

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

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Abstract

Ordinal predictors are commonly used in regression models. However, they are often incorrectly treated as either nominal or metric thus under- or overestimating the contained information. This is understandable insofar as generally applicable solutions or corresponding statistical software are still underdeveloped. We propose a new way of parameterizing regression coefficients of ordinal predictors, which we call monotonic effects. The reparameterization is done in terms of a scale parameter b representing the direction and size of the effect and a simplex parameter ζ modeling the normalized differences between categories. This ensures that predictions increase or decrease monotonically, while changes between adjacent categories may vary across categories. This formulation generalizes to 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 is plausible. Using Stan, we developed a Bayesian estimation method for monotonic effects, which also allows to incorporate prior information and to check the assumption of monotonicity. We have implemented this method in the R package brms, so that fitting monotonic effects in a fully Bayesian framework is now straightforward.

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

Over the last few decades, a substantial amount of statistical research has been devoted to handling ordinal response variables in regression models starting with the seminal paper of McCullagh (1980; see also Agresti, 2010; Bürkner and Vuorre, 2018; Liu and Agresti, 2005;

Tutz, 2011 for an overview). In Psychology, for instance, this kind of data is omnipresent in the form of Likert scale items, which are often treated as continuous out of convenience without ever testing this assumption (Liddell & Kruschke, 2017). With researchers realizing the 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 R (R Core Team, 2018), for instance, several packages are available to fit ordinal models, among others “ordinal” (Christensen, 2018), “VGAM” (Yee, Stoklosa, Huggins, & others, 2015), or “brms” (Bürkner, 2017; Bürkner, 2018) to name the perhaps most general ones.

Ordinal *predictors* seem to have received less attention in statistical research. In R, for instance, the standard treatment of ordinal predictors is still to compute orthogonal polynomials on their integer representations to model linear, quadratic, cubic, etc. terms of the predictors (Chambers, Hastie, & others, 1992). We believe this approach to be suboptimal for various reasons, most notably because it assumes the ordinal categories to be equidistant, which is clearly an oversimplification, and because it yields parameter estimates that are hard to interpret. Apart from that, there are only two lines of research known to the authors of the present paper. One is a penalized regression approach specifically designed for ordinal predictors (Gertheiss, 2014; Gertheiss & Oehrlein, 2011; Gertheiss & Tutz, 2009) and the other are categorical types of isotonic regression (Barlow, Bremner, Brunk, & Bartholomew, 1972; Robertson, Wright, & Dykstra, 1988).

We begin by explaining the former approach. The main idea of the method proposed by 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 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 of the ordinal variable. Depending on the research question and variables under study, this 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* concerns itself with regression models subject to order constraints (Barlow et al., 1972; Robertson et al., 1988). For instance, in some contexts, the effect of a drug may be assumed to be monotonically¹ increasing with an increasing dose – an assumption that we often want to “hard-code” into our models. Depending on the research question and nature of the variable on which we want to impose a monotonicity constraint, different techniques may be more favorable. If the variable is essentially continuous, such as the dose of a drug, we can use parametric functions which are known to be monotonic (e.g., the log or logistic functions in simple cases) or use semi-parametric approaches such as monotonic splines (Kelly & Rice, 1990; Lee, 1996; Leitenstorfer & Tutz, 2007; Pya & Wood,

¹The 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.

2015). If the variable under study is categorical, the monotonicity assumption reduces to an ordering constraint on the group means with respect 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 and Robertson, 1982; Lee, 1981; Wu, Woodroffe, and Mentz, 2001). For the purpose of studying ordinal predictors, we are primarily interested in the categorical type of isotonic regression.

The idea and scope of the two approaches discussed 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 & Oehrlin, 2011). 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 different sets of assumptions which both reflect important aspects of ordinal variables. As we will see later on, we may even combine both aspects (i.e., restricting the direction and penalizing the size of changes) 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 interpret 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 as 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, 2017; Bürkner, 2018), 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., 2011) will be discussed, in which we make extensive use of monotonic effects. We end with a discussion in Section 5. Mathematical proofs about the properties of monotonic effects are presented in the Appendix.

1 Monotonic Effects

A predictor which we want to model as monotonic must have discrete values in an ordered set, which are coded as integers. The integer value 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, in the following, we are going to concentrate on this example of an application for a monotonic predictor. We are going to refer to the values of such a variable as predictor categories. As opposed to a continuous predictor, predictor categories are not assumed 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 , represents the direction and size of the

93 effect similar to an ordinary regression parameter, while an additional parameter vector, ζ ,
 94 estimates the normalized distances between consecutive predictor categories. For a single
 95 monotonic predictor variable, \mathbf{x} , with $x_n \in \{0, \dots, D\}$ (i.e., with a lowest possible value of
 96 zero²), the corresponding predictor term η_n of observation n looks as follows:

$$\eta_n = b D \sum_{i=1}^{x_n} \zeta_i \quad (1)$$

97 For notational convenience, we define $\sum_{i=1}^0 \zeta_i = 0$. The parameter b can take on any
 98 real value, while ζ is a simplex, which means that it satisfies $\zeta_i \in [0, 1]$ and $\sum_{i=1}^D \zeta_i = 1$
 99 with D being the highest possible integer value that \mathbf{x} can take on. Since we start counting
 100 at zero, D is equal to the number of differences between two adjacent categories and also
 101 equal to the total number of categories minus one. If the monotonic effect is used in a
 102 linear model, b can be interpreted as the expected average difference between two adjacent
 103 categories of \mathbf{x} , while ζ_i describes the expected difference between the categories i and $i - 1$ in
 104 the form of a proportion of the overall difference between lowest and highest categories. Thus,
 105 this parameterization has an intuitive interpretation while guaranteeing the monotonicity of
 106 the effect (see Appendix A for a formal proof). For notational convenience we define

$$\text{mo}(x, \zeta) = D \sum_{i=1}^x \zeta_i \quad (2)$$

107 and call $\text{mo}()$ the *monotonic transform*. As visualized in Figure 1, we can understand
 108 monotonic effects as implying a piecewise linear curve of which all components have the
 109 same sign. In a simple linear model, monotonic effects are equivalent to categorical isotonic
 110 regression (see Appendix A for a proof).

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

$$\eta_n = b z_n \text{mo}(x_n, \zeta_x) \quad (3)$$

112 where \mathbf{z} is another predictor. If \mathbf{z} is monotonic as well, then z_n is simply replaced by
 113 $\text{mo}(z_n, \zeta_z)$. One modeling choice to be made is whether different terms including \mathbf{x} should
 114 have the same or different simplex parameters associated with \mathbf{x} . For example, a predictor
 115 term consisting of the main effects and two-way interaction between a monotonic predictor
 116 \mathbf{x} and an arbitrary predictor \mathbf{z} could be formulated as

$$\eta_n = b_1 z_n + b_2 \text{mo}(x_n, \zeta_{xb_2}) + b_3 z_n \text{mo}(x_n, \zeta_{xb_3}), \quad (4)$$

²Note that this convention differs of the one customarily used in statistical software, where indices of vectors, matrices, etc. usually start at one. However, starting at zero simplifies the notation of monotonic effects and so we adopt this approach in the present paper.

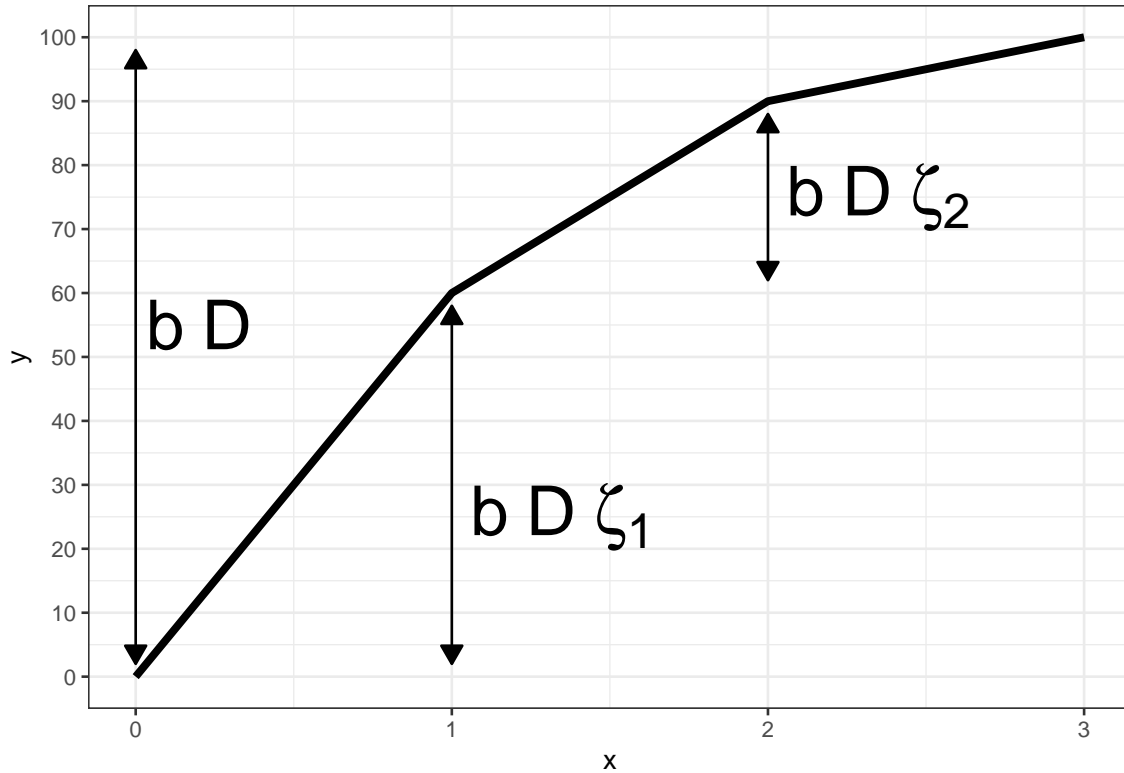


Figure 1. Visualization of a monotonic effect with four categories. Parameters were set to $b = 100/3$ and $\zeta = (0.6, 0.3, 0.1)$.

where ζ_{xb_2} and ζ_{xb_3} are two simplex parameters. Under this formulation, \mathbf{x} may not necessarily be conditionally monotonic for all values of \mathbf{z} (see Appendix A for a counter example). Rather the monotonicity being modeled depends on the chosen parameterization.

For instance, if the predictor \mathbf{z} is dummy coded as 0 and 1 representing the two categories of a dichotomous variable, the formulation above models the effect of \mathbf{x} to be monotonic for category 0 as well as for the *change* between category 1 and 0. Conversely, when using cell mean coding rather than dummy coding for \mathbf{z} , the model assumes a different monotonic effect of \mathbf{x} for both categories of \mathbf{z} . In the latter case, \mathbf{x} is conditionally monotonic on \mathbf{z} . If we fix all simplex parameters corresponding to the same monotonic variable \mathbf{x} to the same value, conditionally monotonicity is achieved in general (proof provided in Appendix A):

Proposition 1. *Let η be an arbitrary linear predictor term containing the monotonic predictor \mathbf{x} with the corresponding simplex parameter ζ being the same across all terms including \mathbf{x} . Then η is monotonic in \mathbf{x} conditionally on all possible combinations of all other predictor variables.*

While fixing all simplex parameters associated with \mathbf{x} to the same vector guarantees conditional monotonicity, it may be too restrictive for many common situations. For instance, if one wanted to model different monotonic effects for two groups, it would imply the shape

135 (ζ) of the predictions to be the same across groups with just their total range (b) to be
 136 different. As explained in Section 3, in brms we make use of both parameterizations (varying
 137 and constant ζ) at different places in the package.

138 1.1 Monotonic effects in a Bayesian framework

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

$$p(\theta|y) = \frac{p(y|\theta)p(\theta)}{p(y)} \quad (5)$$

146 A thorough introduction to Bayesian statistics is outside the scope of the present
 147 paper. Instead, we refer to well established text books such as McElreath (2016), Kruschke
 148 (2014), and Gelman et al. (2013).

149 With respect to monotonic effects, a fully Bayesian framework has two main impli-
 150 cations. First, such a framework allows to incorporate monotonic effects in a large class
 151 of regression models without the need to develop any problem-specific estimators. Second,
 152 it implies that we can think of prior distributions for b and ζ . Such prior distributions
 153 enable us to incorporate information, which does not come directly from data in terms of
 154 the likelihood contribution, such as expert knowledge or findings from previous studies.

155 Priors for b can be derived based on the *a priori* expectation regarding the *average*
 156 *difference* between adjacent categories. Any family of prior distributions typically applied to
 157 regression coefficients can be applied on b , as well. As a weakly-informative prior for b , we
 158 can understand any location shift distribution – such as a normal or student-t distribution –
 159 centered around zero and with a scale parameter large enough to allow for large but plausible
 160 average differences, while penalizing implausibly large differences. This scale will necessarily
 161 depend on the scale of the response distribution and also on the range of the monotonic
 162 predictor. Alternatively, one may use an improper flat prior that treats all real values as
 163 being equally likely *a priori* in the hope that the data alone is sufficient to identify b . We
 164 will return to this in the discussion of our case study.

165 Setting a prior on the simplex parameter ζ requires a different approach. The canonical
 166 prior of a simplex parameter is the Dirichlet distribution, a multivariate generalization of
 167 the beta distribution (Frigyik, Kapila, & Gupta, 2010). It is non-zero for all valid simplexes
 168 (i.e., for ζ with $\zeta_i \in [0, 1]$ and $\sum_{i=1}^D \zeta_i = 1$) and zero otherwise. The Dirichlet prior has a
 169 single parameter vector α of the same length as ζ . Its density is defined as

$$f(\boldsymbol{\zeta}|\boldsymbol{\alpha}) = \frac{1}{B(\boldsymbol{\alpha})} \prod_{i=1}^D \zeta_i^{\alpha_i-1}, \quad (6)$$

where $B(\boldsymbol{\alpha})$ is a normalizing constant (Balakrishnan, 2014). As the *a-priori* expectation of ζ_i is given by $w_i = \mathbb{E}(\zeta_i) = \alpha_i/\alpha_0$, with $\alpha_0 = \sum_{i=1}^D \alpha_i$, higher values of α_i in comparison to the sum over $\boldsymbol{\alpha}$ imply higher *a priori* values of ζ_i . Moreover, the higher the sum over $\boldsymbol{\alpha}$, the higher the certainty in each of the proportions w_i .

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

1.2 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 $\boldsymbol{\zeta}$. 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 $\text{Normal}(0, 5)$ prior. The logic behind this choice is straightforward as 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 $\boldsymbol{\zeta}$. As discussed above, a constant vector $\boldsymbol{\alpha}$ of the Dirichlet prior on $\boldsymbol{\zeta}$ implies a linear trend in expectation. In other words, for constant $\boldsymbol{\alpha}$, the prior means of all changes ζ_i between adjacent categories are the same. The higher the sum over $\boldsymbol{\alpha}$, the higher the certainty in that expectation. Thus, if we expect a linear trend with some certainty, we assign all elements of $\boldsymbol{\alpha}$ 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 (see Balakrishnan, 2014):

$$\text{SD}(\zeta_i) = \sqrt{\frac{\alpha_i(\alpha_0 - \alpha_i)}{(\alpha_0^2(\alpha_0 + 1))}}. \quad (7)$$

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 one's chosen priors. For the default of $a = 1$ and a total of $D = 5$ categories, we get a rather large standard deviation of $\text{SD}(\zeta_i) = 0.19$. If we

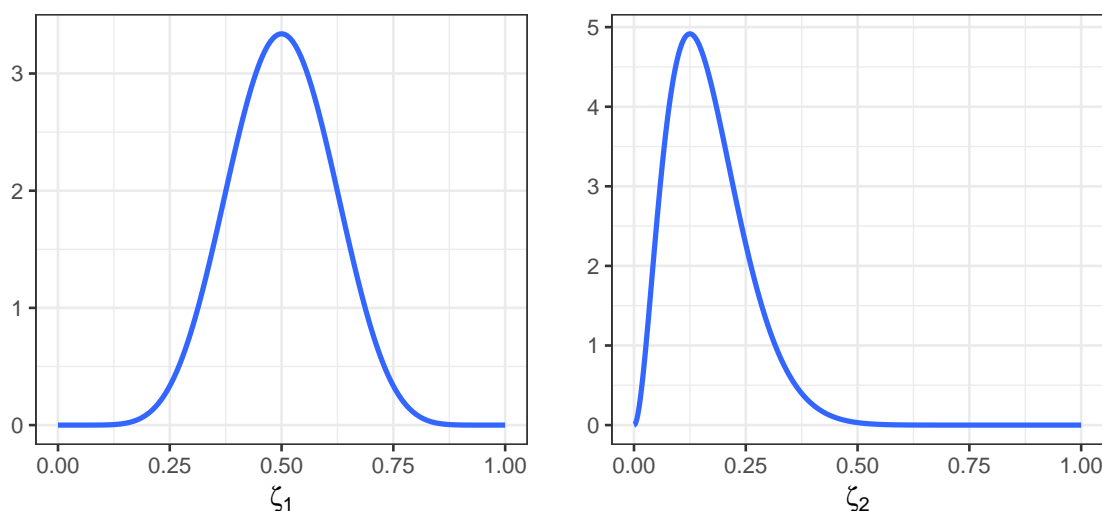


Figure 2. Densities of marginal priors of ζ_1 and ζ_2 for $\alpha = (9, 3, 3, 3)$. The marginal priors of ζ_3 and ζ_4 are in this case identical to the one of ζ_2 .

set, for example, $a = 5$, we get $\text{SD}(\zeta_i) = 0.09$ 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 $D = 5$ 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 else $w_i = 1/6$. As standard deviations, we get $\text{SD}(\zeta_1) = 0.11$ and $\text{SD}(\zeta_i) = 0.09$ else.

Alternatively, and perhaps favorably, we can directly plot the marginals of the Dirichlet distribution. These marginal priors are known to be beta distributions with shape parameters $s_1 = \alpha_i$ and $s_2 = \alpha_0 - \alpha_i$ (Balakrishnan, 2014). For $\alpha = (9, 3, 3, 3)$, the marginal distributions of ζ are exemplified in Figure 2. All of the above approaches to better understand the Dirichlet prior have in common that they ignore the dependencies between elements of ζ . More precisely, elements of ζ are always negatively correlated as an increase in one element needs to be reflected in a decrease in the other elements to satisfy the sum-to-one constraint. A possible solution would be to plot the multivariate density of the Dirichlet prior, but this will become more difficult for higher dimensional ζ (i.e., for variables with more than three categories) and so we do not illustrate this approach in the present paper.

2 Implementation in brms

The brms package (Bürkner, 2017; Bürkner, 2018) provides an interface to fit Bayesian generalized (non-)linear (multilevel) regression 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,

226 and even self-defined mixture models all in a multilevel context.

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

```
y ~ mo(x) + z
```

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

```
y ~ mo(x) * z
```

235 Depending on whether z is a continuous or categorical variable, this will imply a
 236 different predictor term, which is fully determined by and thus consistent with the basic
 237 R formula syntax. If z is monotonic as well, then z is simply replaced by $mo(z)$. Please
 238 note that for models including interactions with monotonic variables, brms will use *different*
 239 simplex parameters for different terms of the same monotonic variable (e.g., for the main
 240 effect of x and the interaction of x and z). This results in much greater modeling flexibility
 241 as explained in the former section.

242 The variable which should be modeled as monotonic may either be integer valued or
 243 an ordered factor. In the latter case, the ordered factor will be transformed to an integer
 244 variable with the lowest factor level being identified with zero as described above.

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

```
y ~ mo(x) + (mo(x) | person)
```

249 The $mo(x)$ term outside the brackets denotes the *average* monotonic effect across per-
 250 sons, while the $(mo(x) | person)$ term indicates that the *difference* between the individual
 251 monotonic effects per person and the average effect should be modeled as well (for more
 252 details on the brms formula syntax see Bürkner (2018)). For this parameterization to make
 253 sense in combination with monotonic effects, we treat the shape (i.e., the simplex parameter
 254 ζ) as constant across persons and only vary the size and direction of the effect (i.e., b) as
 255 varying across persons. This restricts the flexibility of the model but results in much more
 256 stable estimates and less convergence problems in particular if the number of observations
 257 per person (or more generally, per level of the grouping factor) is small.

3 Case study: Measures of chronic widespread pain

To illustrate the application of monotonic effects in practice, we will reanalyze data used to validate measures of chronic widespread pain (CWP) from patients' point of view (Cieza et al., 2004; Gertheiss et al., 2011). There is not universally 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., 2011, p. 378). The applied CWP measures stem 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. (2011) 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 official ICF coding (see Gertheiss et al., 2011 for explanation). Our fully reproducible analysis is available on OSF (<https://osf.io/kvrsg/>).

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. (2011). 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 illustrative purposes, we still manually specify our own priors for each model even if 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 $\text{Normal}(0, 10)$ 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 shape of the effects, we have no particular prior expectations and thus assume a uniform Dirichlet prior as explained in Section 2.1, which is also the default in brms. When specifying the Dirichlet prior for "walking", we have to take into account that the highest category 4 ("complete problem") is actually not present in the data set (we will see how to solve the problem of missing extreme categories later on). Thus, the corresponding prior requires a vector of reduced size. In brms, we can specify the above priors by means of the following code:

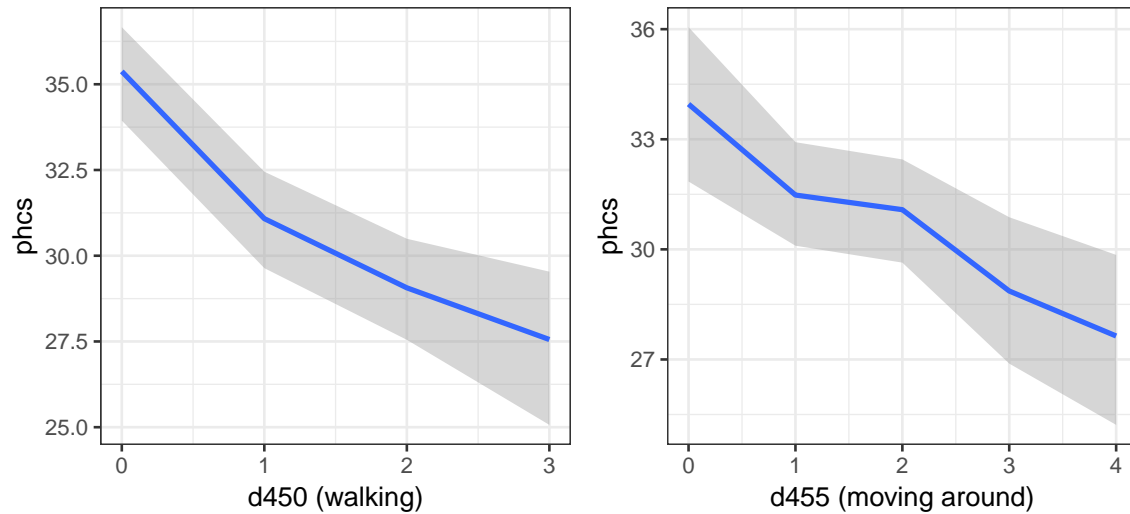


Figure 3. Effects of impairments in walking and moving around on subjective physical health as estimated by model fit1.

```
library(brms)
prior1 <- prior(normal(0, 2.5), class = "b") +
  prior(dirichlet(1, 1, 1), class = "simo", coef = "mod4501") +
  prior(dirichlet(1, 1, 1, 1), class = "simo", coef = "mod4551")
```

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 is only the case for interactions of monotonic effects. Finally, we fit the model in brms via

```
fit1 <- brm(phcs ~ 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

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

and then compute model weights, for instance, by means of the stacking of posterior-predictive distribution (Yao, Vehtari, Simpson, & Gelman, 2017)³:

³In a Bayesian framework, models may be compared by various means for instance Bayes factors (Kass

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]	0.55	0.33	0.79	0.39	0.14	0.64
simo[2]	0.26	0.04	0.50	0.07	0.00	0.24
simo[3]	0.19	0.01	0.42	0.35	0.07	0.64
simo[4]				0.19	0.01	0.48

```
model_weights(fit1, fit2, weights = "loo2")
```

This yields a weight of 96% 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. (2011) 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 to have a considerable non-zero effect on subjective physical health after controlling for all 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 data set containing 420 observations, in particular because of rather high inter-correlations of predictors. For this reason, we impose some regularization on the size parameters b by applying the *regularized horseshoe* prior (Carvalho, Polson, & Scott, 2009; Piironen & Vehtari, 2016; Piironen, Vehtari, & others, 2017). This prior has very fat tails and an infinite spike at zero which results in close-to-zero coefficients to be shrunken to zero, while greater coefficients located in the tails of the prior remain largely unchanged. Thus, the horseshoe prior can be used to guide variable selection (Piironen et al., 2017). There are a lot of 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 expectation about the number of non-zero effects, which we will set to 10%, that is roughly 5 of the total 51 predictors. The smaller `par_ratio`, the stronger the shrinkage towards zero. In brms, we can specify this prior as follows:

& Raftery, 1995), (approximate) cross-validation methods (Vehtari, Gelman, & Gabry, 2017), information criteria (Vehtari et al., 2017; Watanabe, 2010) or stacking of posterior-predictive distributions (Yao et al., 2017). A discussion of the pros and cons of these various approaches is outside the scope of the present paper.

```
prior3 <- prior(horseshoe(par_ratio = 0.1), class = "b")
```

Before we actually fit the model, we add an artificial 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)
```

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 a relevant manner after applying regularization of the horseshoe prior. Most notably, these are impairments in “walking” (`d450`) and “moving around” (`d455`), but also in “community life” (`d910`) and “sensation of pain” (`b280`), which all seem to have a negative effect on subjective physical health after controlling for all other predictors. This does not necessarily imply that other predictors have no additional predictive value. To better understand the latter, different variable selection techniques – for instance those explained in Gertheiss et al. (2011) – may be favorable.

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 stacking of posterior-predictive distributions (Yao et al., 2017) yields a weight of 74% 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 considerably 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, the complexity of a monotonic predictor with a close to zero effect naturally reduces to the complexity of a simple linear predictor.

4 Discussion

In the present paper, we introduced a principled approach to including ordinal predictors in regression models, which we call *monotonic effects*. In simple cases, they coincide with estimates provided by isotonic regression while allowing to penalize larger changes between adjacent categories via prior distributions. Thus, monotonic effects naturally combine

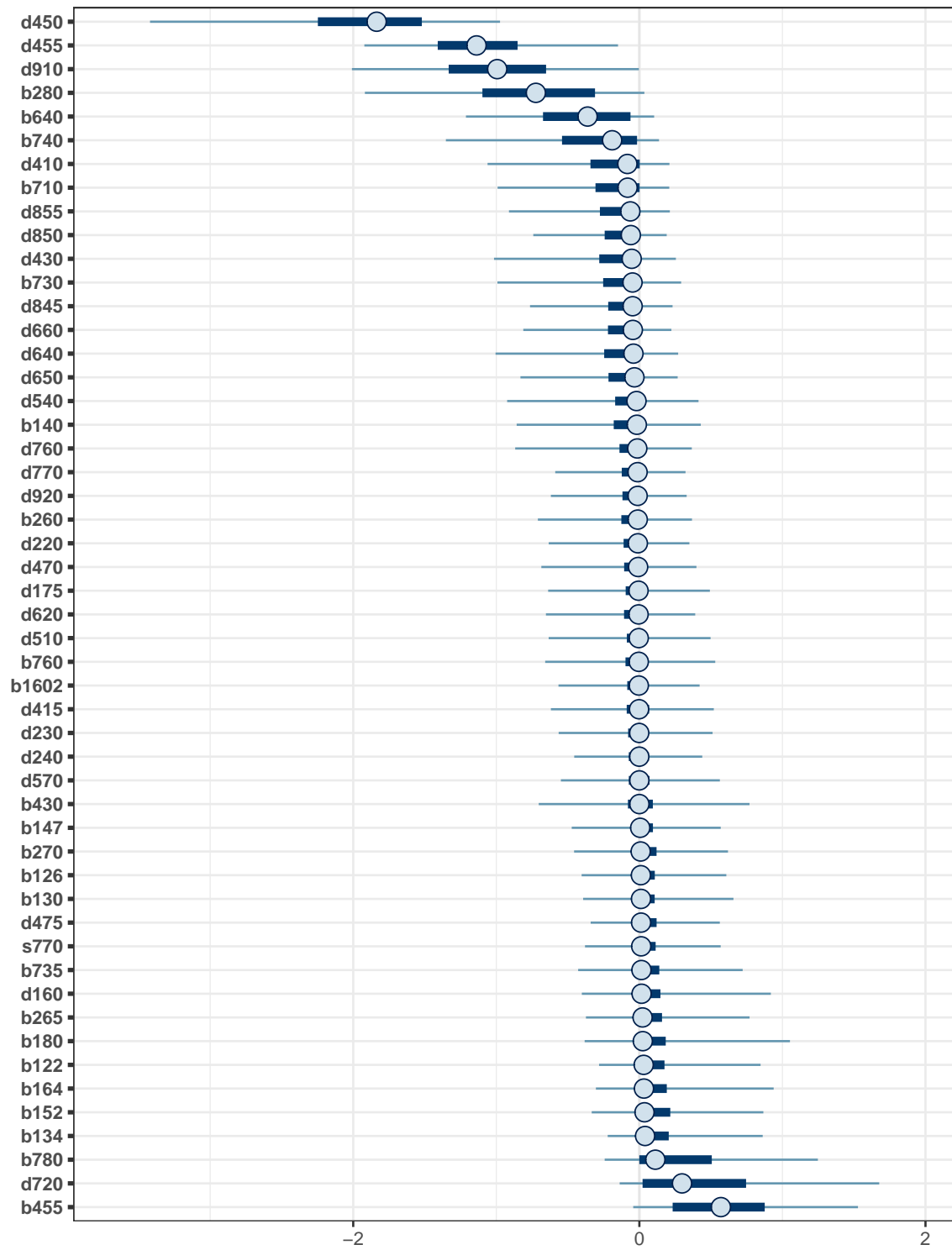


Figure 4. Size parameters of 51 CWP measures as estimated by model fit3. See Gertheiss et al. (2011) for details on the variable names.

important ideas of existing methods for modeling ordinal predictors. Moreover, monotonic effects nicely integrate into the framework of generalized linear regression and can even be used in combination with multilevel structure. By making an informed decision about the parameterization of interactions with monotonic effects, different kinds of monotonicity can be modeled depending on the research question and a-priori information available. Monotonic effects are fully supported in the `brms` R package, which fits Bayesian regression models using Stan and provides an intuitive user interface based on widely known R formula syntax. To date, ordinal predictors are still mostly treated as either nominal or metric thus under- or overstating the contained information. Monotonic effects avoid these problems but still allow for an intuitive interpretation of the estimated parameters. In summary, we hope that monotonic effects can solve some longstanding problems in the treatment of ordinal predictors.

Although our primary focus was the use of monotonic effects for modeling strictly ordinal predictors, we want to point out that they may be applied to other kinds of discrete variables, as well. Such variables may represent, for instance, count data or discrete points in time. As an example for the former, we can think of participants solving a 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. It is plausible to assume the number of correctly solved items to be monotonically related to general intelligence and so the applications of a monotonic effect appears reasonable. As an example for the latter, we could think of a longitudinal study with few measurement points. If the outcome was a skill gradually acquired over time, we would expect time to be monotonically related to it. Of course, time may also be modeled as continuous, but for very few time points, using a monotonic effect may be a more reliable solution without strong assumptions outside of monotonicity.

One potential problem in the Bayesian estimation of monotonic effects is that elements of a simplex tend to be negatively correlated, sometimes rather strongly, thus making MCMC sampling more difficult (Hoffman & Gelman, 2014). However, due to 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), these problems may be alleviated when fitting monotonic effects in Stan – either directly or indirectly through `brms`. Indeed, in the models estimated for the purpose of this paper and more generally in the last two years since implementing monotonic effects in `brms`, sampling efficiency and convergence were good and rarely worse than when using a purely categorical or linear approach. Still, we cannot rule out that in some edge cases or very complex models, convergence problems may occur due to the chosen parameterization of monotonic effects.

For simple cases such as regression models with only a single monotonic effect and normally distributed errors, maximum likelihood estimators can be developed as well (Barlow et al., 1972; Robertson et al., 1988). As we prefer a fully Bayesian approach to statistical modeling, we did not dive deeper into this direction. However, we still believe that developing frequentist estimators and corresponding uncertainty estimates for more complex monotonic models including, for instance, interactions or multilevel structure, may be a worthwhile

endeavor for future research.

Although we focused on the modeling of discrete variables, the general idea of monotonic effects also generalizes to continuous data. In this case, the sum in the definition of monotonic effects becomes an integral and ζ a non-negative function to be integrated over. A similar idea is used in I-splines (i.e., integral splines) whose basis functions represent integrals over the non-negative basis functions of another spline (Ramsay, 1988). In future research, it may thus be worthwhile to study continuous versions of monotonic effects and to relate them to existing methods (e.g., Ramsay, 1988; Pya & Wood, 2015) that ensure monotonicity in the continuous case.

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Appendix

Appendix A: Mathematical Proofs

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

$$\eta(x + 1) - \eta(x) = bD \sum_{i=1}^{x+1} \zeta_i - bD \sum_{i=1}^x \zeta_i = bD \zeta_{x+1}. \quad (8)$$

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

Proof. (Equivalence to categorical isotonic regression) Consider a simple linear model of a continuous response y regressed on a categorical predictor x with categories $j \in \{0, \dots, D\}$. 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

$$y_n = \mu_{x_n} + e_n, \quad (9)$$

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

$$y_n = b_0 + b_1 D \sum_{i=1}^{x_n} \zeta_i + e_n. \quad (10)$$

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

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

$$\eta(x) = b_0 + \sum_{k=1}^K b_k D_k \sum_{i=1}^x \zeta_i = b_0 + \left(\sum_{k=1}^K b_k D_k \right) \left(\sum_{i=1}^x \zeta_i \right). \quad (11)$$

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

Proof. (Counter example to conditional monotonicity for varying simplex parameters) Consider the situation shown in Figure 5, where quite clearly, the effect of \mathbf{x} is monotonic for group G , but non-monotonic for group H . Suppose further that we named the grouping variable \mathbf{z} and applied dummy coding such that $G = 0$ and $H = 1$. Using different simplex

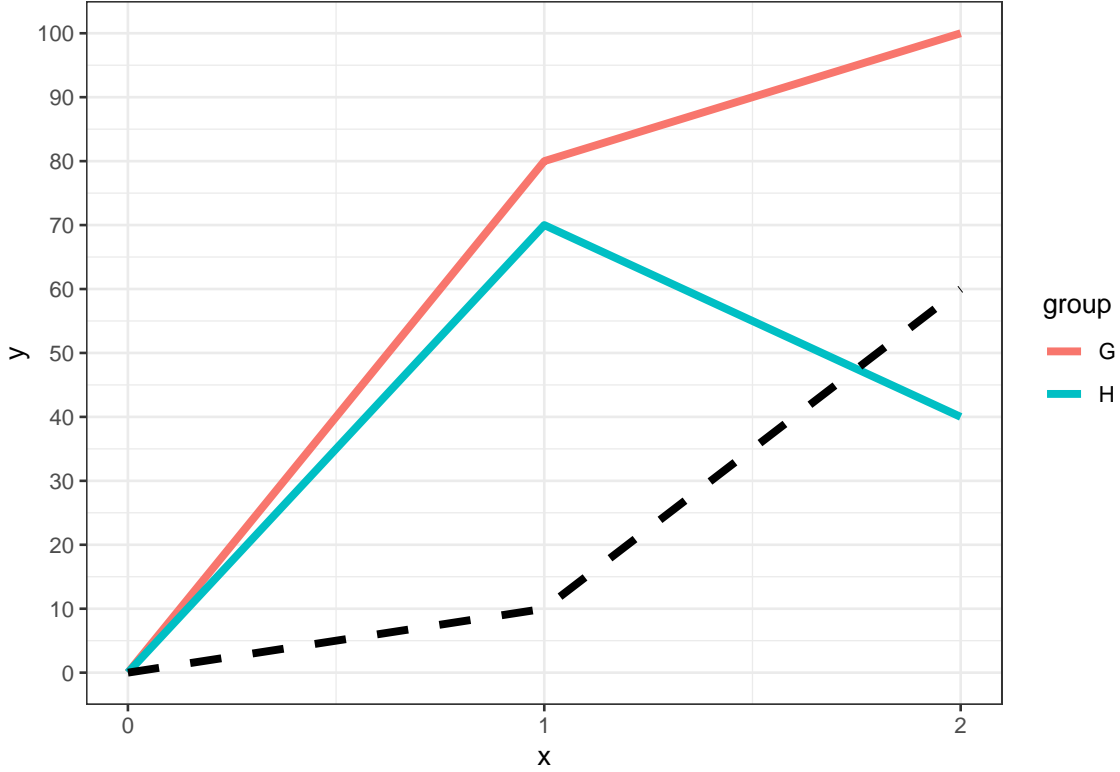


Figure 5. Counter example to the conditional monotonicity for varying simplex parameters. The dashed line shows the difference between the groups a and b as a function of x .

parameters for the main effect of x and the interaction effects between x and z , the linear predictor reads as follows:

$$\eta(x, z) = b_1 z + b_2 \text{mo}(x, \zeta_{xb_2}) + b_3 z \text{mo}(x, \zeta_{xb_3}) \quad (12)$$

For group G this results in $\eta(x, 0) = b_2 \text{mo}(x, \zeta_{xb_2})$ so that $b_2 = 50$ as well as $\zeta_{xb_2} = (0.8, 0.2)$ are completely defined by the curve of group G . For group H , we have

$$\eta(x, 1) = b_1 + b_2 \text{mo}(x, \zeta_{xb_2}) + b_3 \text{mo}(x, \zeta_{xb_3}). \quad (13)$$

As the curve of group H starts at the origin, we have $b_1 = 0$. Due to the chosen parameterization of z , the term $b_3 \text{mo}(x, \zeta_{xb_3})$ models the *difference* between in the effect of x between the two groups, which visualized as a dashed line in Figure 5 and is clearly monotonic. Consequently, we have $b_3 = 30$ and $\zeta_{xb_3} = (\frac{1}{6}, \frac{5}{6})$. Although the assumptions of the monotonic effects are fully met, the effect of x in group H is non-monotonic. Thus, x is not conditionally monotonic given z .

□