eta_n = b \, z_n \, \operatorname{mo}(x_n, \boldsymbol{\zeta}_x) \tag{2}$$

where z is another predictor. If z is monotonic as well, then z_n is simply replaced by mo (z_n, ζ_z) . One modeling choice to be made is whether different terms including x should have the same or different simplex parameters associated with x. For example, a predictor term consisting of the main effects and two-way interaction between a monotonic predictor x and an arbitrary predictor z could be formulated as

$$\eta_n = b_1 z_n + b_2 \operatorname{mo}(x_n, \zeta_{xb_2}) + b_3 z_n \operatorname{mo}(x_n, \zeta_{xb_3}),$$
(3)

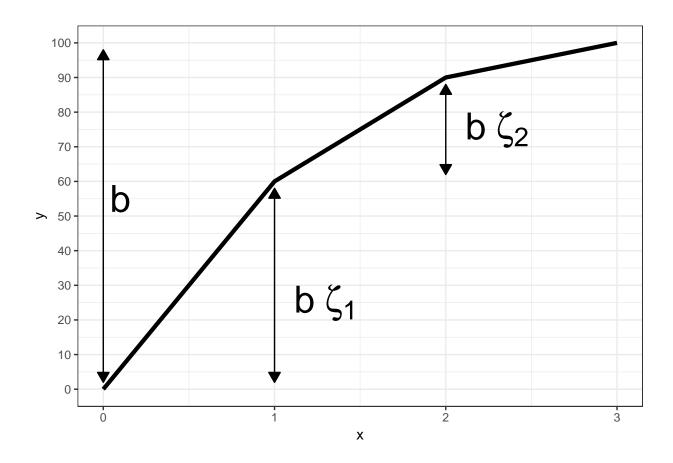


Figure 1. Visualization of a monotonic effect with four categories. Parameters were set to b = 100 and $\zeta = (0.5, 0.3, 0.2)$.

where ζ_{xb_2} and ζ_{xb_3} are two independent simplex parameters. Under this formulation, 126 \boldsymbol{x} may not necessarily be conditionally monotonic for all values of \boldsymbol{z} (see Appendix A for a 127 counter example). Rather the monotonicity being modeled depends on the chosen 128 parameterization. For instance, if the predictor z is dummy coded as 0 and 1 representing 129 the two categories of a dichotomous variable, the formulation above models the effect of x to be monotonic for category 0 as well as for the *change* between category 1 and 0. Conversely, 131 when using cell mean coding rather than dummy coding for z, the model assumes a different 132 monotonic effect of x for both categories of z. In the latter case, x is conditionally 133 monotonic on z. If we fix all simplex parameters corresponding to the same monotonic 134 variable x to the same value, conditionally monotonicty is achieved in general (proof 135

provided in Appendix A):

Proposition 2.1. Let η be an arbitrary linear predictor term containing the monotonic predictor x with the corresponding simplex parameter ζ being the same for all terms including x. Then η is monotonic in x conditionally on all possible combinations of all other predictor variables.

While fixing all simplex parameters associated with \boldsymbol{x} to the same vector quarantees conditional monotonicity, it may be not flexible enough for many common situations. For instance, if one wanted to model different monotonic effects for two groups, it would imply the shape (ζ) of the predictions to be the same across groups with just their total range (b) to be different. As explained in Section 3, in brms we make use of both parameterizations (varying and constant ζ) at different places in the package.

2.1 Monotonic effects in a Bayesian framework

The present paper describes monotonic effects as embedded in a fully Bayesian framework. We consider every statistical models a Bayesian model if it quantifies the uncertainty in all observed and unobserved variables by means of probabilities. This is often expressed in terms of Bayes' Theorem, which states that the posterior distribution $p(\theta|y)$ of the model parameters θ given the data y can be expressed in terms of the product of likelihood $p(y|\theta)$ and prior distribution $p(\theta)$ as well as a normalizing constant p(y):

$$p(\theta|y) = \frac{p(y|\theta)p(\theta)}{p(y)} \tag{4}$$

A thorugh introduction to Bayesian statistics is outside the scope of the present paper.

Instead, we refer to well established text books such as McElreath (2016), Kruschke (2014),
and Gelman et al. (2013).

With respect to monotonic effects, a fully Bayesian framework has two main implications. First, such a framework allows to incorporate monotonic effects in a large class

of regression models without the need to develop any problem specific estimators. Second, it implies that we can think of prior distributions for b and ζ . Such prior distributions enable us to incorporate information, which does not come directly from data in terms of the likelihood contribution, such as expert knowledge or findings from previous studies.

Priors for b can be derived based on the a-priori expectation regarding the differences 163 between highest and lowest category, which we call maximal difference in the following. Any 164 family of prior distributions typically applied to regression coefficients can be applied on b, as well. As a weakly-informative prior for b, we can understand any location shift 166 distribution – such as a normal of student-t distribution – centered around zero and with a scale parameter large enough to allow for large but plausible maximal differences, while 168 penalizing unplausibly large maximal differences. This scale will necessarily depend on the 169 scale of the response distribution and also on the range of the monotonic predictor. 170 Alternatively, one may use an improper flat prior that treats all real values as being equally 171 likely a-priori in the hope that the data alone is sufficient to identify b. We will come back to 172 this in the discussion of our case study. 173

Setting a prior on the simplex parameter ζ requires a different approach. The

canonical prior of a simplex parameter is the Dirchlet distribution, a multivariate

generalization of the beta distribution (Frigyik, Kapila, & Gupta, 2010). It is non-zero for all

valid simplexes (i.e., for ζ with $\zeta_i \in [0,1]$ and $\sum_{i=1}^{C} \zeta_i = 1$) and zero otherwise. The Dirichlet

prior has a single parameter vector α of the same length as ζ . Its density is defined as

$$f(\zeta|\alpha) = \frac{1}{B(\alpha)} \prod_{i=1}^{C} \zeta_i^{\alpha_i - 1}, \tag{5}$$

where $B(\alpha)$ is a normalizing constant. As the a-priori expectation of ζ_i is given by $w_i = \mathbb{E}(\zeta_i) = \alpha_i/\alpha_0$, with $\alpha_0 = \sum_{i=1}^C \alpha_i$, higher values of α_i in comparison to the sum over α imply higher a-priori values of ζ_i . Moreover, the higher the sum over α , the higher the certainty in each of the proportions w_i .

In the absense of any problem specific information, a reasonable default prior on ζ

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would surely be one that assumed all differences between adjacent categories to be the same 184 on average while being considerably uncertain about this expectation. Such a prior would 185 imply, on average, a linear trend but with enough uncertainty to allow for all other possible 186 monotonic trends as well. The Dirichlet prior with a constant $\alpha = 1$ puts equal probability 187 on all valid simplex and can thus be understood as the multivariate generalization of the 188 uniform prior on simplexes. Since we have $w_i = 1/C$, this prior centers ζ around a linear 189 trend with large uncertainty and thus appears to be a good default prior in the absense of 190 any problem specific information. 191

2.2 Penalizing larger changes between categories

In a Bayesian framework, larger differences between adjacent categories can naturally be penalized by means of priors on b and ζ . If we expect the total effect b to be small, we can use a zero-centered prior on b with comparatively small tails. For instance, if we expect b to be between -10 and 10 with probability 95% as well as higher probability for values closer to zero, we can use a Normal(0,5) prior. The straightforward logic behind this prior is that the normal distribution has approximately 95% probability between -2 and 2 standard deviations around its mean.

When it comes to the shape of the monotonic effect, we have to take a closer look at the prior on ζ . As discussed above, a constant vector α of the Dirichlet prior on ζ implies a linear trend in expectation. In other words, for constant α , the prior means of all changes ζ_i between adjacent categories are the same. The higher the sum over α , the higher the certainty in that expectation. Thus, if we expect a linear trend with some certainty, we assign all elements of α to the same value a. To get an intuition about what is a reasonable value for a, we may use the standard deviation of the elements ζ_i , which can be computed as

$$SD(\zeta_i) = \sqrt{\frac{\alpha_i(\alpha_0 - \alpha_i)}{(\alpha_0^2(\alpha_0 + 1))}}.$$
 (6)

Although the standard deviation is an imperfect measure of variability for the Dirichlet

distribution as the latter is not symmetric in general, we still believe the former to be helpful in better understanding the implications of ones chosen priors. For the default of a = 1 and a total of C = 5 categories, we get a rather large standard deviation of $SD(\zeta_i) = 0.19$. If we set, for example, a = 5, we get $SD(\zeta_i) = 0.09$ and thus much higher certainty in changes of equal size.

Of course, the process of increasing α on average works equally well even if we do not expect all changes to be the same a-priori. For instance, if C=5 and we expect a 3-times larger change between the first two categories than between all the other categories with some certainty, we may set $\alpha = (9, 3, 3, 3)$. As a result, we get $w_1 = 1/2$ and $w_i = 1/6$ else. As standard deviations, we get $SD(\zeta_1) = 0.11$ and $SD(\zeta_i) = 0.09$ else.

Alternatively, and perhaps favorably, we can directly plot the marginals of the Dirichlet 218 distribution. These marginal priors are known to be beta distributions with shape parameters $s_1 = \alpha_i$ and $s_2 = \alpha_0 - \alpha_i$. For $\alpha = (9, 3, 3, 3)$, the marginal distributions of ζ are 220 exemplified in Figure 2. All of the above approaches to better understand the Dirichlet prior 221 have in common that they ignore the dependencies between elements of ζ . More precisely, 222 elements of ζ are always negatively correlated as an increase in one element needs to be 223 reflected in a decrease in the other elements to satisfy the sum-to-one constraint. A possible 224 solution would be to plot the multivariate density of the Dirichlet prior, but this will become 225 increasingly hard for higher dimensional ζ (i.e., for variables with more than three 226 categories) and so we do not illustrate this approach in the present paper. 227

3 Implementation in brms

The brms package (Bürkner, 2017b, 2017a) provides an interface to fit Bayesian
generalized (non-)linear multilevel models using Stan (Carpenter et al., 2017; Stan
Development Team, 2017), which is a C++ package for performing full Bayesian inference
(see also http://mc-stan.org/). It supports a wide range of distributions, allowing users to fit
among others – linear, count data, survival, response times, ordinal, zero-inflated, and even

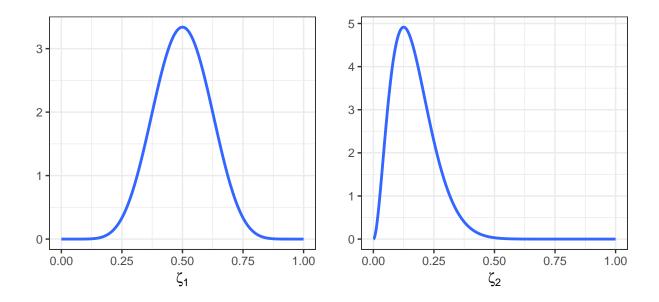


Figure 2. Densities of marginal priors of ζ_1 and ζ_2 for $\boldsymbol{\alpha}=(9,3,3,3)$. The marginal priors of ζ_3 and ζ_4 are in this case identical to the one of ζ_2 .

234 self-defined mixture models all in a multilevel context.

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In brms, monotonic effects are fully integrated into the formula syntax, which builds on and extends standard R formula syntax as well as the multilevel formula syntax initially created for the lme4 package (Bates, Mächler, Bolker, & Walker, 2015). Monotonic predictors can be used like any other predictor variable and, with respect to the formula syntax, behave like a numeric predictor. Suppose the response variable y is predicted by a monotonic variable x and a non-monotonic variable z (i.e., a continuous or categorical variable). Then the corresponding model formula is

$$y \sim mo(x) + z$$

Modeling both main effects and interaction of x and z can be achieved by

```
y \sim mo(x) * z
```

Depending on whether **z** is a continuous or categorical variable, this will imply a
different predictor term, which is fully determined by and thus consistent with the basic R

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formula syntax. If z is monotonic as well, then z is simply replaced by mo(z). Please note that for models including interactions with monotonic variables, brms will use different simplex parameters for different terms of the same monotonic variable (e.g., for the main effect of x and the interaction of x and z). This results is much greater modeling flexibility as explained in the former section.

An especially well developed feature of brms is its multilevel formula syntax allowing to model, for instance, hierarchically nested data structures such as multiple observations per person in a longitudinal study. Suppose we wanted to fit a monotonic effect *per* person in a multilevel model, then we could specify this as follows:

$y \sim mo(x) + (mo(x) \mid person)$

The mo(x) term outside the brackets denotes the average monotonic effect across 254 persons, while the (mo(x) | person) term indicates that the difference between the 255 individual monotonic effects per person and the average effect should be modeled as well (for 256 more details on the brms formula syntax see Bürkner (2017a)). For this parameterization to 257 make sense in combination with monotonic effects, we treat the shape (i.e., the simplex 258 parameter ζ) as constant across persons and only vary the size and direction of the effect 259 (i.e, b) as varying across persons. This restricts the flexibility of the model but results in 260 much more stable estimates and less convergence problems in particular if the number of observations per person (or more generally, per level of the grouping factor) is small. 262

4 Case study: Measures of chronic widespread pain

To illustrate the application of monotonic effects in practice, we will reanalyse data used to validate measures of chronic widespread pain (CWP) from patients' point of view (Cieza et al., 2004; Gertheiss et al., 2011a). There is not universially accepted definition of CWP, but "it may be characterized by pain involving several regions of the body, which causes problems in functioning, psychological distress, poor quality of sleep or difficulties in

daily life" (Gertheiss et al., 2011a, p. 378). The applied CWP measures are coming from the international classification of functioning (ICF; Organization, 2001) and are rated by clinical staff not by patients themselves. Thus, it is important to validate which and to what degree CWP measures actually relate to subjective physical health in order to better understand their implications for patients' life.

For each of the 420 patients, the present data contains information on 67 CWP
measures as well as a subjective measure of physical health based on the SF-36 questionnaire
(Ware & Sherbourne, 1992). The data is freely available in the R package "ordPens"
(Gertheiss, 2015) and is explained in detail in Gertheiss et al. (2011a) and Cieza et al.
(2004). In the data set, the variable of subjective physical health is called phcs while the
CWP measures are named according to their offical ICF coding (see Gertheiss et al., 2011a
for explanation).

In our first model, we will predict the subjective physical health (variable phcs) only
by the impairments in "walking" (variable d450) and "moving around" (variable d455),
which were both measured on a five point scale between 0 ("no problem") and 4 ("complete
problem"). Both of these variables were strong predictors of phcs in the analysis of
Gertheiss et al. (2011a). The category labels of these variables suggest that their
relationship with phcs will be monotonic. More specifically, we expect the subjective
physical health to decrease with an increase in impairments in "walking" or "moving around"
or basically any other everyday functioning.

For the present example – and for most other data sets we have seen so far – the
default priors of brms on monotonic effects work well in terms of sampling efficiency and
convergence. However, for illustrationary purposes, we still manually specify our own priors
for each model if even priors are similar to the default ones. Based on knowledge about the
outcome scale, it is unlikely that any WCP measure across its full range will influence the
subjective physical health by more than 20 points. We code this expectation as a
Normal(0, 10) prior on the size parameters b. That way, |b| will only exceed 10 and 20

outcome points with probabilities of roughly 32% and 5%, respectively. With regard to the 296 shape of the effects, we have no particular prior expectations and thus assume a uniform 297 Dirichlet prior as explained in Section 2.1, which is also the default in brms. When 298 specifying the Dirichlet prior for "walking", we have to take into account that the highest 299 category 4 ("complete problem") is actually not present in the data set (we will see how to 300 solve the problem of missing extreme categories later on). Thus, the corresponding prior 301 requires a vector of reduced size. In brms, we can specify the above priors by means of the 302 following code: 303

```
library(brms)
prior1 <- prior(normal(0, 10), class = "b") +
    prior(dirichlet(1, 1, 1), class = "simo", coef = "mod4501") +
    prior(dirichlet(1, 1, 1, 1), class = "simo", coef = "mod4551")</pre>
```

We use class simo to refer to the simplex parameters of monotonic effects. The required coefficient names "mod4501" and "mod4551" are constructed as mo<variable><index>,
where <index> = 1 unless a single regression term contains multiple simplexes – which only happens for interactions of monotonic effects. Finally, we fit the model in brms via

```
fit1 <- brm(phcs \sim mo(d450) + mo(d455), data = cwp, prior = prior1)
```

As illustrated in Figure 3, both predictors show a strong negative relationship to subjective physical health. Moreover, these relationships are clearly (at least visually) non-linear. For impairments in walking, for instance, changes in the outcome are strongest between the first two categories implying that the most subjective physical health is lost as soon as any problems in walking occur. This impression is confirmed by the summary estimates of the simplex parameters (see Table 1).

We can also show this non-linearity using model comparison. First, we fit a linear

model with the same predictors via

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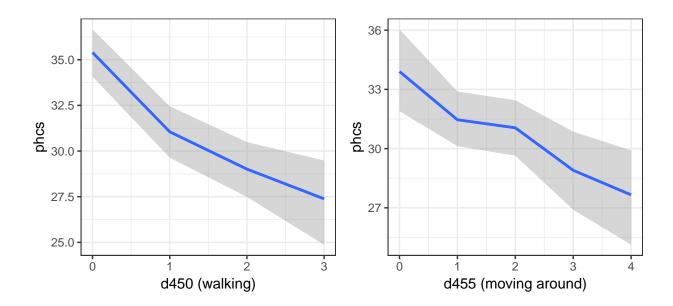


Figure 3. Effects of impairments in walking and moving around on subjective physical health as estimated by model fit1.

```
prior2 <- prior(normal(0, 2.5), class = "b")
fit2 <- brm(phcs ~ d450 + d455, data = cwp, prior = prior2)</pre>
```

and then compute model weights, for instance, by means of the WAIC (Watanabe, 2010):

```
model_weights(fit1, fit2, weights = "waic")
```

This yields a weight of 92% for the monotonic model, again providing evidence that a linear model may be too restrictive to adequately describe the relationship between impairments in walking or moving around and subjective physical health.

In the original study of Gertheiss et al. (2011a) on this data set, the purpose was to select a subset of the total of 67 CWP measures that are related to subjective physical health in a relevant manner. For the purpose of the present case study, we also aim at a form of variable selection but with a somewhat different focus. As most CWP measures show small to medium correlations with at least a few other CWP measures, we expect only few of them

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Table 1 Summary of estimated simplexes for impairments in walking and moving around.

	walking			moving around		
	Estimate	l-95% CI	u-95% CI	Estimate	l-95% CI	u-95% CI
simo[1]	0.54	0.33	0.78	0.39	0.14	0.66
simo[2]	0.26	0.05	0.49	0.07	0.00	0.23
simo[3]	0.20	0.01	0.43	0.35	0.06	0.64
simo[4]				0.19	0.01	0.48

to have a considerable non-zero effect on subjective physical health after controlling for all 326 other measures. For simplicity, we are not including "environmental factor" variables into our analysis as they were measured on a different scale (from -4 "complete barrier to 4 'complete facilitator") as all the other variables (from 0 "no problem" to 4 "complete problem").

This leaves us with a total of 51 predictors, which is still quite a lot to estimate for a 330 data set containing 420 observations, in particular because of rather high intercorrelations of 331 predictors. For this reason, we impose some regularization on the size parameters b by 332 applying the regularized horseshoe prior (Carvalho, Polson, & Scott, 2009; Piironen & 333 Vehtari, 2016; Piironen, Vehtari, & others, 2017). This prior has very fat tails and an infinite 334 spike at zero which results in close-to-zero coefficients to be shrunken to zero, while greater 335 coefficients located in the tails of the prior remain largely unchanged. Thus, the horseshoe 336 prior can be used to guide variable selection (Piironen et al., 2017). There are a lot of 337 options to tune the horseshoe prior, but for the purpose of the present case study, we will only use the par ratio argument. With this argument, we can formalize our prior 339 expectation about the number of non-zero effects, which we will set to 10%, that is roughly 5 340 of the total 51 predictors. The smaller par ratio, the stronger the shrinkage towards zero. 341 In brms, we can specify this prior as follows:

prior3 <- prior(horseshoe(par ratio = 0.1), class = "b")</pre>

Before we actually fit the model, we add an artifical row to our data set which contains
the maximal value (4) for each of the predictor variables and a missing value (NA) for the
subjective physical health measure phcs. This ensures that all size parameters are on the
same scale even if the maximal category was not actually present in the data set, as we had
seen above for impairments in walking. The model including 51 CWP measures as
monotonic predictors is then set up via

fit3 <- brm(phcs | mi() ~ ..., data = cwp, prior = prior3)</pre>

The mi() term on the left-hand side of the formula ensures that the newly added row with a missing value in phcs is actually included in the model, as otherwise it would just have been removed during the data preparation step. The right-hand side abbreviated above as actually contains separate mo() terms for the 51 included CWP measures, which we did not write out due to the length of that expression.

As illustrated in Figure 4, only few predictors have an effect that deviates from zero in 354 a relevant manner after applying regularization of the horseshoe prior. Most notably, these 355 are impairments in "walking" (d450) and "moving around (d455), but also in 'community 356 life" (d910) and "sensation of pain" (b280), which all seem to have a negative effect on 357 subjective physical heath after controlling for all other predictors. This does not necessarily 358 imply that other predictors have no additional predictive value. To better better understand 359 the latter, different variable selection techniques – for instance those explained in Gertheiss 360 et al. (2011a) – may be favorable. 361

Similar to what we did before, we can compare fit of the monotonic model to a corresponding linear model on which we apply the horseshoe prior as well. Performing model comparison by means of the WAIC yields a weight of 94% for the monotonic model, which thus seems to perform better than its linear counterpart even though most of the predictors

actually have an effect very close to zero (see Figure 4). Intuitively, one may expect that
monotonic effects tend to overfit the data in such a case as they have much more parameters
than linear effects. However, this is not what actually happens. If the size parameter b is
close to zero, there is not much to learn about the corresponding simplex parameter ζ , which
will thus have a posterior distribution close to its prior. Still, this uncertainty will not lead to
overfitting as changes in ζ do not influence predictions as long as b is small. In other words, a
monotonic predictor with a close to zero effect naturally reduces to a simple linear predictor.

5 Conclusion

In the present paper, we introduced a principled approach to including ordinal 374 predictors in regression models, which we called *monotonic effects*. In simple cases, they 375 coincide with estimates provided by isotonic regression while allowing to penalize larger 376 changes between adjacent categories via prior distributions. Thus, monotonic effects 377 naturally combine important ideas of existing methods for modeling ordinal predictors. 378 Moreover, monotonic effects nicely integrate into the framework of generalized linear regression and can even be used together with multilevel structures. They are fully supported in the brms R package, which fits Bayesian regression models using Stan and provides an 381 intuitive user interface based on widely known R formula syntax. To date, ordinal predictors 382 are still mostly treated as either nominal or metric thus under- or overestimating the 383 contained information. Monotonic effects avoid these problems but still allow for an intuitive 384 interpretation of the estimated parameters. In summary, we hope that monotonic effects can 385 solve some longstanding problems in the treatment of ordinal predictors. 386

Monotonic effects have been implemented in brms for about two years at the time of writing this paper, which allowed us (and users of brms) to get a reasonable amount of experience with their behavior. From what we have seen in our own data sets and what users reported, sampling efficiency and convergence were good and rarely much worse that when using a purely categorical or linear approach. This is notable insofar, as elements of a

simplex tend to be negatively correlated, sometimes rather strongly, thus making MCMC
sampling more difficult. The fact that this has not been a major issue – at least from our
experience – may be largely due the advanced Hamiltonian Monte-Carlo samplers
implemented in Stan, which are designed to work well even for highly inter-correlated
posteriors (Betancourt, Byrne, Livingstone, & Girolami, 2014; Hoffman & Gelman, 2014).

For simple cases such as regression models with only a single monotonic effect and 397 normally distributed errors, maximum likelihood estimators can be developed as well 398 (Barlow et al., 1972; Robertson et al., 1988). However, we believe them to be of limited 399 practical applicability since the supported models were necessarily of far less complexity as 400 compared to what can be fitted right away in a fully Bayesian framework. Moreover, 401 computing uncertainty estimates for simplex parameters in a frequentist framework is 402 naturally difficult as for finite data, the distribution of their estimators are not necessarily 403 sufficiently normal. This is true in particular for elements of the simplex that come close to 404 the naturally lower or upper boundaries (0 or 1) of the simplex. Thus, any confidence 405 interval constructed based on approximate standard errors will likely be inappropriate in 406 many cases. For these reasons, we chose not to investigate the frequentist properties of 407 monotonic effects any further in the present paper.

Although our primary focus was the use of monotonic effects for modelling strictly 400 ordinal predictors, we want to point out that monotonic effects may be applied to other 410 kinds of discrete variables, as well. Such variables may represent, for instance, count data or 411 discrete points in time. As an example for the former, we can think of participants solving a 412 sequence of figural analogy tasks with the value of interest being the number of tasks solved correctly. This count variable could then be used as predictor of a general intelligence score. 414 It is plausible to assume the number of correctly solved items to be monotonically related to 415 general intelligence and so the applications of a monotonic effect appears reaonsable. As an 416 example for the latter, we could think of a longidutional study with few measurement points. 417 If the outcome was a skill gradually aquired over time, we would expect time to be 418

- 419 monotonically related to it. Of course, time may also be modeled as continuous, but for very
- 420 few time points, using a monotonic effect may be a more reliable solution without strong
- assumptions outside of monotonicity.

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515 Appendix

516 Appendix A: Mathematical Proofs

Proof. (Monotonicity) For all values x between 0 and C-1, we have

$$\eta(x+1) - \eta(x) = b \sum_{i=1}^{x+1} \zeta_i - b \sum_{i=1}^{x} \zeta_i = b\zeta_{x+1}.$$
 (7)

Since $\zeta_{x+1} > 0$, the linear predictor $\eta(x)$ is monotonically increasing if $b \geq 0$ and

monotonically decreasing if $b \leq 0$.

Proof. (Equivalence to categorical isotonic regression) Consider a simple linear model of a continuous response y regressed on a categorical predictor x with categories $j \in \{0, ..., C\}$. Further, let μ_j be the group mean of category j with respect to the response variable. Then the model for observation n can be written as

$$y_n = \mu_{x_n} + e_n, \tag{8}$$

where e_n are errors of the regression. In categorical isotonic regression, we estimate $\mu = (\mu_0, ..., \mu_C)$ under the order-constraint $\mu_0 \le \mu_1 \le ... \le \mu_C$ or $\mu_0 \ge \mu_1 \ge ... \ge \mu_C$. Using a monotonic effect, we write:

$$y_n = b_0 + b_1 \sum_{i=1}^{x_n} \zeta_i + e_n. \tag{9}$$

Hence, we can identify μ_0 with b_0 and μ_j with $b_0 + b_1 \sum_{i=1}^{j} \zeta_i$ for j > 0. This identification is bijective within the set of order-constraint μ .

Proof. (Proposition 2.1) Under the stated assumptions, we can without, loss of generality, write the linear predictor $\eta = \eta(x)$ as

$$\eta(x) = b_0 + \sum_{i=1}^K b_i \operatorname{mo}(x, \zeta) = b_0 + \left(\sum_{i=1}^K b_i\right) \operatorname{mo}(x, \zeta).$$
 (10)

Since all other predictors have been fixed to some constants, their contribution to η can be absorbed by the intercept b_0 and the regression coefficients b_1 to b_K which are all related to

x. If we define $b_x = \sum_{i=1}^K b_i$ we see that $\eta(x)$ is monotonic in x with the sign of the effet determined by the sign of b_x .

Proof. (Counter example to conditional monotonicity for varying simplex parameters)

Consider the situation shown in Figure 5, where quite clearly, the effect of \boldsymbol{x} is monotonic for group a, but non-monotonic for group b. Suppose further that we named the grouping variable \boldsymbol{z} and aplied dummy coding such that a=0 and b=1. Using different simplex parameters for the main effect of \boldsymbol{x} and the interaction effects between \boldsymbol{x} and \boldsymbol{z} , the linear predictor reads as follows:

$$\eta(x,z) = b_1 z + b_2 \, \operatorname{mo}(x, \zeta_{xb_2}) + b_3 z \, \operatorname{mo}(x, \zeta_{xb_3})$$
(11)

For group a this results in $\eta(x,0) = b_2 \mod(x, \zeta_{xb_2})$ so that $b_2 = 100$ as well as $\zeta_{xb_2} = (0.8, 0.2)$ are completely defined by the curve of group a. For group b, we have

$$\eta(x,1) = b_1 + b_2 \operatorname{mo}(x, \zeta_{xb_2}) + b_3 \operatorname{mo}(x, \zeta_{xb_3}).$$
(12)

As the curve of group b starts at the origin, we have $b_1 = 0$. Due to the chosen parameterization of \boldsymbol{z} , the term $b_3 \operatorname{mo}(x, \boldsymbol{\zeta}_{xb_3})$ models the difference between in the effect of \boldsymbol{x} between the two groups, which visualized as a dashed line in Figure 5 and is clearly monotonic. Consequently, we have $b_3 = 60$ and $\boldsymbol{\zeta}_{xb_3} = (\frac{1}{6}, \frac{5}{6})$. Although the assumptions of the monotonic effects are fully met, the effect of \boldsymbol{x} in group b is non-monotonic. Thus, \boldsymbol{x} is not conditionally monotonic given \boldsymbol{z} .

549

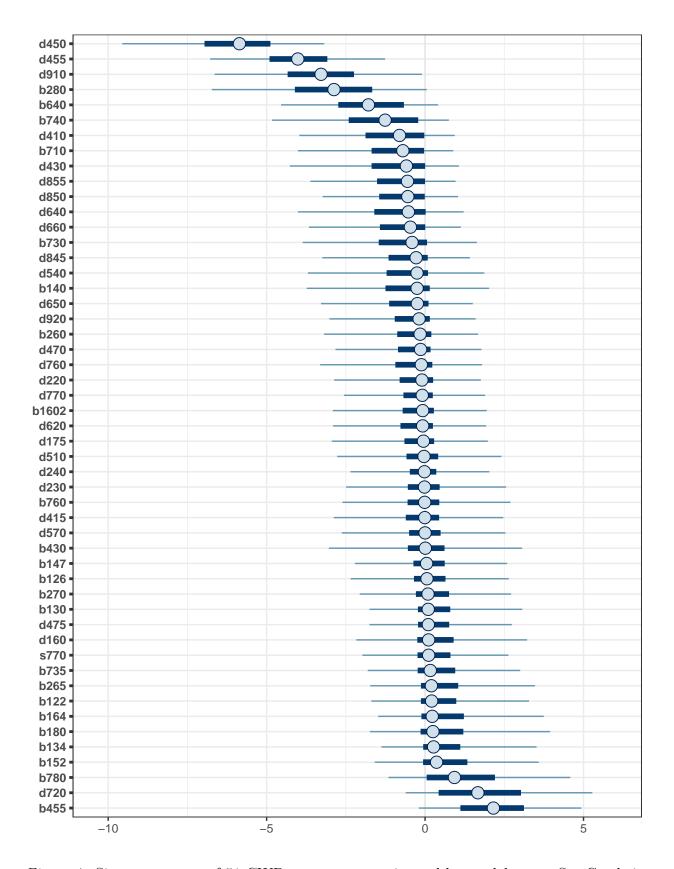


Figure 4. Size parameters of 51 CWP measures as estimated by model fit3. See Gertheiss et al. (2011a) for details on the variable names.

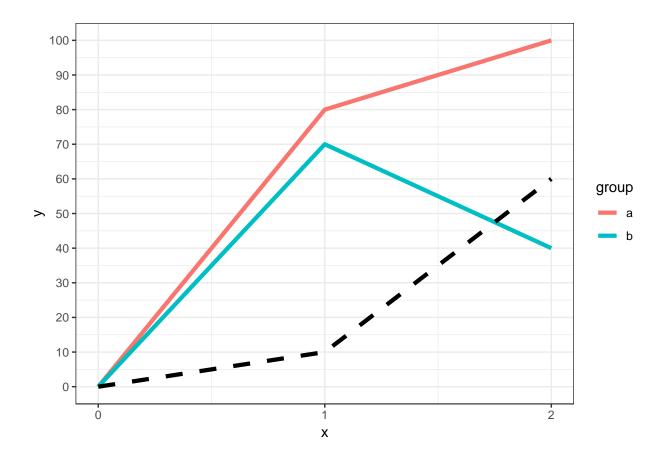


Figure 5. Counter example to the conditional monotonicity for varying simplex parameters. The dashed line shows the difference between the groups a and b as a function of x.