Penalized Non-Linear Principal Components Analysis for Ordinal Variables with an Application to International Classification of Functioning Core Sets

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Abstract

Ordinal data occur frequently in the social sciences. When applying principal components analysis (PCA), however, those data are often treated as numeric implying linear relationships between the variables at hand, or non-linear PCA is applied where the obtained quantifications are sometimes hard to interpret. Non-linear PCA for categorical data, also called optimal scoring/scaling, constructs new variables by assigning numerical values to categories such that the proportion of variance in those new variables that is explained by a predefined number of principal components is maximized. We propose a penalized version of non-linear PCA for ordinal variables that is an intermediate between standard PCA on category labels and non-linear PCA as used so far. The new approach is by no means limited to monotonic effects, and offers both better interpretability of the non-linear transformation of the category labels as well as better performance on validation data than unpenalized non-linear PCA and/or standard linear PCA. In particular, an application of penalized non-linear PCA to ordinal data as given with the International Classification of Functioning, Disability and Health (ICF) is provided.

Keywords: Categorical Data, Chronic Widespread Pain, Likert-Scale, Non-Monotone Principal Components Analysis, Optimal Scaling, Smoothing

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1 Introduction

The objective of principal components analysis (PCA) is to reduce the dimension of the data observed by finding a substantially smaller set of uncorrelated linear combinations of the original variables. These linear combinations – called principal components – should explain as much of the variability in the original data as possible. If PCA is considered an inferential tool, the data at hand should follow (at least approximately) a normal distribution (cf. Jolliffe, 2002, Section 3.7). In practice, however, PCA is also widely used as a descriptive/explorative tool without making distributional assumptions such as normality. Then the methodology is applicable to a wide variety of data. Labovitz (1970) proceeds by assigning numbers to rank order categories treating them as interval scaled and demonstrates via simulations that the resulting errors can be negligible under some circumstances. Nonetheless, since the idea of (pearson) correlation is developed for data of metric nature in the first place, caution may be required when analyzing categorical data. Kolenikov et al. (2004) discuss various methods dealing with categorical data in the context of principal components analysis in an extensive simulation study. Their proposed technique of using polychoric correlations, might indeed be preferable if the statistical properties of the PCA model are of primary interest, but the method is computationally quite intensive. Korhonen and Siljamäki (1998) suggest an approach called ‘ordinal principal component analysis’ with rank correlations to be maximized between the original variables and the ordinal principal component. Again, the suggestion suffers from both high constructional and computational effort for larger data sets. Another procedure is the more established concept of non-linear PCA (Gifi, 1990; Mori et al., 2016). The basic idea of non-linear PCA is to build linear combinations of non-linear transformations of the original variables in order to further increase the variance that is explained by the first principal components.

Here we consider ordinal variables, that is, categorical variables with levels that can be reasonably ordered. Such variables are often found in the social and behavioral sciences. Though many practitioners simply treat category labels as numeric values and apply standard PCA (following the line of Labovitz (1970)), this way of analysis may still be considered questionable, since ordinal variables do not have metric scale level. Hence, variables should be treated at their appropriate measurement level to avoid overestimating the information contained. Furthermore, just as for regression analysis, situations are imaginable, in which it is reasonable to assume the relationships between the variables to be non-linear. Non-linear PCA was designed to take those considerations into account.

Non-linear PCA for categorical data constructs new variables by assigning numerical values to categories such that the proportion of variance in those new variables that is explained by the first, lets say $m$, principal components is maximized. This process is called ‘optimal quantification’, ‘optimal scaling’ or ‘optimal scoring’; cf. Linting et al. (2007) and references therein. However, while
the found transformations—the ‘quantifications’—maximize the explained variance on the data at hand, the ‘training data’, it is by no means clear that they will also work well on new data, sometimes called ‘validation data’ or ‘test data’. In fact, by simply maximizing the explained variance on the training data, the found transformations may rather account for random fluctuations in the data than for substantial non-linearity. In other words, the estimated scores tend to result in ‘overfitting’ the (training) data, which worsens the performance and generalization to new data. In addition, the obtained quantifications are sometimes erratic and thus hard to interpret. To attack those problems, in IBM SPSS Statistics (Version 25.0), for instance, there is an option available for smoothing quantifications by use of spline functions, with the number of (interior) knots being chosen by the user. On the one hand, however, smoothing by using a small and manually chosen number of knots (the default in SPSS is ‘2’) limits the type of functions that can be fitted and may be challenging for the (inexperienced) user (without further guidance on how to choose the number of knots). That is why, state-of-the-art methods for regression splines rather use a large number of basis functions/knots in combination with a smoothing penalty, and a smoothing/penalty parameter that is determined by using a specific, data-dependent criterion such as (generalized) cross-validation; see, e.g., Eilers and Marx (1996), Wood (2008, 2017). On the other hand, splines are defined on a sub-interval of \( \mathbb{R} \), whereas ordinal variables can only take some discrete values. In other words, a spline function may be seen as unnecessarily complex for scaling ordinal/discrete data.

Here, we propose a penalized version of non-linear PCA for ordinal variables that is an intermediate between standard PCA on category numbers and non-linear PCA (without smoothing) as typically used so far. Also, the discrete nature of ordinal data is taken into account. Specifically, we utilize the idea of second-order penalties presented in Gertheiss and Oehrlein (2011) and Gertheiss et al. (2021) in the context of regression with ordinal predictors. The new approach offers both better interpretability of the non-linear transformations (i.e., the scoring/quantification rules) as well as better performance on validation data than unpenalized non-linear PCA and/or standard linear PCA. Also, our implementation provides the option of both non-monotone effects and incorporating constraints enforcing monotonicity, as the latter assumption is reasonable for some practical applications. Based on a related idea of penalizing large differences between adjacent categories, Bürkner and Charpentier (2020) proceeded from a Bayesian point of view to model monotonic effects of ordered independent variables. When using penalization in the framework of PCA or explanatory factor analysis, literature has so far typically been on shrinking loadings towards zero to avoid the drawbacks of the usual hard-threshold approach; see, e.g., Zou et al. (2006), Jin et al. (2018).

A representative example for ordinal variables is the so-called International Classification of Functioning, Disability and Health (ICF; WHO, 2001) core set.
for chronic widespread pain (CWP). Besides observed levels of the 67 ICF variables, the data set at hand (Cieza et al., 2004; Gertheiss and Oehrlein, 2011) also provides a physical health component summary measure, originally constructed from the SF-36 questionnaire by standard, linear PCA (McHorney et al., 1993). The proposed penalized, non-linear PCA seems promising to allow a more intuitive way to derive the overall health condition in an unsupervised fashion directly from the ICF data.

The remainder of the paper is organized as follows. Section 2 provides insights into optimal scaling and the proposed penalized fitting algorithm. Some illustrative simulation studies in Section 3 examine the quality of the proposed methodology under the presence and even absence of monotonicity. In Section 4, we consider the ICF case study dealing with measures of CWP; also, further results are presented on another publicly available data set (Jouvent et al., 1988). In Section 5 we conclude with a discussion. All computations were done using the statistical program R (R Core Team, 2021). To ensure reproducibility, the algorithm together with evaluation on publicly available data as given above is made accessible through R add-on package ordPens (Gertheiss and Hoshiyar, 2021).

2 Penalized Principal Components Analysis

Before introducing our approach for penalized non-linear PCA with ordinal variables, we will first shortly review standard linear PCA and optimal scaling for categorical variables. For proofs and mathematical derivations on principal components, we refer to Jolliffe (2002), as a more detailed introduction to linear PCA would lie beyond the scope of the present work. For background on non-linear PCA and its alternating algorithm, see Kuroda et al. (2013). If particularly interested in interpreting non-linear PCA models, we refer to Linting et al. (2007).

2.1 Linear PCA and Optimal Scaling

As usual in multivariate statistics, we assume that the observed data matrix $X$ has entries $(X)_{ij} = x_{ij}$ denoting the value of the $j$th variable observed at the $i$th subject, $j = 1, \ldots, p, i = 1, \ldots, n$. Furthermore, we assume that variables are centered and scaled to have unit variance. Then, the empirical covariance/correlation matrix is given by $R = n^{-1}X^\top X$. Our goal is to extract the important information from the correlated data, i.e., to achieve dimension reduction with as little loss of information as possible.

The idea of principal components analysis is to find linear combinations $y_r = Xa_r$ that are uncorrelated, i.e., $y_r^\top y_s = 0$ for $r \neq s$. In addition, the variation in the original data that is explained by the first $m$ principal components $a_1, \ldots, a_m$
should be as large as possible. This means
\[
\sum_{r=1}^{m} y_r^\top y_r \sum_{j=1}^{p} x_j^\top x_j
\]
has to be maximized, with \( x_j = (x_{1j}, \ldots, x_{nj})^\top \) and \( m < p \). As the numerator depends not only on the directions but also on the lengths of the vectors \( a_r \), those \( a_r \) are restricted to have unit length, i.e., \( a_r^\top a_r = 1 \) for all \( r \). To ensure uncorrelated scores \( y_r \) and \( y_s \), we further have \( a_r^\top a_s = 0 \) for \( r \neq s \). This (constrained) optimization problem is solved by the first \( m \) eigenvectors \( a_1, \ldots, a_m \) of correlation matrix \( R \), e.g., using singular value decomposition (SVD) of \( X \). Alternatively, the optimum is found by eigenvalue decomposition of matrix \( R \). Here, we follow the former representation in accordance with \( \text{R function stats::prcomp} \), which is also part of our algorithm’s implementation. Then, \( X \) can be decomposed as follows:
\[
X = UDV^\top,
\]
with \( U \) and \( V \) being the left and right singular vectors of \( X \), respectively, where the columns of \( V \) correspond to eigenvectors \( a_r \). Matrix \( D \) contains the square roots of eigenvalues \( \nu_r \), sorted decreasingly.

With ordinal variables, matrix \( X \) (before standardizing) contains only integers 1, 2, \ldots, with entry \( x_{ij} \) indicating the level of the \( j \)th variable that is observed at the \( i \)th subject. As numbers 1, 2, \ldots are just class labels, linearity in these labels as assumed by usual PCA appears to be very restrictive and not necessarily the right choice for categorical data. Therefore, non-linear PCA constructs new variables by assigning numerical values to categories in terms of \( \phi_{ij} = \varphi_j(x_{ij}) \), with scaling functions \( \varphi_j : \mathbb{N} \rightarrow \mathbb{R}, j = 1, \ldots, p \). Then, standard PCA as described above is applied to the recoded variables. As before with data matrix \( X \), recoded variables are standardized to have mean zero and variance one. To find appropriate, or ‘optimal’ functions \( \varphi_j \) to use for recoding, the proportion of variance in the transformed variables that is explained by the first \( m \) principal components is maximized, with \( m \) being fixed at a certain value. For solving this optimization problem, it is useful to consider the usual principal components \( a_1, \ldots, a_m \), \( a_r = (a_{r1}, \ldots, a_{rp})^\top \), and corresponding vectors of component scores \( y_1, \ldots, y_m \), \( y_r = (y_{1r}, \ldots, y_{nr})^\top \), as the solution of the least squares problem
\[
L(Y, A) = \sum_{j=1}^{p} \sum_{i=1}^{n} \left( x_{ij} - \sum_{r=1}^{m} y_{ir} a_{rj} \right)^2 \rightarrow \min,
\]
with \( (Y)_{ir} = y_{ir}, (A)_{jr} = a_{rj}, r = 1, \ldots, m, j = 1, \ldots, p, i = 1, \ldots, n \). For non-linear PCA, criterion
\[
L(\Phi, Y, A) = \sum_{j=1}^{p} \sum_{i=1}^{n} \left( \phi_{ij} - \sum_{r=1}^{m} y_{ir} a_{rj} \right)^2
\]
is minimized as a function of matrices $A$, $Y$ and $\Phi$, with $(\Phi)_{ij} = \phi_{ij} = \varphi_j(x_{ij})$; see Linting et al. (2007). Now, $A$ and $Y$ correspond to principal components and respective scores when using the transformed variables. Scaling function $\varphi_j$ can also be represented by the vector $\theta_j = (\theta_{j1}, \ldots, \theta_{jk_j})^\top$ where $\theta_{jl}$ is the value that is assigned to category $l$ of the $j$th (categorical) variable, and $k_j$ denotes the highest level of variable $j$.

For fixed quantifications $\Phi$, $L(\Phi, Y, A)$ is minimized by the usual PCA solution on data matrix $\Phi$ (note, we just replaced $X$ by $\Phi$). For fixed $Y$ and $A$, minimization of $L(\Phi, Y, A)$ becomes a “regression problem”

$$L(\Phi, Y, A) = \sum_{j=1}^p \sum_{i=1}^n (u_{ij} - z_{ij}^\top \theta_j)^2 \longrightarrow \min,$$

with pseudo response $u_{ij} = \sum_{r=1}^m y_{ir} a_{rj}$, and $z_{ij} = (z_{ij1}, \ldots, z_{ijk_j})^\top$ being a design vector of dimension $k_j$ with entry $z_{ijl} = 1$ if at subject $i$ variable $j$ has value $l$, and zero otherwise. The complete indicator matrix is then given by $Z = (Z_1 | \ldots | Z_p)$ and

$$Z_j = (z_{ijl}) = \begin{pmatrix} z_{1j1} & \cdots & z_{1jk_j} \\ \vdots & \ddots & \vdots \\ z_{nj1} & \cdots & z_{njk_j} \end{pmatrix}.$$ If substantial reasons exist that changes between adjacent categories arise consistently negative or positive, monotonicity constraints are to be imposed. In case of monotonically increasing quantifications, for instance, this can be achieved by introducing the $((k_j - 1) \times k_j)$ difference matrix of first order $D_1$ s.t. the differences

$$D_1 \theta_j = \begin{pmatrix} -1 & 1 \\ \vdots & \ddots \\ -1 & 1 \end{pmatrix} \begin{pmatrix} \theta_{j1} \\ \vdots \\ \theta_{jk_j} \end{pmatrix} = \begin{pmatrix} \theta_{j2} - \theta_{j1} \\ \vdots \\ \theta_{jk_j} - \theta_{jk_j-1} \end{pmatrix} \geq \begin{pmatrix} 0 \\ \vdots \\ 0 \end{pmatrix}$$

are enforced to be non-negative. For finding the final solution, $\Phi$ and $\{Y, A\}$ are alternately fixed at their current value, and it is cycled through the two optimization steps until convergence. For further details on the alternating least squares (ALS) algorithm, see Young et al. (1978). In order to incorporate constraints, such as monotonic quantifications, we make use of the dual routine of Goldfarb and Idnani (1982, 1983) on solving quadratic functions under constraints, as implemented in R add-on package quadprog (Turlach et al., 2019).

### 2.2 Penalized Fitting

When $L(\Phi, Y, A)$ at (3) is minimized as a function of $\theta_1, \ldots, \theta_p$, only the nominal scale level of the variables is used (unless monotonicity constraints are set). In regression problems, it has been proposed to use special penalties to incorporate
the covariates’ ordinal scale level; see, e.g., Tutz and Gertheiss (2014, 2016) for an overview. Similar approaches can be used here. In particular, penalizing non-linearity in the coefficients as done in Gertheiss and Oehrlein (2011) seems promising. Due to the fact that categories considered here are ordered, changes between adjacent levels can be assumed to take place rather smoothly. In order to avoid abrupt jumps between levels, we hence smooth out the coefficient vector during the estimation procedure. The idea is not to minimize $L(\Phi, Y, A)$ at (3) as a function of $\theta = (\theta_1^\top, \ldots, \theta_p^\top)^\top$, but its penalized version

$$L_p(\Phi, Y, A) = \sum_{j=1}^p \sum_{i=1}^n (u_{ij} - z_{ij}^\top \theta_j)^2 + \sum_{j=1}^p \lambda_j J_j(\theta_j),$$

with $\lambda_j = \lambda(k_j - 1)$. For the penalty terms $J_j(\theta_j)$, we choose

$$J_j(\theta_j) = \sum_{l=2}^{k_j-1} ((\theta_{j,l+1} - \theta_{j,l}) - (\theta_{j,l} - \theta_{j,l-1}))^2 = \sum_{l=2}^{k_j-1} (\theta_{j,l+1} - 2\theta_{j,l} + \theta_{j,l-1})^2.$$

To be more concise, equation (5) takes the general form $J_j(\theta_j) = \theta_j^\top \Omega_j \theta_j$ with $(k_j \times k_j)$ penalty matrix $\Omega_j = D_2^\top D_2$ and $((k_j - 2) \times k_j)$ second-order difference matrix

$$D_2 = \begin{pmatrix} 1 & -2 & 1 & \cdots & \cdots & \cdots & \cdots & \cdots & 1 \\ 1 & -2 & 1 & \cdots & \cdots & \cdots & \cdots & \cdots & 1 \\ \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 1 & -2 & 1 \end{pmatrix}.$$  

By using this quadratic, second-order penalty, we penalize non-linearity in the $\theta$-coefficients that belong to the same variable.

The strength of penalization is controlled by parameter $\lambda$. With $\lambda = 0$, optimal scaling for categorical variables as described above is obtained; with $\lambda \to \infty$, coefficients are forced to be linear, which is equivalent to usual PCA using (standardized) class labels $1, 2, \ldots, k_j$ for variable $j$. With $0 < \lambda < \infty$, coefficients are non-linear but smoother than with unpenalized non-linear PCA, which makes good sense for ordinal variables, as wiggly coefficient vectors $\theta_j$ are hard to interpret. How to choose an appropriate value for $\lambda$, will be discussed in Subsection 2.3 below. Before doing so, however, to shed some light on the implementation of the final, penalized non-linear PCA approach, a brief overview of our penalized ALS algorithm is in order.

For initializing the algorithm, $X$ itself serves as initial data/quantification denoted by $\Phi^{(0)}$ (and is standardized if not already). Further let $\Phi^{(t)}$ denote the $j$th column of $\Phi$ in iteration $t$ of the algorithm, i.e., $\Phi^{(t)}$. Then, iteratively:

- **PCA step**: Calculate $A^{(t+1)}$ and $Y^{(t+1)}$ from SVD of $\Phi^{(t)}$ and update the matrix $U^{(t+1)} = Y^{(t+1)} A^{(t+1)^\top}$. 


Quantification step: Columnwise, calculate estimates \( \hat{\theta}_j^{(t+1)} \) by minimizing (4) using the entries of \( U^{(t+1)} \) obtained from the PCA step above, and subject to constraints (i) standardization/unit variance w.r.t. \( \hat{\phi}_j^{(t+1)} = Z_j \hat{\theta}_j^{(t+1)} \), and (ii) monotonicity (if so) w.r.t. \( \hat{\theta}_j^{(t+1)} \); (i) is realized by use of the estimate from the iteration before, more precisely, optimization is done subject to constraint \((\hat{\phi}_j^{(t)})^T Z_j \hat{\theta}_j^{(t+1)} = 1\), where \( \hat{\phi}_j^{(t)} \) is the (standardized) estimate from iteration \( t \). (ii) is done as described above. Update \( \hat{\phi}_j^{(t+1)} = Z_j \hat{\theta}_j^{(t+1)} \).

Once a user-specified convergence criterion has been reached, apply a final (usual) PCA to the quantified data matrix. The criterion we use is

\[
\frac{1}{np} \sum_{i=1}^{n} \sum_{j=1}^{p} (\hat{\phi}_{ij}^{(t)} - \hat{\phi}_{ij}^{(t+1)})^2 < \epsilon,
\]

where \( (\hat{\Phi}^{(t)})_{ij} = \hat{\phi}_{ij}^{(t)} \), and \( \epsilon \) is a small, positive constant such as \( \epsilon = 10^{-7} \). At this point we would like to highlight the importance of standardizing the data matrix/matrix of quantifications before applying any PCA. Otherwise, we could just assign arbitrarily large values to the levels of an arbitrary set of \( m \) variables, while setting the remaining variables to zero. Then, trivially, 100% variance would be explained by \( m \) principal components.

### 2.3 Selection of the Tuning Parameter

In the algorithm above, the penalty parameter \( \lambda \) was fixed at some value. The choice of an optimal value for \( \lambda \), however, should be made using the data at hand. Common strategies in penalized regression involve information criteria or cross-validation techniques. If PCA is used as an explorative tool without distributional assumptions as done here, \( K \)-fold cross-validation can be used, since it does not require a likelihood. The general procedure is that the data is randomly split into \( K \) folds/subsets \( k = 1, \ldots, K \) of similar size. Given the \( k \)th subset is used as the so-called validation set, unknown parameters are fitted on the remaining \( K - 1 \) parts of the data (the so-called training set). Using those parameters, an appropriate measure of performance \( M_k \) is calculated on the \( k \)th part of the data. Specifically, with penalized non-linear PCA as proposed here, the parameters of interest are the scaling functions. So we use the quantifications as estimated on the training set to scale the validation data (the \( k \)th subset). Then, we run a (standard) PCA on the scaled validation data and use the proportion of variance that is explained by the first \( m \) principal components as the measure of performance \( M_k \) of the fitted scaling function. Recall, the basic idea behind optimal scaling is to maximize the variance that is accounted for (VAF) by the first \( m \) principal components. For instance, if the scaling function rather fits noise in the training data than results from substantial non-linearity, it will perform...
worse on independent validation data than a simpler, rather linear function. Since
the quantifications in our case depend on the value of the penalty parameter $\lambda$, $M_k$ also depends on $\lambda$, and is hence written as $M_k(\lambda)$. Then, cycle through all
$k = 1, \ldots, K$ partitions and calculate

$$CV(\lambda) = \frac{1}{K} \sum_{k=1}^{K} M_k(\lambda).$$

Now, over a fine grid $G$ of sensible values $\lambda \in G$, the optimal $\lambda$ can be determined by maximizing the cross-validated VAF.

Cross-validation, however, can be time-consuming, since parameters need to be fitted repeatedly. Interestingly, in many practical applications of penalized non-linear PCA, also a simple graphical tool can be used to find an appropriate value for $\lambda$. Instead of cross-validated VAF, for each candidate value of $\lambda$ the parameters are only fitted once, using the entire data set as training data. Then, the VAF on the training data is drawn as a function of $\lambda$. By definition of penalized non-linear PCA, this function, $\text{VAF}(\lambda)$, is monotonically decreasing (as with a smaller $\lambda$ more emphasis is put on the data). However, it is often found that this function is almost constant for $\lambda$ below some $\lambda_0$ (and for $\lambda$ above some $\lambda_1$). Consequently, $\lambda_0$ may be used as a good compromise between fit to the data and interpretation. In other words, with $\lambda < \lambda_0$ we run into ‘over-fitting’, where more pronounced non-linearity (obtained for smaller $\lambda$) only leads to marginal improvement with respect to VAF. With $\lambda > \lambda_0$, on the other hand, we observe a substantial drop in VAF. Examples where this behavior of $\text{VAF}(\lambda)$ is observed, are found in Section 4.

As an alternative to the purely graphical approach, we can, e.g., choose $\lambda_0$ as the largest $\lambda$ still fulfilling the condition

$$\text{VAF}(0) - \text{VAF}(\lambda) = \frac{1}{p} \sum_{r=1}^{m} \nu_r(0) - \frac{1}{p} \sum_{r=1}^{m} \nu_r(\lambda) \leq \delta,$$

where $\nu_r(\lambda)$ denotes the $r$th (largest) eigenvalue obtained in the final PCA with penalty parameter $\lambda$, and $\delta$ being a small (preselected) constant, e.g., $1\%$; $\text{VAF}(\lambda)$ denotes the corresponding VAF on the training data.

3 Numerical Experiments

Before applying penalized non-linear PCA as proposed to real world data, we carry out some illustrative numerical experiments to confirm that the method is able to identify the underlying structure used for data generation. This allows us to gain some insight into statistical properties such as the so-called bias-variance trade-off, which is commonly seen for smoothing techniques (compare,
e.g., Fahrmeir and Tutz (2001)). To be concrete, a larger value of the penalty parameter is typically associated with a larger bias and comparatively low variance, and vice versa. A related aspect of interest is whether and to what extent the procedure is qualified to detect relationships beyond linearity. Note, however, that the term ‘bias’ is rather used informally/qualitatively speaking here, since there is no ‘true’ scoring rule the obtained quantifications could be compared to in a strict sense by taking differences (mainly due to the method of creating ordinal observations from continuous data by thresholding, see below).

3.1 Experimental Design

For illustration and evaluation of our method, we conducted this simulation with varying design level parameters such as the tuning parameter, sample size and the standard deviation of noise overlaying the data obtained as linear combinations of some latent factors. For $\lambda$ we opt for different values according to no penalization (purely non-linear PCA), small, medium and large penalization, with the latter tending towards standard, linear PCA. We chose a rather large sample size of $n = 500$, which is comparable to our empirical example on the ICF data, along with a quite small value of $n = 100$ to illustrate the method’s potential limitations. In the latter case, we ran the algorithm with $\lambda = 0, 0.1, 2, 5$. Since the effect of the penalty tends to vanish off as the sample size exceeds a certain value, the tuning parameters are adjusted to $\lambda = 0, 0.1, 5, 10$ in the case of $n = 500$. The number of variables ($p = 20$) and the number of principal components/latent factors ($m = 5$) are kept fixed. While varying one parameter ($\lambda$ or $n$), we keep the other constant such that we observe a total of 8 scenarios. For reasons of simplicity, we chose a design assuming a five-point scale for each variable. For the eigenvalues $\nu_r$, $r = 1, \ldots, 5$, which correspond to the variances of the underlying factors, we assume the descending sequence 6, 5, 4, 3, 2. The (true) loadings matrix $A$ is block diagonal, such that each component loads on a distinct set of variables; more precisely

$$A = \begin{pmatrix} a_{(1)} & \cdots & \cdot \\ \cdot & \ddots & \cdot \\ \cdot & \cdot & a_{(5)} \end{pmatrix},$$

with $a_{(r)}$ being a normalized $((7 - r) \times 1)$ vector with entries $1/\sqrt{7 - r}$. By doing so, we achieve a sparse matrix, having a positive loading on one factor only for each variable, which is ideally wished for factor interpretation in practice. Matrix $A$ doesn’t change over scenarios. For generating the five latent factors, we draw i.i.d. normal data, with zero means and variances corresponding to the eigenvalues given above. The resulting ($n \times 5$) (latent) data matrix $\tilde{Y}$ is multiplied by $A^\top$, and overlaid with i.i.d. gaussian error with variance $\tau^2$. The resulting matrix, say $\tilde{X} = \tilde{Y} A^\top + E$, is then discretized by applying cut-points (similarly to a threshold mechanism known from cumulative ordinal regression.
models). Those cut-points are chosen such that five different types of quantifications are obtained, involving monotonic as well as non-monotonic effects: V-shaped (variables 1–6), S-shaped (variables 7–11), linear (variables 12–15), square root (variables 16–18) and quadratic (variables 19–20). For simplicity, the same transformation is applied to each variable within the same PC (compare matrix $A$ above), leading to a construction where the V-shaped variables load on PC 1, S-shaped on PC 2, and so on. In case of a monotone (i.e., S-shaped, linear, square root and quadratic) scoring rule, cut-points are simply obtained by applying corresponding transformations on some equidistant grid-points. For the non-monotonic quantifications, we use two cut-points $\zeta_1$ and $\zeta_2$ only, with latent/continuous observations falling into $[\zeta_1, \zeta_2]$ being randomly assigned to level 2 or 4, and observations above $\zeta_2$ being denoted as level 1 or 5 (also chosen at random). The remaining data points (i.e., below $\zeta_1$) are interpreted as level 3. The motivation/interpretation behind this is that the latent factor merely determines whether extreme categories are observed or not. The entire process of data generation, transformation/discretization, and penalized, non-linear PCA was repeated 500 times. Result are discussed below.

### 3.2 Results

To check whether the method presented in Section 2 is qualified to recover the underlying transformations of the data, we will examine the estimated quantifications $\hat{\theta}$ for different values of penalty parameter $\lambda$, given a certain sample size $n$ and error variance $\tau^2$.

Since, for simplicity, the same transformation/categorization is applied to all variables within each principal component, we will only present the results for variables 1, 7, 12, 16, 19, which display the V-shaped, S-shaped, linear, square root and quadratic transformation, respectively. Figures 1 and 2 show the respective subsets of coefficient vector $\hat{\theta}$ averaged over 500 iterations (black lines) along with pointwise uncertainty bands ($\pm 2$ standard deviations, grey error region), where $\tau^2 = 0.2, n = 100$ and $n = 500$, respectively. Since both eigenvectors/principal components and quantifications are only defined up to the sign, further restrictions need to be involved when plotting/comparing results across iterations. For (truly) monotone quantifications, we generally request that the overall trend/shape is rather increasing than decreasing, that means, quantifications are multiplied by $-1$ if necessary. For (truly) non-monotone but symmetric(!) quantifications, we request that the shape is rather V than inverted V. Technically speaking, the choice whether to multiply by $-1$ (i.e., flip the fitted quantifications or not) is based on first/second-order differences, i.e., discrete versions of first/second derivative.

From Figure 1 (column/variable 1) we see that, under true and substantial non-monotonicity, (penalized) non-linear PCA with small $\lambda$ clearly outperforms penalized non-linear PCA with large $\lambda$ regarding both bias and variance. At
first glance, this result is counterintuitive having results from smooth, non-linear regression in mind. However, it can be explained as follows. If $\lambda$ is large, scoring rules are forced to be approximately linear with arbitrary orientation. Then, the V-shape transformation (i.e., flip, if necessary) leads to the butterfly-shaped grey/uncertainty regions (Figure 1, bottom left). But note, suchlike transformation to obtain a (rather) convex scoring rule for variables 1–6 (instead of a transformation yielding (rather) increasing rules for variable 7–20) is necessary to see that small $\lambda$ indeed gives to the true, underlying categorizations. Figure 2 with $n = 500$ clarifies, that the increase in sample size outweighs in a way that
PCA even with $\lambda = 10$ is able to detect non-monotonicity, but still suffers from higher variance. As before, one way of explaining this is that penalizing deviations from linearity (together with the potential flip to obtain a V-shaped scaling function) still has some influence regardless of the sample size. On the other hand, we see that, under true monotonicity (Figure 1 and 2, columns 2-5), penalized non-linear PCA is clearly superior to usual non-linear PCA ($\lambda = 0$) with regard to estimation uncertainty. Even under true non-linearity (variable 7, 16 and 19), purely non-linear PCA seems to be problematic if the number of observations is relatively small. Here, the variance observed reaches values of undesirable amount.
Fortunately, a small change in penalty ($\lambda = 0.1$, second row) is already able to attack the problem, which allows us to capture the non-linear structure while keeping the amount of uncertainty comparatively low. Also if the number of observations is high, penalized non-linear PCA with $\lambda = 0.1$ performs best (among the results shown) as it represents a good compromise yielding low variance while keeping the true, possibly non-linear, shape.

4 Application to Real World Data

While the simulation studies in the previous section provided some illustration on and insight into the proposed method’s behavior, the real potential/benefit is only seen from real data applications. For that purpose, we will consider two, publicly available data sets, with the main focus being on the ICF core set for chronic widespread pain already mentioned in Section 1.

4.1 The ICF Core Set for Chronic Widespread Pain

The ICF core set for CWP, available from R package \texttt{ordPens}, contains 420 observations of 67 ordinally scaled variables measuring difficulties in functioning, activities and reduction of life quality of patients with CWP. Each ICF factor is associated with one of the following four types: ‘body functions’, ‘body structures’, ‘activities and participation’, and ‘environmental factors’. The latter are measured on a nine-point Likert scale ranging from $-4$ ‘complete barrier’ to $+4$ ‘complete facilitator’. All remaining factors are evaluated on a five-point Likert scale ranging from 0 ‘no problem’ to 4 ‘complete problem’. Due to space limitations, we refer to the online supplementary material for an overview on the data analyzed, covering, inter alia, a description of the 67 ICF categories along with observed frequencies (Table S1, Figures S1–S2). For more detailed information on the ICF, we refer to Cieza et al. (2004) and Gertheiss et al. (2011).

For validating the core set for CWP, ICF evaluations have been compared to the general purpose short-form health survey SF-36 (Ware and Sherbourne, 1992). More specifically, this has been done by regressing a physical health component summary calculated from the SF-36 on the ICF data (Gertheiss et al., 2011; Bürkner and Charpentier, 2020). The SF-36 summary measures, a physical and a mental health component score, however, were originally constructed by (standard, linear) principal components analysis (McHorney et al., 1993). So for constructing rather disease-specific, ICF-based summary scores, PCA on the ICF data itself appears to be a (more) sensible approach.

4.1.1 Smoothing Coefficient Vectors

Penalized non-linear PCA is to be applied to detect (latent) dimensions of life quality reducing symptoms and caused problems as measured by the most im-
important principal components. In analogy to McHorney et al. (1993), we perform PCA with \( m = 2 \) components, as also resulting from the scree test, see Figure 5 and details as given in Section 4.1.3 below. Figure 3 illustrates the estimated coefficients of selected variables for different values of the penalty parameter \( \lambda \). The black lines refer to \( \lambda \to 0 \), the red dashed lines refer to \( \lambda = 0.5 \), and the green dotted lines to \( \lambda = 5 \). It is noticeable that with an increasing penalty parameter quantifications become increasingly linear.

For the variable ‘touch function’ in Figure 3, for instance, the impact of the penalty can be clearly seen with regularization towards linearity; see also variable \( b265 \) (ICF code) in the online appendix (Table S1, Figure S3). In general, for all variables of type ‘body functions’, ‘body structures’, or ‘activities and participation’, such as ‘touch function’, ‘walking’ and ‘moving around’ (all of which having coding schemes ranging from ‘no problem’ to ‘complete problem’), we restrict ourselves to monotone scoring rules, as activities (like ‘moving around’) or body functions (like the ‘touch function’) are typically affected more and more with
worsening CWP. For the scale $-4$ ‘complete barrier’ to $+4$ ‘complete facilitator’ on the other hand, as given with ‘environmental factors’, such restriction would lead in the wrong direction. As observed in Figure 3 (bottom row), some very non-monotonic effects can be discovered if using a rather small $\lambda$, which can be seen as a clear benefit of non-linear PCA over usual (linear) PCA. When using the penalized method proposed (see, e.g., the red triangles), quantifications are smoother than for unpenalized non-linear PCA (black circles), which is desirable, as wiggly coefficients are hard to interpret. Due to a lack of space, results for the other ICF categories are not presented here, but can be found in the online supplements (Figures S3–S8). Finally, it should be noted that $\lambda \to 0$, i.e., $\lambda > 0$ instead of $\lambda = 0$, enables fitting of quantifications (via linear intra/extrapolation) even for levels that are not observed in the data (compare, e.g., level 4 of ‘walking’ in Figure 3).

4.1.2 Smoothing Parameter Selection

For evaluating the performance of our approach and selecting the right amount of penalization, we use 5-fold cross-validation as described above. That means, the data is split into 5 roughly equal-sized parts; then, in turn, 4 of these parts are used to determine the scaling rule and the performance of the rule is evaluated on the part of the data that has been left out. The performance of the quantification rule is measured by the proportion of variance that is explained by the first $m = 2$ principal components when the respective rule is used for scaling the categorical variables, as given in Figure 4. The optimal smoothing parameter, as determined...
on the validation set(s), is indicated by the dashed line in Figure 4 (right). Cross-
validation results indicate that non-linear PCA can indeed be enhanced when 
using the suggested penalized method. Although penalized scaling functions are 
less complex, and thus easier to interpret, performance improves on the validation 
data up to a certain $\lambda$ value and deteriorates from there. Based on those results, 
we can use $\lambda \approx 0.5$ (where the proportion of variance explained on the validation 
data reaches its maximum) to find the final scaling rule; compare the dashed 
vertical line in Figure 4 (right). Results on training data only, are shown in the 
left panel of Figure 4, and look exactly as sketched in Section 2.3. Hence, an 
optimal penalty parameter could alternatively be found using the training-data-
only approach described there.

### 4.1.3 Selecting the Number of Components and Further Interpretation of Results

To extract a suitable number of principal components, we consider the scree cri-
terion (Cattell, 1966) by plotting the PCs against their eigenvalues and detecting 
the first break (‘elbow’). Figure 5 depicts the scree plot for $m = 2$ (solid black) 
in the penalized algorithm if using the optimal $\lambda$ (as chosen via cross-validation, 
see above) along with the scree plot for standard, linear PCA (dotted red). One 
sees that the first two components are by far the most relevant and that the 
additional amount of variance accounted for after the second drop can be ne-
glected, as the line levels off. In addition, we see again (compare Figure 4, left) 
the amount of variance explained by the first two principal components is in-
creased substantially if allowing for non-linear/non-monotone scoring rules, as 
the first two black circles are well above the red dots. The supplementary mate-
rial gives further insight to the data set covering also the extracted eigenvectors

![Figure 5: Scree plots for $m = 2$ (solid black) using the proposed method and standard, linear PCA (dotted red).](image-url)
(Table S2) and the varimax rotated matrix of loadings (Table S3). In summary, the most important, first principal component (which accounts for roughly 33% of variance with $\lambda \approx 0.5$ here, compare Figure 5) can be interpreted as overall CWP condition, with bad health being associated with large values of ‘body functions’, ‘body structures’, or ‘activities and participation’, e.g., ‘moving around’ and ‘walking’. With respect to ‘drugs’ ($e_{1101}$) both large and small values indicate poor overall condition (compare Figure 3). In other words, patients with a milder form of CWP are much less affected by the medication, as the latter is much less described as either ‘barrier’ to ‘facilitator’. It should be pointed out again here, that this would have been impossible to find by standard, linear PCA (or non-linear PCA with monotonicity constraint). Loadings of the other environmental factors are comparatively high (in absolute values) for the second principal component/latent factor. In other words, the second dimension is mainly characterized by those factors. Again, many of those factors show very non-linear or even non-monotone behavior (compare Figure 3 and the online appendix). More broadly speaking, this example highlights the potential of allowing for non-monotonic effects together with penalization in (ordinal) PCA. Combining the scree test and cross-validation (or some other method for choosing $\lambda$ as described) appears to provide a good compromise between model complexity, fit to the data, and interpretation.

4.2 Further Example: Depressive Mood Scale Data

Next, we will illustrate the proposed method on another publicly available data set for reproducibility. We will investigate the ehd data from R package psy (Falissard, 2009). Example R code for running ordinal PCA as proposed here on the ehd data, is also found in ordPens. The ehd data consists of 269 observations of 20 ordinally scaled variables forming a polydimensional rating scale of depressive mood (Jouvent et al., 1988). Each item is measured on a five-point scale. We scale the variables by using the presented technique for non-linear PCA with $m = 5$ and additional restriction of monotonicity. Figure 6 shows some of the obtained quantifications for different values of smoothing parameter $\lambda$. For the sake of uniformity, the black lines again refer to unpenalized non-linear PCA (i.e., $\lambda \to 0$), the red lines refer to $\lambda = 0.5$, and the green lines to $\lambda = 5$. As before, it is nicely seen that with larger $\lambda$ quantifications become more and more linear, which is equivalent to standard (linear) PCA using just the category labels. In this example, a further analysis of the data without monotonicity restrictions led to some non-monotone coefficient estimates. As the affected variables of the ehd data are supposed to have consistent, negative association with depressive mood, however, it seems reasonable to assume monotonicity. In other words, content-motivated considerations should be incorporated to enhance interpretability of the estimated effects. To obtain an optimal amount of smoothing, $\lambda$ was again determined based on 5-fold cross-validation. Figure 6(e) and (f) shows the mean...
Figure 6: Category quantifications/scores for $\lambda \to 0$ (solid black), $\lambda = 0.5$ (dashed red), $\lambda = 5$ (dotted green) with monotonicity constraint (a)--(d); VAF by the first 5 principal components: (e) training data, (f) validation data.

The proportion of variance explained as a function of penalty parameter $\lambda$ (on a logarithmic scale) for both the training data as well as the validation data, respectively. On the training data, this function is of course monotonically decreasing in $\lambda$, as with smaller $\lambda$ more emphasis is put on the data. For $\lambda \to 0$, the original non-linear PCA is obtained, where the explained variance is maximized by construction. On the validation data, however, it’s a different story: both (linear) PCA, which is obtained for $\lambda \to \infty$, and un-penalized/purely non-linear PCA (see $\lambda \to 0$, i.e., $\log_{10}(\lambda) \to -\infty$) are clearly worse than penalized, non-linear PCA with $\lambda$-values between $10^{-1} = 0.1$ and $10^0 = 1$. That means, results of non-linear PCA can be improved by using the penalized fitting algorithm. To obtain a distinct $\lambda$-value for the final scaling rule, cross-validation results as given in Figure 6(f) can be used as before. Consequently, for the ehd data, we would use $\lambda = 10^{-0.3} \approx 0.5$ (again), where the explained variance on the validation data is maximized (compare the dashed vertical line in Figure 6(f)).
5 Summary and Discussion

In the present work, we proposed a new approach to apply principal components analysis on ordinal variables. Those type of data occur often in social and behavioral sciences, but are typically treated as numeric using standard linear PCA, or they are treated as categorical using non-linear PCA (also known as optimal scoring/scaling/quantification). While the former assumes relationships between variables to be linear per construction, the latter can detect non-linear effects but tends to over-fit the data and can lead to estimates that are hard to interpret. To attack those problems, we presented penalized non-linear PCA as an intermediate between the aforementioned methods where the degree of smoothness can be controlled by a tuning parameter. We proceeded by introducing second-order penalties to incorporate the variables’ ordinal scale by smoothing out coefficients of adjacent levels, more specifically, penalizing non-linearity in the coefficients. The new approach offers both better interpretability of the non-linear transformations of the category labels as well as better performance on validation data than un-penalized non-linear PCA. The method proposed is implemented in R and publicly available on CRAN through add-on package ordPens.

Numerical experiments were set up to shed light on the method’s capability to parameter recovery and comparison to linear and fully non-linear PCA. We presented a setting involving linear relationships between the variables together with more challenging, non-linear and even non-monotonic effects. Following the concept of bias-variance trade-off, we would associate a large penalty with smaller variance but larger bias (tendency to under-fitting). Comparing estimated coefficients, we indeed detected higher variation going along with purely non-linear PCA, especially given a small sample size. This leads us to the conclusion that overall, it can be preferable to use the proposed penalization technique with an appropriate amount of penalty. Fortunately, already a slight portion of penalization was sufficient to reduce variance while still detecting non-linearity in the scoring rules in our simulations. In practice, cross-validation techniques can be used to find the optimal penalty parameter. The proportion of variance explained on the validation samples also visualizes the potential advantage of penalized PCA against purely non-linear and linear PCA.

To illustrate the application and potential benefits of penalized non-linear PCA in practice, we considered the publicly available ICF core set data for chronic widespread pain. We found that two principal components are to be extracted in order to detect the main dimensions of health status in the context of CWP. Results on the validation data and non-linearity detected in the majority of quantified variables, signalize the potential impact of non-linear transformations when aiming at dimension reduction, feature extraction and factor selection, compared to both standard, linear and purely non-linear PCA. Penalized, non-linear PCA as proposed here also allows for monotonicity constraints to enforce monotonic scoring rules/quantifications. The latter often makes sense as seen with ICF vari-
ables of type ‘body functions’, ‘body structures’, and ‘activities and participation’ (or the ‘depressive mood scale data’ also considered). Sometimes, however, non-monotonic transformations provide valuable, additional insight, as it was the case with ICF environmental factors.

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Supporting Information

The following supporting information may be found in the online edition of the article:

**Figure S1.** Summary for ICF categories corresponding to ‘body functions’, ‘body structures’, ‘activities and participation’ (prefix ‘b’, ‘d’, ‘s’) on individual level. Coding scheme for categories: 0 ‘no problem’, 1 ‘mild problem’, 2 ‘moderate problem’, 3 ‘severe problem’, 4 ‘complete problem’.

**Figure S2.** Summary for ICF categories corresponding to ‘environmental factors’ (prefix ‘e’) on individual level. Coding scheme for categories: -4 ‘complete barrier’,..., -1 ‘mild barrier’, 0 ‘no barrier or facilitator’, 1 ‘mild facilitator’,..., 4 ‘complete facilitator’.

**Figure S3.** Category quantifications/scores for $\lambda \to 0$ (solid black), $\lambda = 0.5$ (dashed red), $\lambda = 5$ (dotted green). Monotonicity constraint only applied to variables corresponding to ‘body functions’, ‘body structures’, ‘activities and participation’ (prefix ‘b’, ‘d’, ‘s’).

**Figure S4.** Category quantifications/scores for $\lambda \to 0$ (solid black), $\lambda = 0.5$ (dashed red), $\lambda = 5$ (dotted green). Monotonicity constraint only applied to variables corresponding to ‘body functions’, ‘body structures’, ‘activities and participation’ (prefix ‘b’, ‘d’, ‘s’).

**Figure S5.** Category quantifications/scores for $\lambda \to 0$ (solid black), $\lambda = 0.5$ (dashed red), $\lambda = 5$ (dotted green). Monotonicity constraint only applied to variables corresponding to ‘body functions’, ‘body structures’, ‘activities and participation’ (prefix ‘b’, ‘d’, ‘s’).

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**Figure S7.** Category quantifications/scores for $\lambda \to 0$ (solid black), $\lambda = 0.5$ (dashed red), $\lambda = 5$ (dotted green). Monotonicity constraint only applied to variables corresponding to ‘body functions’, ‘body structures’, ‘activities and participation’ (prefix ‘b’, ‘d’, ‘s’).

**Figure S8.** Category quantifications/scores for $\lambda \to 0$ (solid black), $\lambda = 0.5$ (dashed red), $\lambda = 5$ (dotted green). Monotonicity constraint only applied to variables corresponding to ‘body functions’, ‘body structures’, ‘activities and participation’ (prefix ‘b’, ‘d’, ‘s’).

**Table S1.** ICF categories included in the Comprehensive ICF Core Set for chronic widespread pain.

**Table S2.** Eigenvectors of ICF data.

**Table S3.** Varimax rotated loadings of ICF data. The higher loading for each variable is highlighted.
Penalized Non-Linear Principal Components Analysis for Ordinal Variables with an Application to International Classification of Functioning Core Sets

Supplementary Material

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| Body Functions | Activities and Participation |
|----------------|-----------------------------|
| **b122** Global psychosocial functions | **d160** Focusing attention |
| **b126** Temperament and personality functions | **d175** Solving problems |
| **b130** Energy and drive functions | **d220** Undertaking multiple tasks |
| **b134** Sleep functions | **d230** Carrying out daily routine |
| **b140** Attention functions | **d240** Handling stress and other psychological demands |
| **b147** Psychomotor functions | |
| **b152** Emotional functions | **d410** Changing basic body position |
| **b160** Content of thought | **d415** Maintaining a body position |
| **b164** Higher level cognitive functions | **d430** Lifting and carrying objects |
| **b180** Experience of self and time functions | **d450** Walking |
| **b260** Proprioceptive function | **d455** Moving around |
| **b265** Touch function | **d470** Using transportation |
| **b270** Sensory functions related to temperature and other stimuli | **d475** Driving |
| **b280** Sensation of pain | **d510** Washing oneself |
| **b330** Haematological system functions | **d540** Dressing |
| **b55** Exercise tolerance functions | **d620** Acquisition of goods and services |
| **b640** Sexual functions | **d640** Doing housework |
| **b710** Mobility of joint functions | **d650** Caring for household objects |
| **b730** Muscle power functions | **d660** Assisting others |
| **b735** Muscle tone functions | **d720** Complex interpersonal interactions |
| **b740** Muscle endurance functions | **d760** Family relationships |
| **b760** Control of voluntary movement functions | **d770** Intimate relationships |
| **b780** Sensations related to muscles and movement functions | **d815** Acquiring, keeping and terminating a job |
| | **d850** Remunerative employment |
| | **d855** Non-remunerative employment |
| | **d910** Community life |
| | **d920** Recreation and leisure |
| **e1101** Drugs | **s770** Additional musculoskeletal structures related to movement |
| **e310** Immediate family | |
| **e325** Acquaintances, peers, colleagues, neighbours and community members | |
| **e355** Health professionals | |
| **e410** Individual attitudes of immediate family members | |
| **e420** Individual attitudes of friends | |
| **e425** Individual attitudes acquaintances, peers, colleagues, neighbours and community members | |
| **e430** Individual attitudes of people in positions of authority | |
| **e450** Individual attitudes of health professionals | |
| **e455** Individual attitudes of health-related professionals | |
| **e460** Societal attitudes | |
| **e465** Social norms, practices and ideologies | |
| **e570** Social security services, systems and policies | |
| **e575** General social support services, systems and policies | |
| **e580** Health services, systems and policies | |
| **e590** Labour and employment services, systems and policies | |

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Figure S6: Category quantifications/scores for $\lambda \to 0$ (solid black), $\lambda = 0.5$ (dashed red), $\lambda = 5$ (dotted green). Monotonicity constraint only applied to variables corresponding to ‘body functions’, ‘body structures’, ‘activities and participation’ (prefix ‘b’, ‘d’, ‘s”).
Figure S7: Category quantifications/scores for $\lambda \to 0$ (solid black), $\lambda = 0.5$ (dashed red), $\lambda = 5$ (dotted green). Monotonicity constraint only applied to variables corresponding to 'body functions', 'body structures', 'activities and participation' (prefix 'b', 'd', 's').
Figure S8: Category quantifications/scores for $\lambda \to 0$ (solid black), $\lambda = 0.5$ (dashed red), $\lambda = 5$ (dotted green). Monotonicity constraint only applied to variables corresponding to ‘body functions’, ‘body structures’, ‘activities and participation’ (prefix ‘b’, ‘d’, ‘s’).
|       | PC1  | PC2  |       | PC1  | PC2  |
|-------|------|------|-------|------|------|
| b1602 | 0.13 | 0.09 | d475  | 0.10 | 0.04 |
| b122  | 0.12 | 0.02 | d510  | 0.13 | 0.04 |
| b126  | 0.14 | 0.05 | d540  | 0.13 | 0.06 |
| b130  | 0.15 | 0.09 | d570  | 0.11 | -0.01|
| b134  | 0.15 | -0.01| d620  | 0.16 | 0.02 |
| b140  | 0.15 | 0.10 | d640  | 0.16 | -0.02|
| b147  | 0.14 | 0.04 | d650  | 0.15 | 0.00 |
| b152  | 0.16 | 0.03 | d660  | 0.12 | -0.02|
| b164  | 0.14 | 0.07 | d720  | 0.16 | -0.04|
| b180  | 0.11 | 0.07 | d760  | 0.13 | -0.04|
| b260  | 0.12 | 0.04 | d770  | 0.10 | -0.05|
| b265  | 0.13 | 0.04 | d845  | 0.11 | 0.03 |
| b270  | 0.12 | 0.03 | d850  | 0.11 | 0.01 |
| b280  | 0.15 | 0.09 | d855  | 0.07 | -0.10|
| b430  | 0.04 | 0.01 | d910  | 0.12 | 0.02 |
| b455  | 0.13 | -0.04| d920  | 0.13 | 0.04 |
| b640  | 0.10 | 0.04 | e1101 | 0.10 | -0.08|
| b710  | 0.12 | 0.11 | e310  | 0.11 | -0.14|
| b730  | 0.15 | 0.10 | e325  | 0.09 | -0.18|
| b735  | 0.15 | 0.07 | e355  | 0.07 | -0.25|
| b740  | 0.14 | 0.10 | e410  | 0.12 | -0.13|
| b760  | 0.11 | 0.08 | e420  | 0.11 | -0.15|
| b780  | 0.14 | 0.04 | e425  | 0.09 | -0.21|
| d160  | 0.15 | 0.06 | e430  | 0.06 | -0.23|
| d175  | 0.15 | 0.01 | e450  | 0.07 | -0.26|
| d220  | 0.16 | 0.01 | e455  | 0.07 | -0.26|
| d230  | 0.16 | -0.02| e460  | 0.05 | -0.26|
| d240  | 0.16 | 0.03 | e465  | 0.05 | -0.25|
| d410  | 0.14 | 0.09 | e570  | 0.04 | -0.29|
| d415  | 0.13 | 0.10 | e575  | 0.04 | -0.30|
| d430  | 0.14 | 0.04 | e580  | 0.07 | -0.25|
| d450  | 0.14 | 0.06 | e590  | 0.04 | -0.28|
| d455  | 0.14 | 0.02 | s770  | 0.12 | 0.06 |
| d470  | 0.13 | -0.04|       |      |      |

Table S2: Eigenvectors of ICF data.
| Variable | PC1  | PC2  | Variable | PC1  | PC2  |
|----------|------|------|----------|------|------|
| b1602    | 0.65 | 0.01 | d475     | 0.46 | -0.06|
| b122     | 0.56 | -0.15| d510     | 0.60 | -0.11|
| b126     | 0.68 | -0.10| d540     | 0.65 | -0.07|
| b130     | 0.75 | -0.03| d370     | 0.49 | -0.22|
| b134     | 0.66 | -0.27| d620     | 0.72 | -0.22|
| b140     | 0.75 | 0.01 | d640     | 0.69 | -0.31|
| b147     | 0.64 | -0.11| d650     | 0.65 | -0.23|
| b152     | 0.73 | -0.19| d660     | 0.50 | -0.24|
| b164     | 0.70 | -0.06| d720     | 0.66 | -0.35|
| b180     | 0.57 | -0.00| d760     | 0.55 | -0.30|
| b260     | 0.55 | -0.10| d770     | 0.41 | -0.29|
| b265     | 0.62 | -0.12| d845     | 0.52 | -0.11|
| b270     | 0.57 | -0.11| d850     | 0.48 | -0.14|
| b280     | 0.73 | -0.01| d855     | 0.25 | -0.35|
| b430     | 0.21 | -0.04| d910     | 0.55 | -0.15|
| b455     | 0.53 | -0.30| d920     | 0.63 | -0.11|
| b640     | 0.46 | -0.05| e1101    | 0.38 | -0.35|
| b710     | 0.61 | 0.08 | e310     | 0.36 | -0.51|
| b735     | 0.73 | -0.00| e325     | 0.23 | -0.59|
| b740     | 0.73 | 0.02 | e410     | 0.39 | -0.51|
| b760     | 0.57 | 0.01 | e420     | 0.33 | -0.54|
| b780     | 0.64 | -0.11| e425     | 0.23 | -0.65|
| d160     | 0.73 | -0.09| e430     | 0.07 | -0.66|
| d175     | 0.65 | -0.22| e450     | 0.09 | -0.76|
| d220     | 0.72 | -0.23| e455     | 0.06 | -0.75|
| d230     | 0.69 | -0.30| e460     | -0.00| -0.70|
| d240     | 0.74 | -0.17| e465     | -0.01| -0.69|
| d410     | 0.70 | -0.01| e570     | -0.10| -0.76|
| d415     | 0.68 | 0.03 | e575     | -0.08| -0.79|
| d430     | 0.65 | -0.11| e580     | 0.08 | -0.72|
| d450     | 0.67 | -0.09| e590     | -0.09| -0.74|
| d455     | 0.62 | -0.18| e770     | 0.60 | -0.04|
| d470     | 0.54 | -0.31| s770     | 0.60 | -0.04|

Table S3: Varimax rotated loadings of ICF data. The higher loading for each variable is highlighted.