

# EXPLORATORY DATA STRUCTURE COMPARISONS: THREE NEW TOOLS BASED ON PRINCIPAL COMPONENT ANALYSIS

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Abstract

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Key words: keywords...

## 1. Introduction

Classical statistical methodology is aimed at analyzing data from designed experiments and historically, statistical analyses have been done by researchers who knew the design and origin story of the data set well. However, the origin stories of data sets have changed over time and today a lot of data is accumulated without a specific purpose in mind. This is due to vast amounts of data being registered online and to a trend towards more open source research. The latter phenomenon in particular poses new challenges wrt. data quality assessment. When data are collected and made public without a specific end-point in mind, how do we ensure that differences in, say, choice measurement instruments, mode of administration, or sampling frame do not cause the data to be effectively divided into subsets that are simply not comparable? Three examples of this are

- Surveys often use mixed modes of administration, e.g. mail and telephone, and while this can improve response rates, the mode of administration can affect results Brambilla and McKinlay (1987); McHorney et al. (1994) and differences in response behavior can lead to biased results. Powers, Mishra and Young (2005) report effects of mode of administration on changes in mental health scores that are of a magnitude that is considered to be clinically meaningful.
- The rapid growth of web surveys, due to low cost, timeliness, and other factors, generate large data sources that lack a sampling frame of the general population. However, it can be problematic to combine online panels (pre-recruited profiled pools of respondents) with intercept samples (a pool of respondents obtained through banners, ads, or promotions) Liu (2016).
- Large scale open source data sets such as the PISA data and ESS (European Social Survey) data. In these data sets, data analysts are far away from the data producers and problem-specific recommendations about potential instrument-induced challenges in the data sets are not available for the data analysts.

Maybe something here about what PCA is usually used for, e.g. dimension reduction, exploratory data analysis, ...

Assume that we have two data sets with the same variables, but different observations represented as a data set with a subset-inducing variable. Assume next that we wish to compare structures without specifying a model, or even a variable of interest. The central question is whether the two data sets can readily be combined for the purpose of later data analysis, or if the subset-inducing variable implies heterogeneity across the subset division.

Sophisticated methods for addressing this question are available when we are willing to assume a statistical model, but when these models are taken away, a remarkable void of methods is left behind. What is needed is a procedure that compares differences in overall data structures in two (or more) subsets of a data set without assuming neither directional nor hierarchical relationships between the variables. Using parametric models is not a general data structure comparison method, but rather a fitted-model comparison method. It addresses the interplay between the model and the data, not the data alone. Simple methods like variable-by-variable

tests in distributional differences suffer from the drawback that they only address marginal differences and not to the interplay between variables. Entry-by-entry comparison of the two empirical correlation matrices quickly becomes unmanageable as the number of variables increase. For these methods significant  $p$ -values are likely to abound as the sample size increases. Parametric models using, e.g., latent variable models moves beyond the marginal approach, but need a pre-specified model.

We propose a suite of three new tools for this task, which we will refer to collectively as Principal Component Analysis-based Data Structure Comparisons (PCADSC). These methods employ the principal component decomposition of the empirical covariance matrix performed on two subsets of a dataset in order to create intuitive visualizations of data structure differences. Software for using these tools is available in an R-package. [how to refer to our package?](#) This yields a solution that is largely independent of the sizes of the two subsets of data. Thereby, a lot of methods that compare each subset to the full data set in some sense are excluded.

This manuscript is structured as follows: First, in Section Section 2, we describe the PCADSC procedures, including a brief introduction to principal component analysis (PCA) in general. In Section 3, we present a worked data example using open source, online available data on psychological well-being in three European countries. More specifically, we compare data from Denmark, which has repeatedly been rewarded "happiest country in the world", with data from Bulgaria and Sweden, respectively, to investigate whether or not psychological well-being - and thus happiness - is really a concept that is universal beyond country borders, or if such rankings of happiness are inherently meaningless. At last, we discuss limitations and merits of the PCADSC tools in Section 4.

## 2. PCA-based tools for data structure comparisons

As mentioned above, the purpose of PCADSC is comparing overall data structures in two or more subsets of a dataset. But before we can get further into describing the PCADSC tools, we must first define the exact meaning of *overall structures* in this context. One such definition is the structure of the covariance matrix of the dataset. If we assume all variables in the dataset to be jointly normal with zero means, the covariance matrix is a sufficient statistic for describing the simultaneous distribution of all the variables. This gives it a very nice interpretation as a measure of the overall structure. If we do not accept the normality assumption, pairwise correlations and marginal variable variances are still interesting quantities that say something about the interrelations between the variables in the data. All in all, the empirical covariance matrix is a reasonable place to start looking for differences in *overall data structures*.

A naive approach for data structure comparisons might therefore be to compute the empirical covariance matrices on each of the two data subsets and simply compare these matrices. Though the idea perhaps sounds appealing at first, it is quite difficult to assess similarity of matrices, and moreover, it becomes increasingly difficult for large numbers of variables and thus high dimensional covariance matrices. There is simply too much information to consider at once. However, by use of linear algebra, we can decompose and recompose the covariance matrix such that the distinct dimensions of information withheld in it are clearly separated and ordered according to their relative importance. In particular, we find a new representation of the

covariance matrix that makes it possible to gain an overview of the most interesting aspects of the data. On such decomposition strategy is using *principal component analysis* (PCA), which uses eigenvalue decomposition in order to obtain a new representation of the covariance matrix.

### 2.1. A brief introduction to Principal component analysis

Consider  $n$  observations  $x_1, \dots, x_n \in \mathbb{R}^d$  of  $d$  variables, let  $\bar{x} = (\bar{x}_1, \dots, \bar{x}_d)^\top = \frac{1}{n} \sum_{i=1}^n x_i$  denote their averages, and let  $S = \frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})(x_i - \bar{x})^\top \in \mathbb{R}^{d \times d}$  denote the empirical covariance matrix of the full data matrix,  $X$ . We assume in the following that all variables of  $X$  have a numerical interpretation, e.g. by being continuous or ordinal and categorical. For a given  $q \leq d$ , principal component analysis (PCA) is a tool for finding a new representation of the dataset of dimension  $q$  such that the least possible amount of information is lost. More specifically, we wish to minimize the loss when looking at a projection of  $X$  onto a  $q$ -dimensional space, rather than the original  $d$ -dimensional one. Formally, we define the *rank- $q$ -reconstruction error* as the minimal squared error that is achievable by linear subspaces  $K_q \subset \mathbb{R}^d$  of dimension  $q < d$ , that is

$$\min_{K_q} \sum_{i=1}^n \min_{z \in K_q} \|x_i - \bar{x} - z\|^2 = \min_{K_q} \sum_{i=1}^n \|x_i - \bar{x} - \text{proj}_{K_q}(x_i - \bar{x})\|^2.$$

and the theory of *Principal component analysis* (PCA) not only ensures the existence of a subspace  $\hat{K}_q \subset \mathbb{R}^d$  that attains this minimum, it also provides an explicit description of  $\hat{K}_q$  and the rank- $q$ -reconstruction error. [Reference here?](#) [Maybe to like original Pearson article?](#)

More specifically, the rank- $q$ -reconstruction error is attained when we choose

$$\hat{K}_q = \text{span}\{\eta_1, \dots, \eta_q\}$$

where  $\eta_1, \dots, \eta_q$  are the  $q$  first eigenvectors of the empirical covariance matrix,  $S$ , as ordered by the size of their associated eigenvalues,  $\lambda_1, \dots, \lambda_d$ . In the PCA framework, we refer to the eigenvectors as *loadings*. The eigenvalues may be understood as *variance components*, as the sum of the marginal empirical variances is preserved under eigenvalue decomposition, that is,

$$\text{trace}(S) = \sum_{j=1}^d \hat{V}(X_j) = \sum_{j=1}^d \hat{V}(\eta_j^\top X^\top) = \sum_{j=1}^d \lambda_j$$

where  $X_j \in \mathbb{R}^n$  denotes the  $j$ th variable of  $X$  and  $\hat{V}$  is the empirical variance function. This again emphasizes that we do not change the covariance structure of a dataset when performing PCA; we merely use linear algebra to make it easier to describe. And as eigenvalues are uniquely defined, and eigenvectors are uniquely defined up to a change of sign whenever the eigenvalues are different, the representation hereby obtained is a valid object of inference. If  $n < d$  or if the covariance matrix does not have full rank, it is possible to obtain non-unique eigenvalues, e.g.  $\lambda_i = \lambda_{i+1} = \dots = \lambda_0$ , but even in this case, the associated eigenvectors  $\eta_i, \eta_{i+1}, \dots, \eta_j$  are uniquely defined up to a common rotation.

The  $j$ th loading can also be found iteratively as the unit vector  $u \in \mathbb{R}^d$  orthogonal to  $\hat{K}_{j-1}$  that maximizes the variation of the associated scores:

$$\eta_j = \operatorname{argmax}_{u \in \mathbb{R}^d: u \perp \hat{K}_{j-1}} \sum_{i=1}^n \|u^\top (x_i - \bar{x})\|^2, \quad \lambda_j = \frac{1}{n-1} \sum_{i=1}^n \|\eta_j^\top (x_i - \bar{x})\|^2.$$

where the initial subspace is defined as  $\hat{K}_0 = \{0\}$ . It is worth emphasizing that this greedy approach of successively adding the next direction  $\eta_j$  explaining most of the remaining variation, also gives the sequence  $\hat{K}_q = \hat{K}_{q-1} \oplus \operatorname{span}\{\eta_q\}$  of subspaces minimizing the rank- $q$ -reconstruction error. This strong interpretation of PCA, which is often overlooked in the literature, means that the sequence of loadings  $\eta_j$  and their associated variation components  $\lambda_j$  yield a simultaneous description of the structure of the data set for all approximating dimensions  $q$ . This implies that the loadings and the variation components can be used to investigate the structure of the data set without the need to decide on an approximating dimension,  $q$ , a priori.

## 2.2. Using PCA for data structure comparisons

All in all, PCA qualifies as an appealing first step in structural comparisons of two datasets containing the same variables, and especially the loadings and variance components are meaningful quantities to compare across such different datasets. Usually, when performing PCA with other purposes in mind, the main interest lies in the *scores*, i.e. the projections  $\eta_j^\top (x_i - \bar{x})$  of the observations onto the loadings. But where the scores describe the observations, the variation components and the accompanying loadings describe the usage of the variables. If two different datasets with the same variables, but different samples of observations, have similar loading patterns, then the variables appear to be measuring the same underlying quantities in both datasets. This can be the case while the two sets of scores could be arbitrarily different, which e.g. could happen if the two datasets were taken from two different populations of subjects. On the other hand, if the loading patterns are different in the two datasets, then this indicates that the variables are used differently in the two data situations, and hence it would be criticizable to use these variables for comparisons across the two datasets.

The tools presented in this paper are all based on comparing the PCA results across two different datasets that contain the same variables. We denote these two datasets by  $X_1$  and  $X_2$ , respectively, with  $X_1$  consisting of  $n_1$  observations of  $d$  variables  $x_{11}, \dots, x_{1n_1} \in \mathbb{R}^d$ , and similarly,  $X_2$  consisting of  $n_2$  observations of the  $d$  variables,  $x_{21}, \dots, x_{2n_2} \in \mathbb{R}^d$ . For each of these two datasets, we complete the following steps:

1. Standardized each of the variables to have mean zero and unit standard deviation. Let  $\tilde{x}_{ij} \in \mathbb{R}^d$  for  $i = 1, 2$  and  $j = 1, \dots, n_i$  be the standardized datasets.
2. Form the principal component analysis

$$S_i = \frac{1}{n_i - 1} \sum_{j=1}^{n_i} \tilde{x}_{ij} \tilde{x}_{ij}^\top = \sum_{k=1}^d \lambda_{ik} \eta_{ik} \eta_{ik}^\top \quad \text{for } i = 1, 2.$$

thereby obtaining loadings  $\eta_{ik}$  and variance components  $\lambda_{ik}$  for  $i \in \{1, 2\}$  and  $k \in 1, \dots, d$ .

The hereby obtains PCA decompositions of the covariance matrices can then be compared. We present three diagnostics plots that are designed to shine a light on different types and nuances of data structure differences. These three plots are

**The CE plot:** The CE (cumulative eigenvalue) plot can be used to illustrate differences in variance components, that is, in the relative importance of the directions identified by the PCA. The CE plot is accompanied by two permutation-tests, testing the hypothesis of no difference in variance components.

**The angle plot:** The angle plot compares both loadings and variance components at once and it can be used to understand the information loss if the data structure of one dataset is superimposed on the other, thereby revealing which principal components (i.e. loading and variance component pairs) that are most similar and most different across the two datasets

**The chroma plot:** The chroma plot is primarily an illustration of the loading patterns and it targets the question of how the roles of the original variables are different between the two datasets, thus leading the data structure comparison question back to its original, empirical context.

For the deepest understanding of the data structure differences in two datasets, we suggest using all three steps in the above order.

But before diving deeper into the details of the *CE plot*, the *angle plot* and the *chroma plot*, a general remark about standardization in PCA is in place. We would like to emphasize that PCA is sensitive to scaling, as the procedure deconstructs the covariance matrix in components according to the most explained variance. This implies that if a variable has a very large sample variance (possibly because of its scale), this variable will be always be deemed highly influential, no matter the structure of the data. Therefore, the variables should always be scaled prior to performing PCA. Note that the covariance matrix for the standardized variables is the same as the correlation matrix for the original variables, so this simply corresponds to performing data structural comparisons of the correlation matrices rather than the covariance matrices. The standardization makes the variables comparable on the same scale, i.e. units of standard deviation, and it implies that the diagonal elements of  $S$ ,  $S_1$ , and  $S_2$  all equals 1, and thus also that  $\sum_{k=1}^d \lambda_k = \sum_{k=1}^d \lambda_{1k} = \sum_{k=1}^d \lambda_{2k} = d$ .

### 2.2.1. The cumulative eigenvalue plot

The cumulative eigenvalue (CE) plot compares the variation components, i.e. the eigenvalues of the covariance matrix. In order to investigate whether the same proportion of the total variation can be described by the same number of principal components in the two datasets, we plot a piecewise linear curve connecting the points

$$(0, 0), \quad (\lambda_1, \lambda_{11} - \lambda_{12}), \quad (\lambda_1 + \lambda_2, \lambda_{11} + \lambda_{12} - \lambda_{21} - \lambda_{22}), \quad \dots, \quad \left( \sum_{j=1}^d \lambda_j, \sum_{j=1}^d \lambda_{1j} - \sum_{j=1}^d \lambda_{2j} \right).$$

This may be seen as a cumulative Bland-Altman plot for the variation components ([reference to cumulative residuals and to Bland-Altman](#)). Note that due to the standardization, the last point will always be equal to  $(d, 0)$ . Thus, this curve will begin and end at the x-axis. And the larger excursions it makes away from the x-axis, the less alike the cumulative variation components for the two datasets are. Moreover, a positive cumulative differences implies that dataset 1 holds more information in the first components than dataset 2 does.

In order to test whether these cumulative differences are statistical artifacts or if they represent something real, we have implemented both the *Kolmogorov-Smirnov* and the *Cramér-von Mises* test statistics, which are given by

$$\text{KS} = \max_{k=1, \dots, d} \left| \sum_{j=1}^k \lambda_{1j} - \sum_{j=1}^k \lambda_{2j} \right|, \quad \text{CvM} = \sum_{k=1}^{d-1} \frac{\lambda_k + \lambda_{k+1}}{2} \left( \sum_{j=1}^k \lambda_{1j} - \sum_{j=1}^k \lambda_{2j} \right)^2.$$

We conduct the tests as *permutation tests*, that is, by randomly reallocating the combined and standardized datasets into two new datasets of  $n_1$  and  $n_2$  observations, respectively, and then redoing the CE plot steps and recalculating the test statistics. This should be done a large (e.g. 10000) number of times. Then, a  $p$ -value is obtained by computing the proportion of reallocated datasets that lead to even larger test statistics than the one we found for the original datasets.

The permutation test results are also used to visualize the uncertainty of the CE curve in the plots. In the CE plots shown in the following section, we plot the observed curve together with 20 of the resampled curves, as well as a shaded region visualizing pointwise 95 % coverage intervals. If the observed curve is very different from the resampled curves or if it is substantially outside the shaded region, then this also indicates differences between the two datasets.

### 2.2.2. The angle plot

This plot simultaneously compares the variation components and the loadings. Let  $\lambda_{\max} = \max\{\lambda_{11}, \lambda_{21}\}$  be the largest variation component for the two datasets. The empirical correlation matrix  $S_1$  for the first dataset has the following orthogonal decomposition in the coordinate system of the second dataset

$$S_1 = \sum_{k=1}^d \lambda_{1k} \eta_{1k} \eta_{1k}^\top = \lambda_{\max} \sum_{k=1}^d \left( \sum_{j=1}^d \sqrt{\frac{\lambda_{1k}}{\lambda_{\max}}} \eta_{2j} (\eta_{2j}^\top \eta_{1k}) \right) \left( \sum_{j=1}^d \sqrt{\frac{\lambda_{1k}}{\lambda_{\max}}} \eta_{2j} (\eta_{2j}^\top \eta_{1k}) \right)^\top,$$

and we have a similar decomposition of  $S_2$  in the coordinate system of the first dataset [Anne: it was not completely clear to me what this meant the first xx times I read it - expand?](#). We propose to visualize these two decompositions in a  $d \times d$  grid display. In the  $j$ th row and  $k$ th column of this display we plot two arrows based at the lower left corner of the grid cell. The first arrow has length  $\mu_{jk}$  and angle  $\theta_{jk}/2$  counterclockwise from the diagonal, and the second arrow has length  $\nu_{jk}$  and angle  $\theta_{jk}/2$  clockwise from the diagonal. To facilitate the following description we will refer to the arrows drawn counterclockwise as the blue arrows, and the arrows drawn

clockwise as the red arrows. The lengths  $\mu_{jk}$  and  $\nu_{jk}$  and the angle  $\theta_{kj}$  are given by

$$\mu_{jk} = \sqrt{\frac{\lambda_{1k}}{\lambda_{\max}}} |\eta_{1k}^\top \eta_{2j}|, \quad \nu_{jk} = \sqrt{\frac{\lambda_{2j}}{\lambda_{\max}}} |\eta_{2j}^\top \eta_{1k}|, \quad \theta_{jk} = \arccos(|\eta_{1k}^\top \eta_{2j}|).$$

Note that for two  $d$ -dimensional, unit length vectors  $a$  and  $b$ ,  $a^\top b = \langle a, b \rangle = \tilde{c}(a, b)$ , where  $\tilde{c}$  denotes the sample correlation. Thus, in the angle plot, we are essentially looking at the absolute values of correlations between loadings that have been scaled according to their variance component contributions. The absolute value of the projection  $\eta_{1k}^\top \eta_{2j}$  is inserted due to the indeterminacy of the direction of loading vectors. This indeterminacy implies that the angle between loadings from the two datasets always can be chosen to be in the interval  $[0, \pi/2]$ , and hence the decomposition of  $S_1$  and  $S_2$  can be visualized in a joint plot by dividing the angles by two and using counterclockwise and clockwise shifts from the diagonal. Furthermore, the scaling of the lengths by  $\lambda_{\max}$  is made so that the longest arrow has at most unit length.

In the *angle plot*, the blue arrows in the  $k$ th column of the grid display visualize the decomposition of the  $k$ th principal component for the first dataset in the coordinate system of the second dataset. Similarly, the red arrows in the  $j$ th row visualize the decomposition of the  $j$ th principal components for the second dataset in the coordinate system of the first dataset. **Can we expand on this in a non-technical way?** If the structures of the two datasets are identical, then we will have coinciding blue and red arrows along the diagonal in the grid display, and nothing else as arrows in the off-diagonal cells would have zero length. Differences in the variation components are visualized as differences in the lengths of the blue and the red arrows, also in the diagonal. And loadings in other directions than the corresponding loading from the other dataset are visualized as angle separation of the blue and the red arrows in the diagonal cells, as well as arrows of non vanishing length in the off-diagonal cells.

### 2.2.3. The chroma plot

This plot compares the loadings of the two datasets. The chroma plot consists of two panels, one for each dataset, made up of colored bars. These bars each represent a principal component and their coloring illustrates the relative weights of the  $d$  original variables, that is, their absolute, normalized loading contributions. More specifically, when illustrating the  $i$ th principal component, we plot a vertical bar of length one that has been divided into  $d$  segments of different colors and the wideness of the  $j$ th such segment is given by

$$\omega_{ij} = \frac{|(\eta_i)_j|}{\sum_{k=1}^d |(\eta_i)_k|}$$

where  $(\eta_i)_j$  denotes the  $j$ th entry of  $\eta_i$ . Due to the indeterminacy of the sign, all the signs are removed from the coefficients in the loadings. The bars are ordered according to the variation components and they are annotated with the cumulative percentage explained variance of that component, that is, the scaled and summed variance component contributions,

$$\sigma_c = \frac{\sum_{j=1}^i \lambda_j}{\sum_{k=1}^d \lambda_k} = \frac{\sum_{j=1}^i \lambda_j}{d}$$



Especially when  $d$  is large, we recommend plotting only a select set of interesting principal components, e.g. as identified by use of the angle plot. In this scenario, the annotations should rather be the non-cumulative variance contributions,  $\frac{\lambda_i}{d}$ .

The plots resulting from this procedure should be inspected focusing on two properties: Similarities in loading patterns, which will correspond to similar visual impressions, and similarities in variance contributions. For each component, the loadings describe how influential the different variables are on that component. Therefore, the chroma plot allows us to make qualitative statements about the original datasets, such that *"variable  $x$  is generally more influential in subset 1 than it is in subset 2"*, thereby helping us to understand where and why the data structure differences are found.

### 3. European differences in psychological well-being: A data example

We will now turn to a concrete data example in order to illustrate the capabilities of the methods presented above. We use data from the 2012 version of the European Social Survey (ESS) project to investigate inter-country differences in psychological well-being and happiness. This investigation is motivated by an increasingly popular new tendency to publish miscellaneous rankings of countries in fields as different as educational quality (ref: PISA stuff), XXX and citizen happiness (ref OECD?). From a methodological point of view, such international rankings are very concerning, as they rely on the fundamental assumption that the measured concepts are inherently the same across countries. The PCADSC tools qualify as a suite of methods for exploring the validity of this assumption empirically.

In the rankings of happiness, Denmark has repeatedly been awarded with the title of "happiest country" (ref?). However, little critical discussion has been aimed at whether or not this title is in any way meaningful. Does there exist such a thing as a universal, internationally valid concept of happiness? Or do different aspects of psychological well-being or happiness simply do not have the same relative meaning in different cultural and socioeconomic settings? This is in fact a question concerning comparability of data structures. If two countries differ e.g. in terms of how social networks are typically build and structured, with one emphasizing family relations and the other mostly focusing on other social relations, having a weak family connection does not have the same implications in the first country as it does in the second one. More specifically, whereas in the first country, lack of familial network might be related to loneliness, lack of general social capital and isolation, in the second country, the quality of the family network might not be informative at all about other aspects of a person's social or psychological well-being. The two countries thus differ in how different aspects or measures of psychological well-being are interrelated, which is essentially a difference in data structures. And therefore, comparing the two countries in these measures is not a meaningful endeavor.

In this section we will use the PCADSC tools to unveil such differences between Denmark and Bulgaria. These two countries have previously been highlighted to be very different in terms of what defines happiness (REF: ESS6 Topline Results Series 5). This might be the result of large, cultural and socioeconomic differences between the two countries. Therefore, a successful method for data comparisons should be able to detect these differences by looking at data on psychological well-being from these two countries.

	Denmark			Bulgaria			Sweden		
	$Q_1$	$M$	$Q_3$	$Q_1$	$M$	$Q_3$	$Q_1$	$M$	$Q_3$
Evaluative wellbeing	8.00	8.75	9.50	3.50	5.00	7.00	7.00	8.00	9.00
Emotional wellbeing	7.22	8.33	8.89	5.00	6.67	7.78	6.67	7.78	8.89
Functioning	6.93	7.57	8.21	5.50	6.68	7.68	6.39	7.04	7.68
Vitality	6.67	7.50	8.33	5.83	7.50	8.33	6.67	7.50	9.17
Community wellbeing	5.83	6.77	7.57	3.70	4.67	5.70	5.66	6.57	7.37
Supportive relationships	7.42	8.25	8.92	6.17	7.25	8.08	7.42	8.25	8.75

TABLE 1.

The 1st quartile, the median and the third quartile of the distributions of each of the six dimensions of psychological well-being, stratified by country. Note that the scales are constructed such that they all run from 0-10.

We also compare the Danish data with Swedish data in order to illustrate that the PCADSC tools actually do have some discriminatory power. Denmark and Sweden are both Scandinavian countries and are often deemed very similar in terms of culture and history. Therefore, we expect fundamental concepts such as psychological well-being to similar across these two countries.

All computations and figures presented in this section were created using our R package PCADSC, which is available online at [www.github.com/AnnePetersen1/PCADSC](https://www.github.com/AnnePetersen1/PCADSC) [maybe do a CRAN submission instead?](#).

### 3.1. Data

The ESS 2012 data contains a total of 626 variables collected from 54673 citizens in 29 countries. Here, we will only work with a subset of 35 questionnaire items that are all related to psychological well-being. These 35 items can be divided into 6 distinct scales, namely *Evaluative wellbeing*, *Emotional wellbeing*, *Functioning*, *Vitality*, *Community wellbeing* and *Supportive relationships*. More details on these scales is to be found in (ref: ESS6 Topline Results Series 5). We represent each of these scales by a single variable, which is calculated as the average score within the items related to that variable (ref to someone that says that is sensible?) and scaled such that it takes a value between 0 and 10. For simplicity, we use only complete cases for this construction and thus exclude all participants that did not answer all the 35 questionnaire items used below. This gives us  $n_{DK} = 1498$  observations in the Danish sample,  $n_{BG} = 1798$  observations in the Bulgarian sample and  $n_{SE} = 1736$ . Table 1 summarizes the marginal distributions of the six dimensions of psychological well-being, stratified by country.

### 3.2. Comparing Denmark and Bulgaria

Figure 1 presents the CE plot and the angle plot obtained from comparing the Danish and Bulgarian psychological well-being scales. The CE plot shows a remarkable degree of lacking comparability: The cumulative difference in the eigenvalue by far exceeds what could come about randomly if there really was no difference in the data structure. This is also confirmed by the Kolmogorov-Smirnov and the Cramér-von Mises tests, which both result in  $p$ -values that are virtually zero.

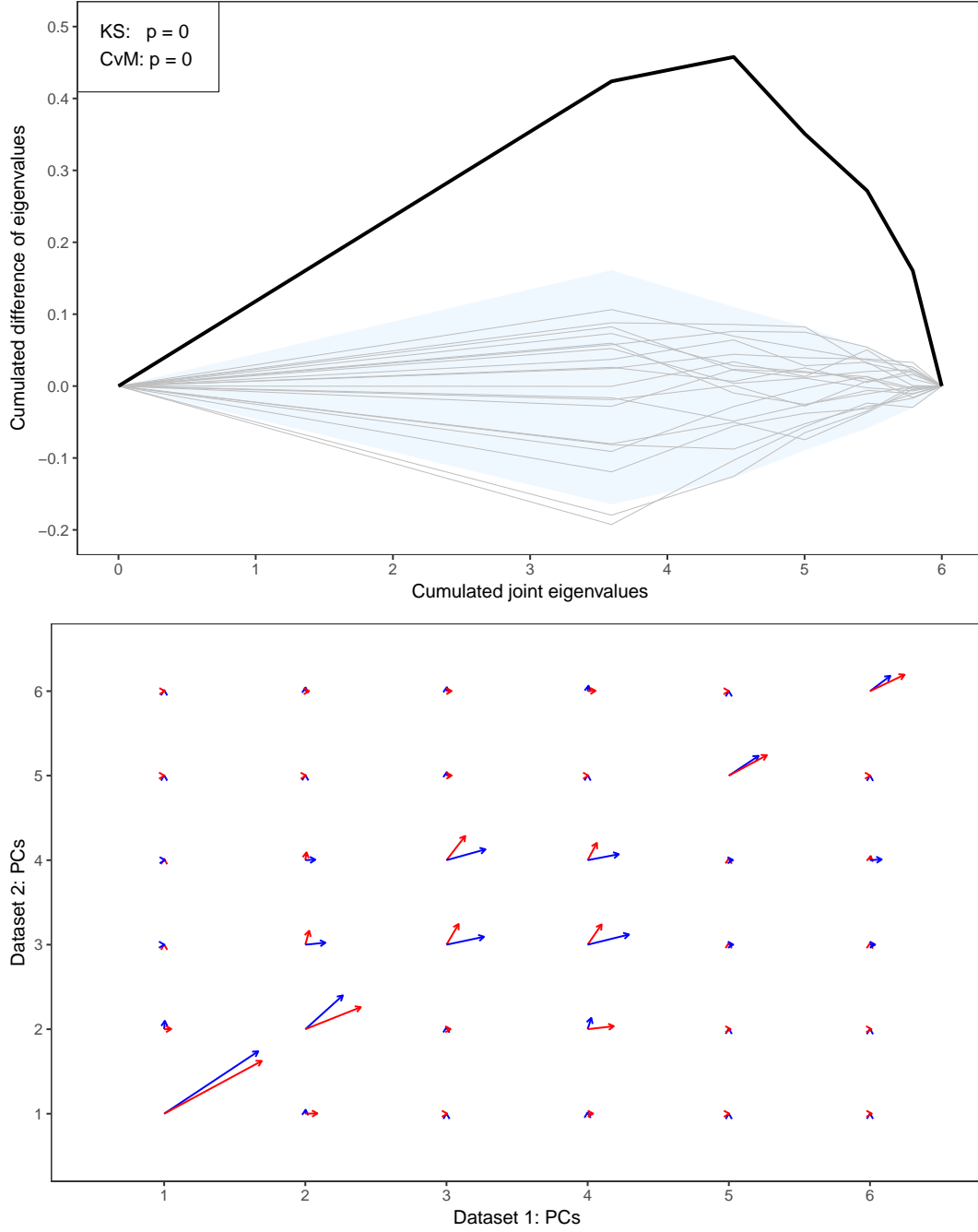


FIGURE 1.

The CE plot (top) and the angle plot (bottom) resulting from comparing Bulgarian and Danish data on psychosocial well-being. Dataset 1 refers to the Bulgarian subsample, while Dataset 2 is the Danish data. The CE plot is annotated with the  $p$ -values of the Kolmogorov-Smirnov and the Cramér-von Mises tests of the assumption of no difference in data structures. In the angle plot, the blue arrows show the principal components of the Bulgarian dataset decomposed in the coordinate system of the principal components of the Danish dataset, while the red arrows illustrate the reverse.

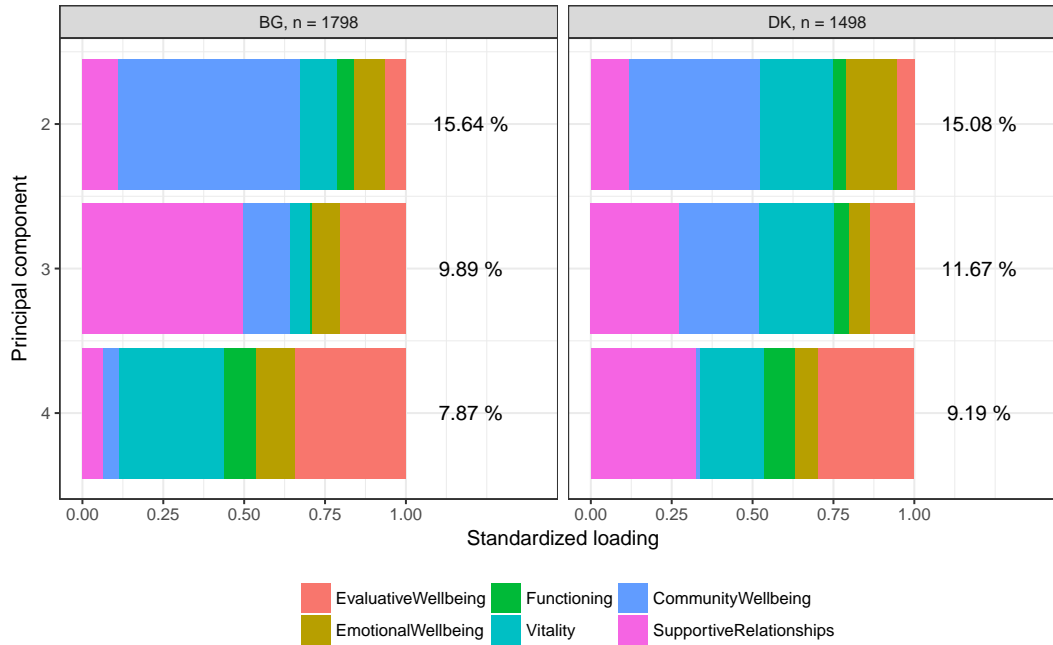


FIGURE 2.  
something

Moving on to the angle plot, we find that the differences are primarily to be found in the second, third and fourth principal components (PCs): The blue arrows visualize the decomposition of the principal components for the first dataset in the coordinate system of the second dataset. We see that PC2 also loads on PC3, that PC3 also loads on PC4, and that PC4 also loads on PC2 and PC3. The red arrows visualize the decomposition of the principal components for the second dataset in the coordinate system of the first dataset. Here, we see that PC2 also loads on PC4, that PC3 also loads on PC2 and PC4, and that PC4 also loads on PC3. Thus, if we wish to understand why differences in the data structures occur, an inspection of the loadings of components 2, 3 and 4 might be informative.

The chroma blot in Figure 2 allows us to look closer into these components. Here, we find that the relative importance of the *Community wellbeing* and *Supportive relationships* scales is much larger in the Bulgarian sample than in the Danish. In the Danish data, on the other hand, we find that *Vitality* and *Emotional well-being* seem to play bigger roles, as they appear with larger loadings in more high-ranking components in this sample, relative to the Bulgarian.

All in all, we find that psychological well-being does not seem to be the same concept in Bulgaria as in Denmark. The two countries disagree both in how many dimensions are needed to capture the most important parts of the concept (as illustrated by the differences in eigenvalue) and in how these dimensions are then weighted among the 6 scales (as illustrated by the angle and chroma plots). In Bulgaria, interpersonal features seem to be more informative of psychological wellbeing, whereas in Denmark, individual characteristic play a relatively bigger

role. Thus, the datasets are fundamentally different and that we should therefore be wary about combining them in a joint analysis, which was also the conclusion of the ESS authors, though based on country-level aggregated statistics.

I have dropped the Wally-plots for now, as I'm not really sure they are that useful.

### 3.3. Comparing Denmark and Sweden

We now turn to the comparison of Denmark and Sweden in terms of psychological well-being. Figure 3 show the CE and angle plots for these two countries. In the CE plot, we now find the cumulative eigenvalue curve to be just within the acceptance region of the null-hypothesis. This is also reflected by the two tests, which now produce  $p$ -values of  $p_{KS} = 0.14$  and  $p_{CvM} = 0.09$ , respectively, thus accepting the null-hypothesis at the typical 5% level, but not with overwhelming evidence.

The angle plot from Figure 3 shows that the two datasets agree very strongly about the relative importance of the six scales in the six PCs, as almost all off-diagonal arrows are practically non-existent. This implies that if one already has e.g. the information held in the first PC from the Danish data, this information is in itself mostly sufficient to describe the first PC of the Swedish data.

Looking at the chroma plot in Figure 4, the same tale is told once again: Here, we find remarkably similar loading patterns in the first three components (which are responsible for almost 80 % of the variance in both datasets), and slight, but increasing, differences in the remaining three components. We therefore conclude that any differences in the data structures of the Danish and the Swedish samples are related to the least important dimensions of the datasets and that these dimensions are only responsible for less than 25 % of the variance in both datasets. In particular, this means that we can combine and compare the Danish and Swedish datasets in a meaningful way and e.g. conclude using Table 1 that in general, Danes seem to be somewhat more happy than Swedes, and in particular, the unhappy people in Denmark (represented by the 1st quartiles) are generally a lot happier in Denmark than they are in Sweden. A more thorough, statistical investigation could now be put to work on answering *why* this seems to be the case.

## 4. Discussion

When deciding whether to combine two data sets for analysis, the issue of heterogeneity across data sets must be addressed. Simple methods suffer drawbacks and will likely scale poorly. Parametric models using, e.g., latent variable models moves beyond the marginal approach, but need a pre-specified model.

New tools, referred to collectively as Principal Component Analysis-based Data Structure Comparisons (PCADSC), for the task of deciding if the two two data sets can be combine for analysis were proposed and discussed in the paper. They employ the principal component decomposition of the empirical covariance matrix performed on two subsets of a dataset in order to create intuitive visualizations of data structure differences yielding a solution that is largely independent of the sizes the two data sets.

The methodology is quite general and in principle any plot that can be made can be included ('di-scree plot') ... [rephrase!!]

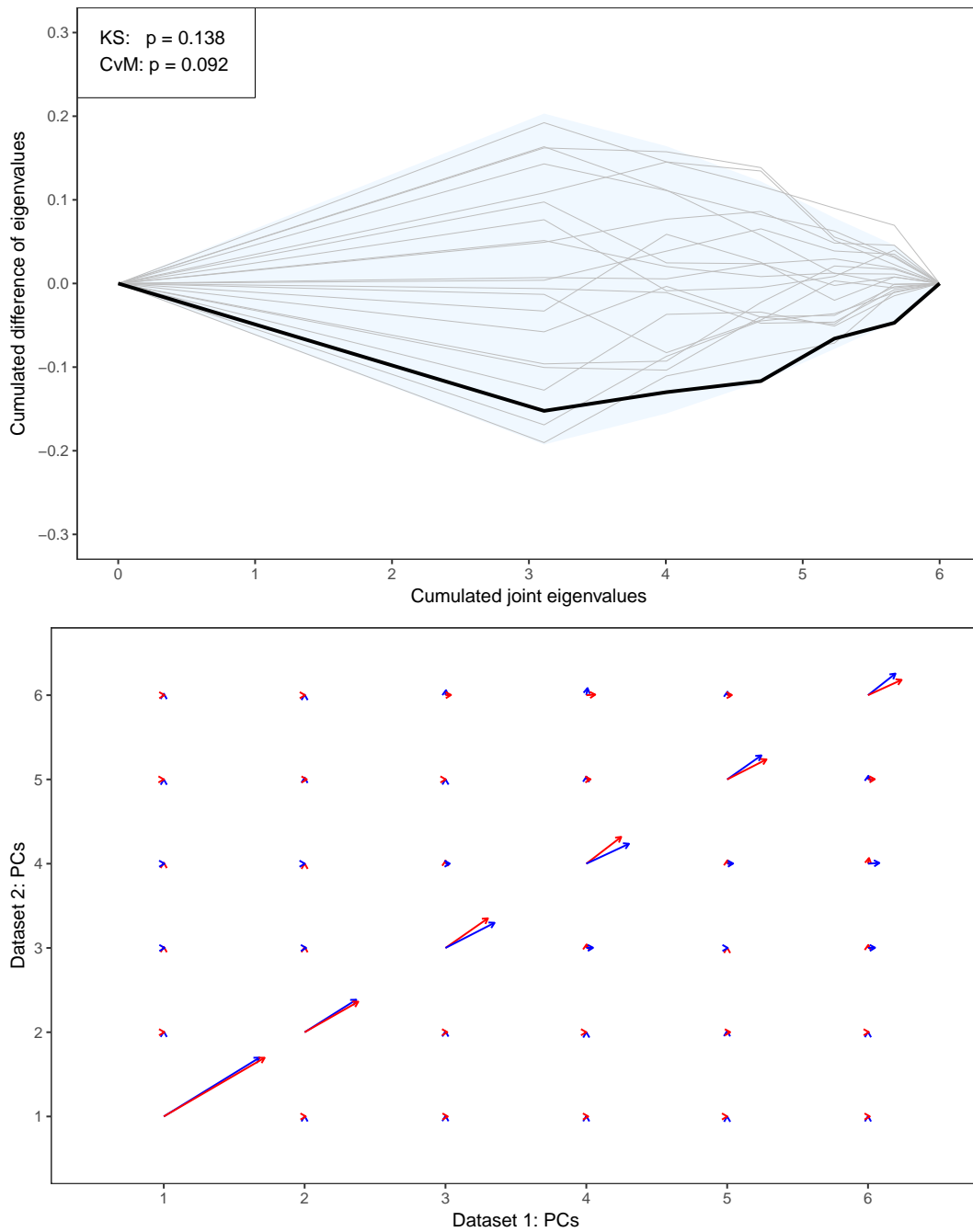


FIGURE 3.

A CE (top) and a hair (bottom) plot for comparing the Danish (Dataset 1) and the Swedish (Dataset 2) psychological well-being data. The blue arrows show the principal components of the Danish dataset decomposed in the coordinate system of the principal components of the Swedish dataset, and the red arrows illustrate the reverse.

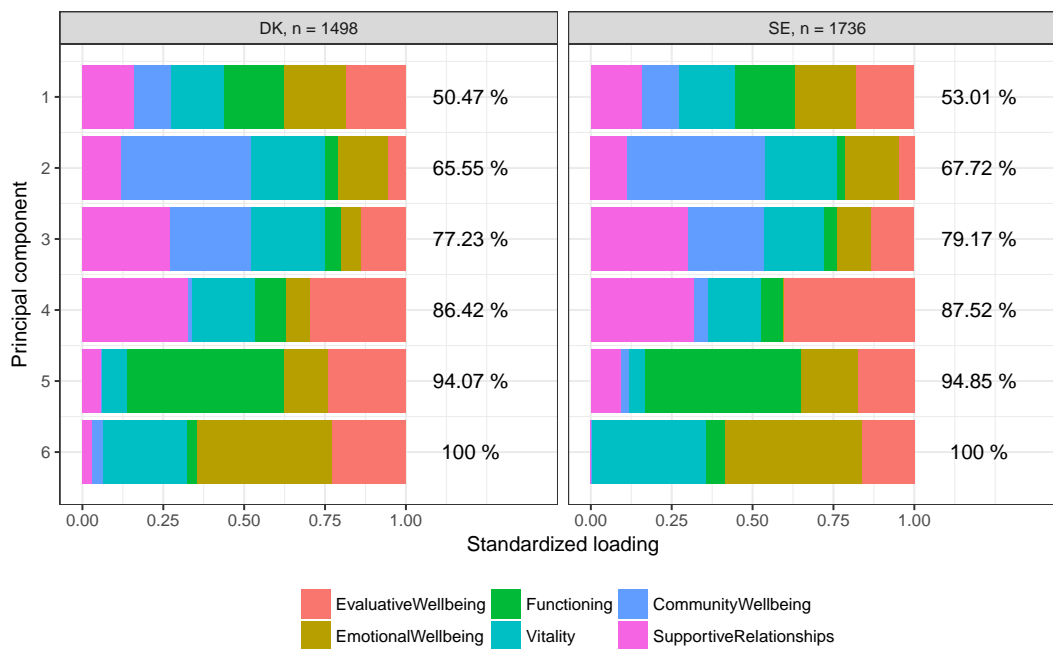


FIGURE 4.

A chroma plot for comparing the loading patterns of the Danish and the Swedish subsamples. Note that the bars for each component is annotated with its cumulative variance score, that is, how much variance can be explained by having information of this and the preceding components.

Further topics need to be addressed. These include generalizing the methods to be able to address (i) binary, ordinal or even nominal categorical variables, (ii) covariance matrices that are not of full rank.

More evaluation of the performance is also needed. Investigating sensitivity towards the sample sizes  $n_1$  and  $n_2$

The limitations of the PCADSC procedures should also be studied in more detail. It seems unlikely that the procedure would be able to disclose differences in scaling, since all variables are standardized in the procedure. This type of heterogeneity should thus be adjusted for in later analyses of the combined data set.



## References

- Brambilla, D. J. and McKinlay, S. M. (1987). A comparison of responses to mailed questionnaires and telephone interviews in a mixed mode health survey. *American journal of epidemiology*, 126(5):962–71.
- Liu, M. (2016). Comparing data quality between online panel and intercept samples. *Methodological Innovations*, 9:2059799116672877.
- McHorney, C. A., Kosinski, M., and Ware, J. E. (1994). Comparisons of the costs and quality of norms for the SF-36 health survey collected by mail versus telephone interview: results from a national survey. *Medical care*, 32(6):551–67.
- Powers, J. R., Mishra, G., and Young, A. F. (2005). Differences in mail and telephone responses to self-rated health: use of multiple imputation in correcting for response bias. *Australian and New Zealand journal of public health*, 29(2):149–54.