Penguins Go Parallel: a grammar of graphics framework for generalized parallel coordinate plots

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Abstract

Parallel coordinate plots (PCP) are a valuable tool in exploratory data analysis of high-dimensional numerical data. The use of PCPs is limited when working with categorical variables or a mix of categorical and continuous variables. In this paper, we propose generalized parallel coordinate plots (GPCP) to extend the ability of PCPs from just numeric variables to dealing seamlessly with a mix of categorical and numeric variables in a single plot. In this process we find that existing solutions for categorical values only, such as hammock plots or parsets become edge cases in the new framework. By focusing on individual observations rather than a marginal frequency we gain additional flexibility. The resulting approach is implemented in the R package ggpcp.

Contents

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Broad Comments:

- Replace fleas with penguins
- Make colors consistent - gentoo are always ___ color - but with a different (but consistent) color scheme in the clustering example.
- Leave out missing data until it's explicitly discussed in the example with labeled ? points

1 Introduction

Few approaches in data visualization exist that are truly high-dimensional. Most visualizations are projections of data into two or three dimensions enhanced by facetting or additional mappings to plot aesthetics, such as point size and color. Parallel coordinate plots are one of the exceptions: in parallel coordinate plots we can actually visualize an arbitrary number of variables to get a visual summary of a high-dimensional data set. In a parallel coordinate plot, each variable takes the role of a vertical (or parallel) axis; giving the visualization its name. Multivariate observations are then plotted by connecting their respective values on each axis across all axes using polylines (cf. Figure 1). For just two variables this switch from orthogonal axes to parallel axes is equivalent to a switch from the familiar Euclidean geometry to the projective space. In the projective space, points take the role of lines, while lines are replaced by points, i.e. points falling on a line in the Euclidean space correspond to lines crossing in a single point in the projective space. This duality provides a good basis for interpreting geometric features observed in a parallel coordinate plot [Inselberg, 1985].

The origins of parallel coordinate plots date back to the 19th century and are, depending on the source, either attributed to d'Ocagne [1885] or Gannett [1880]. Modern era parallel coordinate plots go back to Inselberg [1985] and Wegman [1990]. Parallel coordinate plots are used in an exploratory setting as a way of getting a high-level overview of the marginal distributions involved, identifying outliers in the data, and finding potential clusters of points. In the absence of those, Parallel Coordinate Plots are often criticized for the amount of clutter they produce, resembling a game of mikado (also known as pickup-sticks – if you are not familiar with the game, imagine spilling a box of spaghetti) rather than organized data. This clutter is sometimes mitigated by the use of α-blending [Miller and Wegman, 1991], density estimation [Heinrich and Weiskopf, 2009], or edge-bundling parallel coordinate plots [McDonnell and Mueller, 2008]. For a detailed overview of these and other techniques see Heinrich and Weiskopf [2013].

While parallel coordinate plots are a powerful tool using categorical variables alongside quantitative variables is a great challenge. In current solutions, levels of categorical variables are transformed to numbers and variables are then used as if they were numeric. This introduces ties into the data, and the resulting parallel coordinate plot becomes uninformative, as it only shows a mesh of lines from each level of one variable to each level of the next variable. Some versions of parallel coordinate plots have been specifically developed to deal with categorical data: parallel set plots [Kosara et al., 2006], Hammock plots [Schonlau, 2003], and common angle plots [Hofmann and Vendettuoli, 2013], but these solutions do not accommodate quantitative variables. Instead, they are intended for use with tabular data and show bands of observations from one categorical variable to the next. Hammock plots and common angle plots mitigate effects of the sine-illusion [Day and Stecher, 1991, VanderPlas and Hofmann, 2015] on parallel sets plots. An attempt to combine categorical and numeric variables in a parallel coordinate plot is introduced in the categorical parallel coordinate plots of Pilhöfer and Unwin [2013] by treating factor variables as numeric. Similar to parallel sets, this approach is also based on marginal frequencies for the categorical variables. Categorical parallel coordinate plots are the closest of these variations to our solution, but the `extracat` package has not been updated recently and is no longer on CRAN.

The remainder of the paper is organized as follows: section 2 introduces the `ggpcp` syntax and explains the improvements in `ggpcp` over other parallel coordinate plot software packages. section 3 describes the data processing for parallel coordinate plots and how this wrangling is separated from the plot rendering in `ggpcp`. section 4 discusses the rendering of parallel coordinate plots and factors such as plotting order

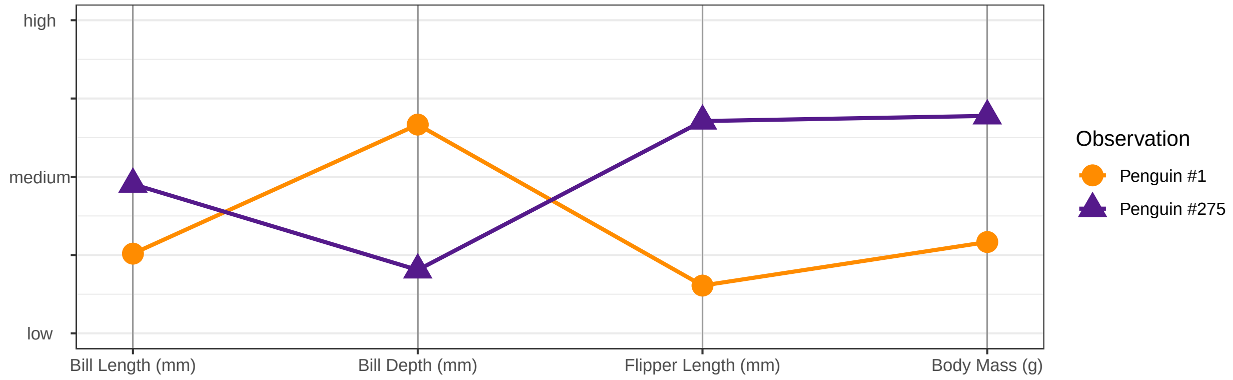


Figure 1: *Sketch of a parallel coordinate plot of two observations in four dimensions. Each dimension is shown as a vertical axis, observations are connected by polylines from one axis to the next.Two penguins from the Palmer Penguin data set (see section 5) were sampled for this example.*

and tie-breaking which are important for the design of PCPs. **??** provides three examples which highlight the use of generalized PCPs in exploratory settings.

2 Motivation and Package Usage

An important motivation for the 'ggpcp' package is that other implementations of parallel coordinate plots for categorical variables make it difficult to follow a single observation across the chart. 'ggpcp' alleviates this difficulty with two new developments: careful treatment of categorical variables to prevent line intersections at vertical axes, which maintains the visual ability to follow individual cases across the chart, and methods for ordering observations within categorical variables to reduce the amount of visual clutter. Together, these features allow for easier perception of lines in generalized parallel coordinate plots: by reducing the number of intersecting lines at pivot points along the vertical axes, we allow our brains to leverage the gestalt principle of good continuation to follow one line across the plot. Reducing the number of line crossings at non-axis points simplifies the plot, reducing the overall cognitive load required to "untangle" (literally and metaphorically) the individual observations.

Listing 1: *A demonstration of ggpcp's data wrangling and plotting API.*

```
pcp <- penguins %>%                       # data management:
  pcp_select(species, 3:6, sex) %>%       #   variable selection, see section 3.1
  pcp_scale(method="uniminmax") %>%       #   setting scaling method, see section 3.2
  pcp_arrange() %>%                       #   arranging categorical data
  ggplot(aes_pcp()) +                     # plotting the chart:
    geom_pcp_axes() +                     #   vertical lines for axes
    geom_pcp(aes(colour = species))       #   parallel coordinate line segments
```

In addition, ggpcp leverages the full ggplot2 philosophy instead of using highly specific wrapper functions, allowing users to focus on the data, rather than the names of various parameters used for customization. ggpcp adopts tidy conventions for data wrangling, separating the necessary data manipulation to generate a parallel coordinate plot from the visual rendering. Scaling, ordering of cases, and the arrangement of the parallel axes are completed using `pcp_select`, `pcp_arrange`, and `pcp_scale`,respectively; the resulting data frame is then passed directly into the familiar `ggplot()` call. During the plotting state, the only modification from default `ggplot2` syntax is the use of `aes_pcp()` in place of `aes()`; this is necessary to handle the multiple axes in a parallel coordinate plot while maintaining the ability to map all other variables of the original data frame to aesthetics such as linetype and color. The user has complete control over layers such as PCP lines (`geom_pcp`), labels (`geom_pcp_labels`), and boxes around categorical variables (`geom_pcp_boxes`), but there are additional advantages to the use of `ggplot2`. Users can also augment their parallel coordinate plots with additional information, such as boxplots or violin plots, with standard ggplot2 syntax.

One of the strengths of `ggplot2` is its handling of small multiple plots with `facet_grid` and `facet_wrap`; these functions are fully supported in `ggpcp`.

In addition, basing `ggpcp` on `ggplot2` expands the functionality available to users without much additional code, thanks to other packages such as `plotly` [Sievert, 2020] which leverage `ggplot2` to create interactive graphics for the web and `gridSVG` [Murrell and Potter, 2020] which exposes vectorized graphics to allow programmable changes, such as elementary interactions with graphical elements.

3 Data management

One of the ideas behind this re-implementation of parallel coordinate plots is to expose parallel coordinate plots at a functional level. Rather than using a single function with parameters controlling every aspect, we separate the data management from the visual rendering. In particular, we separate out the data management into three parts:

1. Variable selection and reshaping data,
2. Scaling of axes, both at the individual level and in the relationship of the axes to each other, and
3. Treatment of ties in categorical axes.

XXX Cite subfigure above with code XXX

The modularization of the data wrangling process has the additional advantage of laying out the necessary elements in successive steps. Some of these steps are optional - e.g. scaling variables might not be necessary, if all variables are already on the same scale (i.e. method 'raw' in GGally); similarly, using pcp_arrange to break ties is only necessary if there are any factor variables, and if we actively want to spread these observations out. In addition, by exposing these elements of the pcp data wrangling process, we allow users to create additional functions for handling these tasks.

The treatment of ties is an aspect not generally addressed in the original parallel coordinate plots of Inselberg [1985] and Wegman [1990]. We have found a need to deal with ties, because ties are visually the main obstacle of allowing the viewer to follow an observation from axis to axis through the high-dimensional space. If we can track a single observation through the high-dimensional space, we have the ability to look beyond the two-variable associations of adjacent axes. This allows users to more easily summarize main trends and identify observations which do not follow those trends. When ties cannot be separated and users cannot follow individual observations, higher-dimensional insights are next to impossible.

3.1 Variable Selection and Order of the Variables

One of the biggest strengths of the Grammar of Graphics is its mapping between data variables and visual aesthetics. In standard plots any mapping is a function between one data variable and one aesthetic. In a parallel coordinate plot, this one-to-one mapping between data and plot aesthetics is seemingly turned into a one-to-many mapping between arbitrarily many data variables to the x axis. By transforming the wide form of the data set into a long form [Wickham, 2014, 2021], we get to a version of the dataset in which we achieve a one-to-one mapping to a now discrete x axis consisting of the (names of the) original data variables.

From the user's perspective this data reshaping is purely a form of a data selection, while the data wrangling is going on behind the scenes in `pcp_select`:

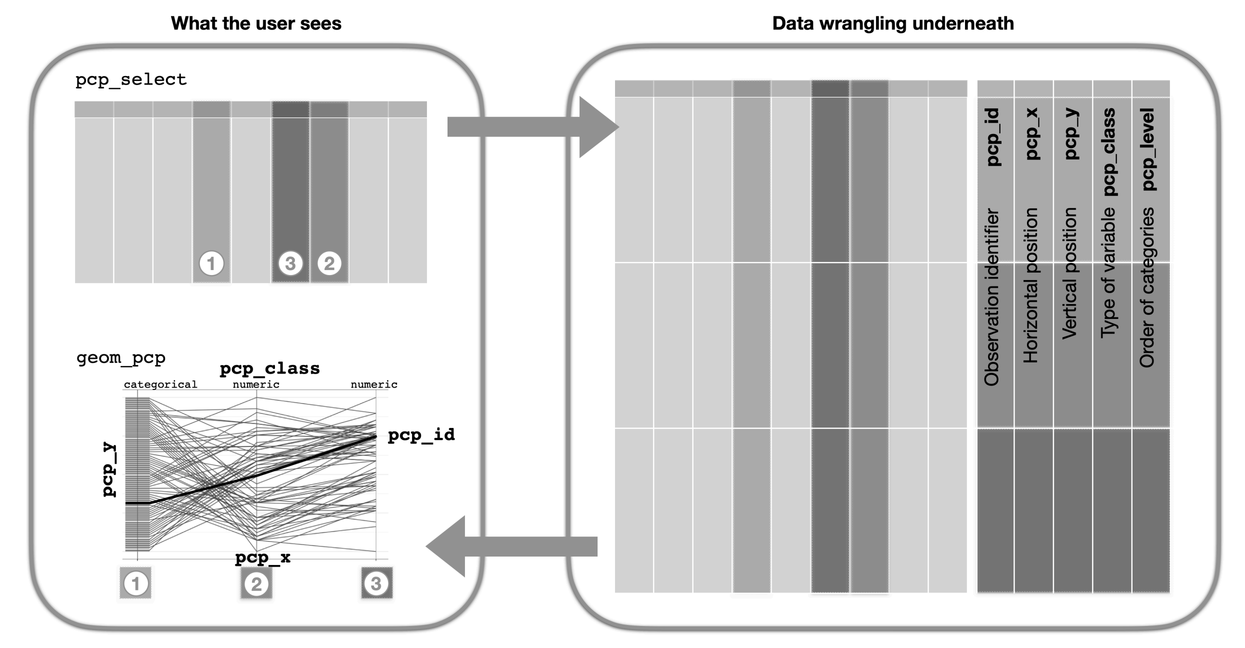


Figure 2: *The user selects a set of three variables (top left). On the right, an overview of the data wrangling step before a parallel coordinate plot can be drawn (bottom left). Note that the order in which variables are selected is reflected in the order in which variables are included in the parallel coordinate plot.*

`pcp_select(data, ...)` selects the variables to be included in the parallel coordinate plot. Variables can be specified by any combination of the following methods:

- position, e.g. `1:4, 7, 5, 4,`
- name, e.g. `class, age, sex, aede1:aede3` or
- using pattern selectors, e.g. `starts_with("aede")`, see `?tidyselect::select_helpers`

Variables can be selected multiple times and will then be included in the data and the resulting plot multiple times. Note that the order in which variables are selected determines the order in which the corresponding axis is drawn in the parallel coordinate plots. `pcp_select` transforms the selected variables to long form and embellishes the data set with a number of additional variables. All of the newly created and added variables start with the prefix `pcp_`:

- `pcp_id`: integer variable identifying each observation in the original dataset. This variable is used as the grouping variable to identify which values should be connected by a line segment in the parallel coordinate plot.
- `pcp_x`: discrete variable consisting of the names of the selected variables in the order that they were selected - this is the order in which the variables will be included in the plot.
- `pcp_y`: numeric variable containing the values of all of the selected variables. In case a selected variable is not numeric, it is converted to a factor variable and the (numeric) factor levels are saved in `pcp_y`.
- `pcp_class`: character variable containing the class information of a selected variable.
- `pcp_level`: character variable containing the factor levels of selected data variables. In case of numeric variables, the data values are stored (in textual form). The ordering of factor variables will be discussed below but is implemented using this added variable.

As a consequence of these design decisions, users have several ways of performing different tasks within the flow of generating data for a parallel coordinate plot. For instance, users can reorder variables using `pcp_select` or after variable selection using the `pcp_x` variable.

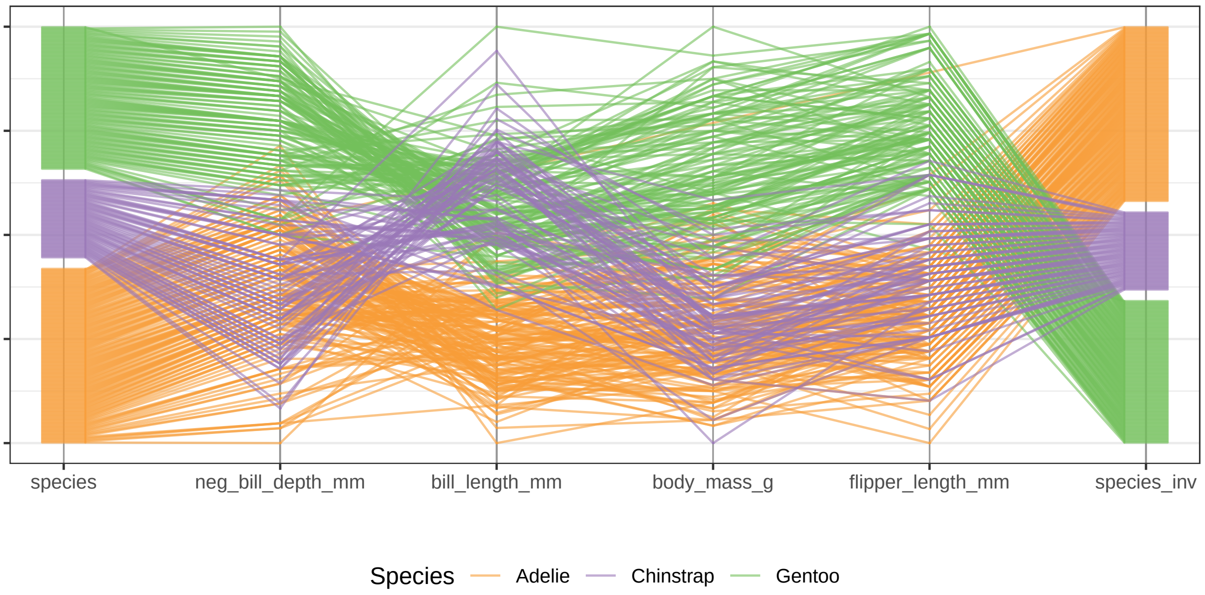


Figure 3: *The left-most axis shows species, where the right-most axis shows the same variable with categories reordered; similarly, `neg_bill_depth_mm` shows the bill depth, multiplied by -1 to invert the order of data points.*

Users can transform individual variables, reordering factors or reversing an axis, using a mutate statement bfeore variable selection, as shown in Listing 2, which generates Figure 3. Univariate transformations like these may be useful to reduce the overall visual complexity of a parallel coordinate plot by reducing the number of anticorrelated axes in sequence.

Listing 2: *Mutations before the `pcp_select` stage can be used to reorder factors or transform numerical variables, as shown in Figure 3.*

```
penguins %>%
  mutate(
    species_inv = factor(species, levels = rev(levels(.$species))),
    neg_bill_depth_mm = —bill_depth_mm) %>%
  pcp_select(species, neg_bill_depth_mm, 3, 6, 5, species_inv) %>%
  pcp_scale(method="uniminmax") %>%
  pcp_arrange() %>%
  ggplot(aes_pcp()) +
    geom_pcp_axes() +
    geom_pcp(aes(colour = species), alpha = 0.6) +
    geom_pcp_labels()
```

Ordering of levels in factor variables (XXX not sure where to put this, yet): What we are doing with the ordering of levels in factor variables, is to stick with the basic interpretation of factor variables as a type of variable that has both labels and an ordering of those labels. Whenever we assign a numeric value to the ordering, we refer to the associated score, which is an integer value from one to the number of categories, if not specified explicitly otherwise. Ordered factors are plotted from the lowest level upwards. If a factor legend is included, it will need to be reversed to match this order. Use `guides(color = guide_legend(reverse=TRUE))` as shown in the example in subsection 5.2.

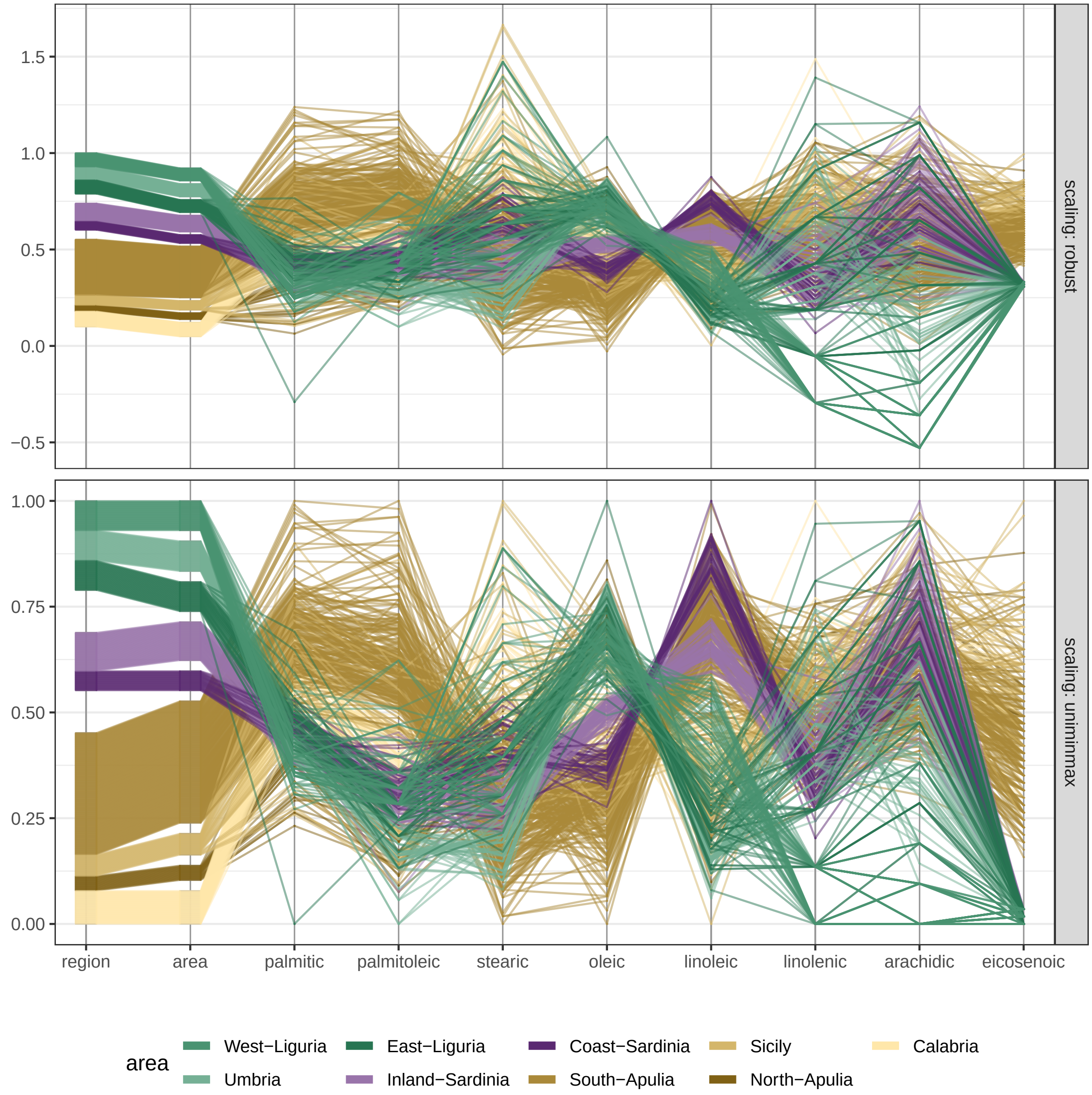


Figure 4: *Two scaling methods showing fatty acid compositions of olive oils from different regions in Italy, areas within each region are colored using similar hues within region (green for Northern Italy, purple for Sardinia, and tans for Southern Italy).robust scale: median to 0 check units XXX The two scaling methods roughly allow the same conclusions.*

3.2 Scaling

`pcp_scale(data, method)` scales the values on each axis and determines the relative relationship of the axes to each other.

`method` is a character string specifying the method to be used when transforming the values of each variable onto a common y axis. By default, the method `uniminmax` is chosen, which univariately scales each variable onto a range of [0,1] with the minimum at 0 and the maximum at 1. `globalminmax` maps the values across all axes onto a an interval of [0,1]. This method should only be used if the values across all variables are comparable. The method `robust` normalizes values univariately by mapping the median value to 0.5 and a robust 95% confidence interval (based on the median absolute deviation) to an interval of 0 to 1.

Figure 4 shows two of the scaling methods applied to the olive oil data [Forina et al., 1983, Wickham et al., 2011]: Measurements of fatty acids in 572 olive oils from three different regions in Italy are visualized as parallel coordinate plots. Similar to the findings in Cook and Swayne [2007], we see that eicosenoic acid is only found in increased quantities in olive oils from Southern Italy. Quantities of oleic and linoleic acids allow a separation between olive oils from Sardinia and Northern Italy. Both scaling methods enable us to find these conclusions. While uniminmax scaling uses the space allotted to the chart most efficiently, the robust normalization method emphasizes the heavy tails and skewness of some of the measurements, such as the percentages of stearic and arachidic fatty acids.

4 Visual Rendering

4.1 Breaking ties on categorical axes

XXX How to deal with ties has a huge visual impact. In order to get to that we need to do some more data wrangling. This subsection is somewhere between data management and visualization.

XXX it might be good to separate the section into ’how’ (data) and ’why’ (visual aspects).

Assigning all cases of the same level to the same point on the axis of a categorical variable makes it impossible to distinguish them. The approach of ‘ggpcp‘ is to draw boxes proportional to the numbers of cases in each level and to order the cases within their boxes so that visual clutter is minimised and individual cases can be followed. This idea is implemented in the ‘ggpcp‘ function `pcp_arrange(data, method, space)`. The two implemented methods are `"from-left"` and `"from-right"`, meaning that ties are broken using a hierarchical ordering determined by variables values from the left or the right, respectively. The parameter `space` specifies the amount of the y axis to use for space between levels of categorical variables. By default, 5% of the axis is used for spacing.

XXX hierarchical ordering seems to minimize line crossings - but I don’t have a proof. If we have a reference on ordering metrics this might go well here

Figure 5 shows several approaches of dealing with categorical variables in parallel coordinate plots. The left-most panel shows two categorical variables and the typical net of lines that forms between them in an original parallel coordinate plot. The other three panels show three different approaches of breaking the ties resulting from the categorical variables, with our favored solution shown on the right: all observations are spaced out evenly. This results in a natural visualization of the marginal frequencies along each axis (additionally enhanced by the lightly greyed boxes grouping observations in the same category). The ordering of the observations within the level is such that a minimal number of line crossings occurs between the axes. This method of dealing with categorical variables is the one we propose in the generalized parallel coordinate plot. While it is aesthetically pleasing, it also allows us in the spirit of the original parallel coordinate plots to follow an individual observation from left to right through the plot even for categorical variables. The other two solutions in the middle panels of Figure 5 show two intermediary solutions of breaking ties in categorical variables: jittering and equi-spaced (unordered) values.

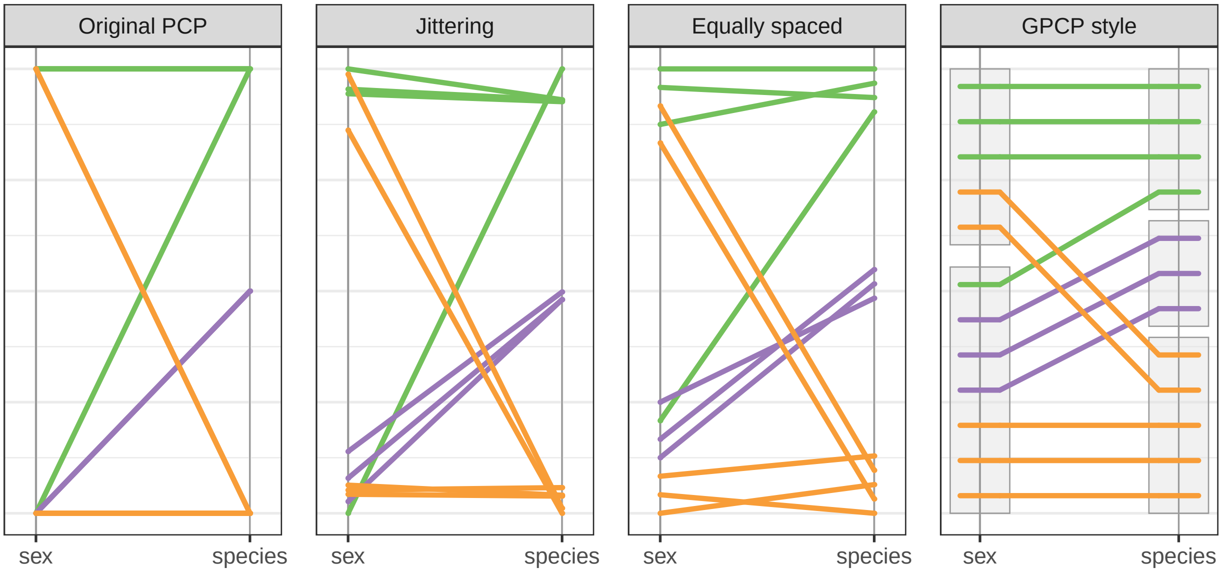


Figure 5: *Using 12 randomly sampled penguins from the Palmer penguin data, we show four different approaches of dealing with categorical variables: the panel on the left shows the typical net of lines resulting from categorical variables in regular parallel coordinate plots. In the other three panels, ties in categorical levels are broken using different approaches (from left to right): jittering, equi-spaced line segments and ordered equi-spaced line segments are shown.*

4.2 Plotting Order of line segments

XXX We need to include some code somewhere to also show the 'how'.

XXX Order of levels and order of variables are important. Drawing pcps depends on what your goal might be.

One of the primary advantages of the generalized approach to dealing with categorical variables is the ability to follow a single observation throughout the plot. As the number of observations increase, this becomes less feasible because of overplotting of line segments, particularly for slightly larger data sets. As more observations and line segments are drawn, more lines cross each other, increasing the effort required to follow a polyline from one side of the plot to the other. XXX the order in which crossing lines are drawn is only visible when the lines have different colors. As a countermeasure we carefully control the order in which line segments are plotted.

Two methods to control this order are implemented and are regulated by the parameter `overplot`:

1. `"small-on-top"` groups of lines (defined by the same color) between categorical variables are are ordered by size and drawn from largest to smallest group.

2. `"none"` the order of the observations is left un-touched by the data wrangling process. This option allows the user to specify a certain order before plotting.

additional counter-measures: use α-blending

the option of `"none"` is very flexible.

5 Examples

5.1 Palmers Penguins

Several aspects in Parallel Coordinate Plots depend on orderings: order of variables along the x axis, order of levels in a categorical variable, and order in which lines are drawn. Different orders emphasize different aspects of the data. Changing orders should therefore (a) have good defaults, and (b) be easily changeable.

XXX Drawing pcps depends on what your goal might be. It reminds me of rotating plots and all the optimisation criteria that were suggested for a variety of purposes. They did not necessarily work well, but they suggested some ways to proceed and generally improved things a bit. What criteria might be similarly helpful for pcps?

Figure 6 shows a generalized parallel coordinate plot of the Palmer penguins data [Horst et al., 2020]. The data consists of body measurements, such as weight, flipper length, bill length, and depth, of three species of penguins. What can be seen is that Adelie penguins generally have smaller bill lengths than the other two species, while Gentoo penguins can be distinguished from the other two species by their relatively larger flipper lengths.

5.1.1 Distinguishing species

Figure 6 shows the effect of re-ordering the levels of both the 'species' and the 'island' variable in the generalized parallel coordinate plots. This re-ordering of factor levels has the effect of emphasizing the fact that Gentoo penguins and Chinstrap penguins are each found on only one island, while Adelie penguins are found on all three islands.

study ID is what? ordering in second plot allows us to see that about the same amount of datat from penguins in each species was collected.

figure 6 and 7 look quite similar, but are quite different - visual emphasis? Maybe use colors[1] and colors [3]?

In addition to the ordering of factor levels, it is also important to carefully order the variables on the x-axis, as shown in Figure 7, where the variables have been re-ordered to allow the viewer to see what body measurements distinguish the species. Note that besides the re-ordering, the axes for bill depth is also reversed. XXX explain why this helps Again, this reversal helps with distinguishing between species: Gentoo penguins have the lowest bill depth, while generally having the longest flippers. Reversing the axis for bill depths, aligns the smallest bill depths with the longest flippers, thereby moving Gentoo penguins closer together as a group. The plot shows that the Gentoo penguins are bigger, that Gentoo and Chinstrap are both only found on single islands, and, finally, that Adelie and Chinstrap are distinguished by the lengths of their bills.

Note that we are using facetting by penguins' sex in Figure 7. While all of the results are the same for the two sexes, any variability of body measures due to sex is removed from the plot by facetting. This makes the results stand out more.

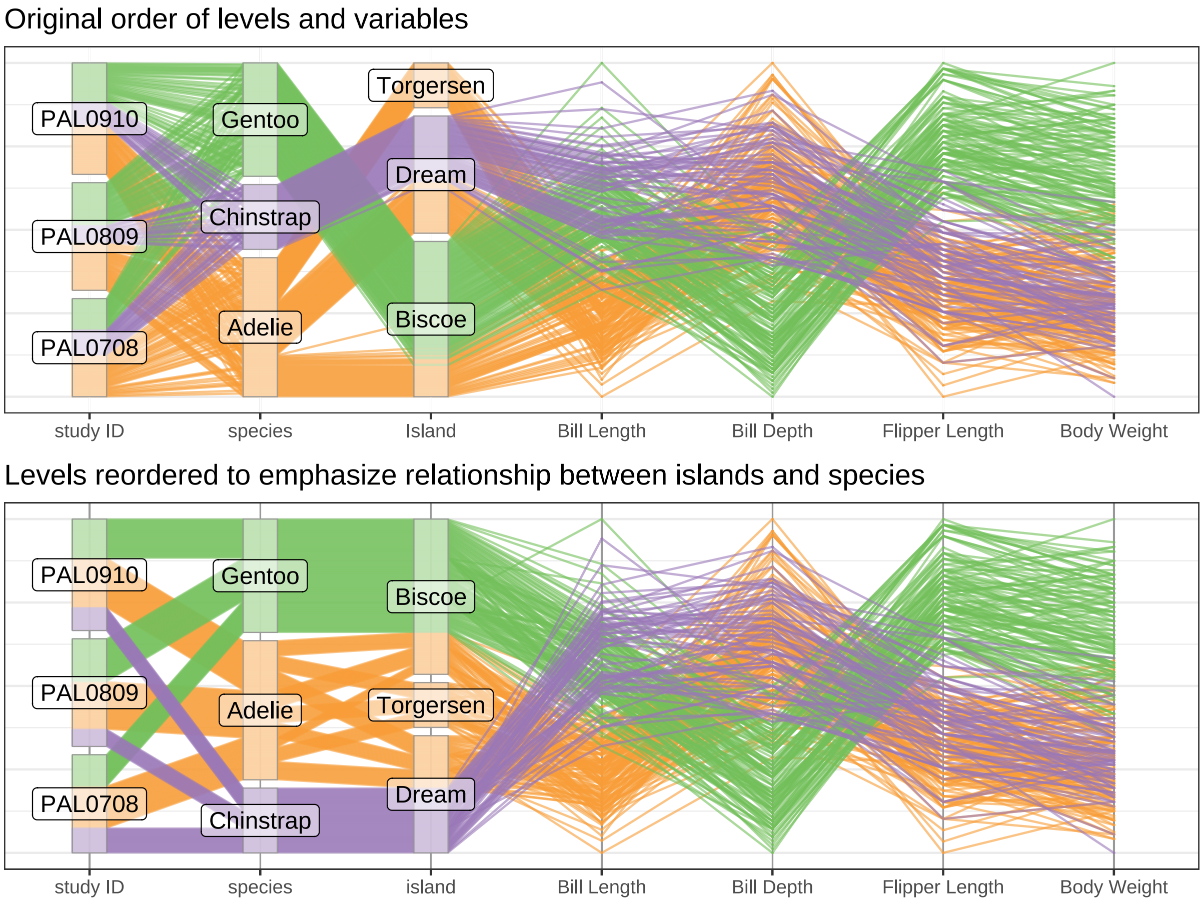
Interestingly, some potential outliers that were not visible previously, now become visible. Note for example the two Gentoo males with particularly short flippers.

XXX Possible other ordering approaches would be to use some kind of association measure or a matrix reordering algorithm for two categorical variables, medians by category or R2 from a linear model for continuous and categorical, correlations for two continuous variables.

5.1.2 Determining sex

XXX intro to ... now we are shifting focus to draw generalized pcps to determine sex.

The lines in Figure 8 are colored by sex of penguins. What can be seen is that within each species, the males tend to be larger in size and heavier than the females. For several of the penguins, sex could not be determined because either the sexing primer did not amplify or no blood sample was obtained [Gorman et al., 2014]. These penguins are represented by dark lines. Based on these penguins' body measurements within the context of the other penguins, we can make some suggestions regarding their sex. In Figure 9 we explore this idea a bit further. This figure is based on the same data as Figure 8, however, we exclude Chinstrap penguins as researchers were able to sex all of those penguins. The body measurements of all sexed penguins are summarised by two ribbons for each sex and species.The inner ribbons are bounded by the 25% and the 75% percentile values on each axis. The lighter ribbon covers 95% of each sex within its


Original order of levels and variables

Levels reordered to emphasize relationship between islands and species

Figure 6: *Both of the levels of the island and the species variable re-ordered to reflect that two of the species are each only found on one island.*

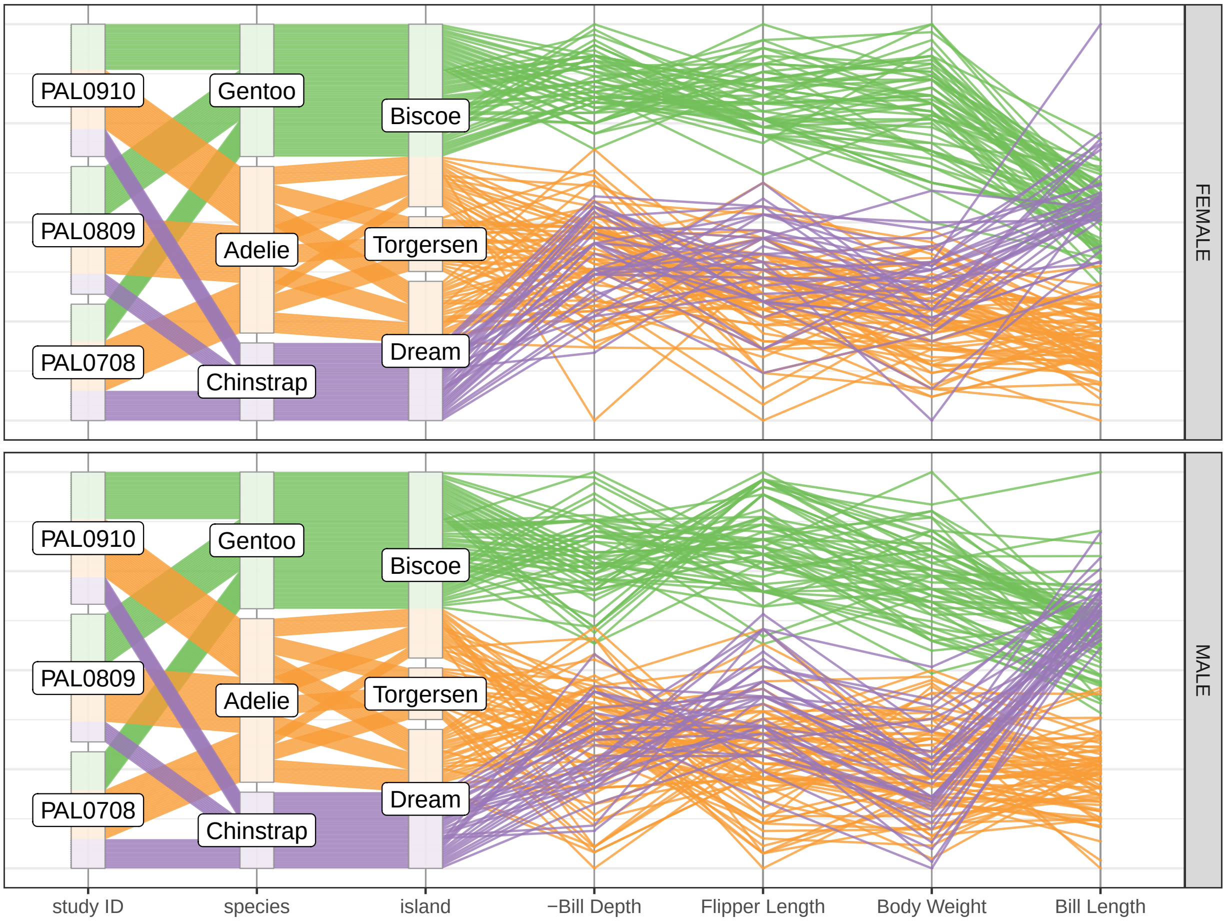


Figure 7: *Changing the order of the variables along the x-axis emphasizes the differences in body measurements between the species.*

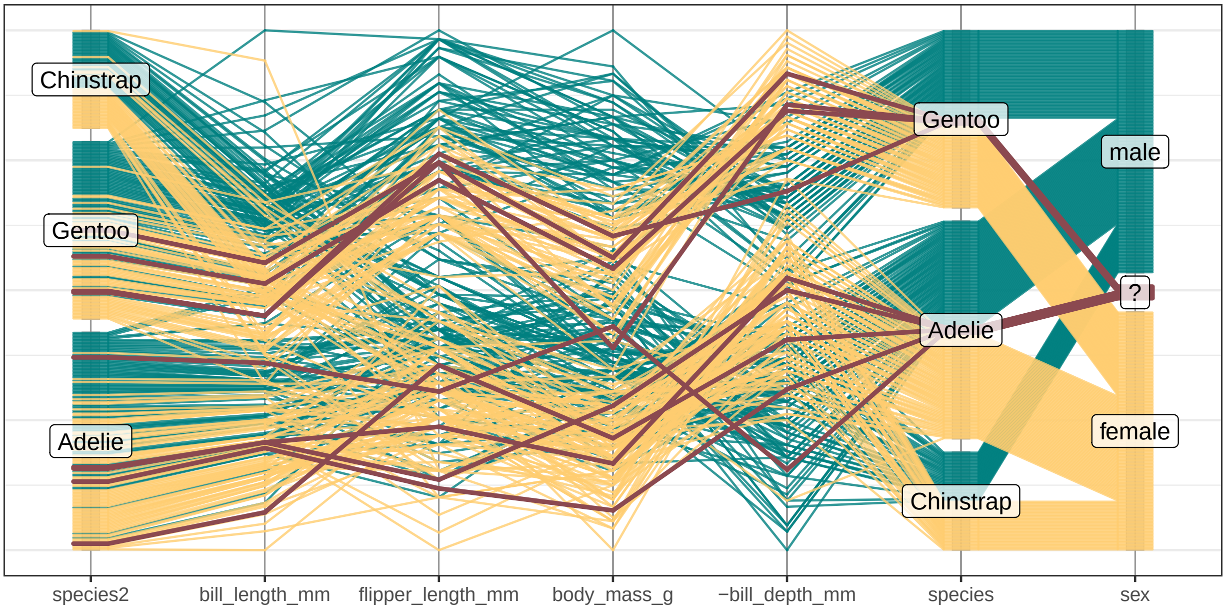


Figure 8: *Generalized Parallel Coordinate Plot of the Palmer penguins data with sex of penguin mapped to color. Dark lines represent penguins for which sex could not be determined. We see that researchers were able to sex all of the Chinstrap penguins. Note that species is included twice (with different order of the levels). XXX reason for that here or in the text?*

species. We use these ribbons to reduce the noise introduced by individual lines. Body measurements of the unsexed animals are represented as line segments on top of the ribbons. This helps us to evaluate and assess the lines drawn for individual, unsexed penguins within the context of the marginal distributions (in this case their putative sex and species).

While we facet both by species and sex, note that the axes are re-scaled within each species to make use of the full range in y. However, we use the same scale between the two sexes of each species. This different treatment of facetting variables is achieved by the use of the grouping variable. The listing below shows the code for prepping the data shown in Figure 9. By grouping on species but not on sex (see line 9), data is being rescaled within species but the same scaling is used across males and females. Measurements for unsexed animals are shown as line segments on top of inter-quantile ribbons of both sexes. Viewers are encouraged to draw a conclusion about an animal's sex based on their values within the (2d density) context of their species and putative sex. Statistically, this comparison relates to a likelihood ratio test: the viewer is asked to make an assessment of the likelihood to observe the measurements of an animal under each of the two competing hypotheses of sex.

Listing 3: *Code to prepare data for Figure 8 by relabling penguins with NA sex as '?' and ordering sex so that penguins of unknown sex are between the male and female labels.*

```
 1  penguins_pcp <- penguins %>%
 2    filter(species != "Chinstrap") %>%                 # no unsexed animals in Chinstrap
 3    mutate(
 4      sex = ifelse(is.na(sex),"?", as.character(sex)),  # make assignment more readable
 5      sex = factor(sex, levels = c("female", "?", "male"))
 6    ) %>%
 7    filter(!is.na(body_mass_g)) %>%
 8    pcp_select(6:5, 3:4) %>%
 9    group_by(species) %>%                              # re-scale by species
10    pcp_scale() %>%
11    pcp_arrange()
```

Chinstrap penguins are excluded (line 2) because all of their individuals in the data have a sex assigned. The general pattern of measurements of the Gentoo penguins suggests that three of the four individuals with missing sex information are female (the three with the lowest bill depth). The fourth animal has an exceptionally deep bill, however, all other measurements suggest that this animal, too, is female. For further evidence, we find from the original data that their nest partners are all sexed as male; this additional information is shown in Figure 9. While assuming that nest partners are male and female is not a perfect method, in particular, for penguins, which have been shown to live in same-sex partnerships, in all three of the studies considered for this data only nests with breeding successes have been considered. More details can be found in Gorman et al. [2014]. For Adelie penguins determining sex is not quite as clear-cut, but based on body mass and bill length measurements the three lightest penguins might be female, while the heaviest one could be male. The fifth penguin exhibits measurements that are neither typically male not typically female. Trying to confirm these putative assignments is a bit more tricky, because four of the five unsexed penguins are nest partners. The lightest unsexed penguin is the partner of a sexed male penguin. The putative assignments do not contradict the hypothesis that each nest is host to a male and a female penguin. Using this assumption, the last unsexed penguin would be resolved as the male of the nest.

let's go back to inter-quantile ranges.

5.2 Getting a second, third, ... and seventh opinion

Figure 10 shows data from Agresti [2002] published as part of the `poLCA` package [Linzer and Lewis, 2011]. Seven pathologists were asked to assess the same 118 slides for the presence or absence of carcinoma in the uterine cervix. Binary responses for each slide were recorded (yes/no). Pathologists all agreed on about 25% of slides, which they considered to be carcinoma free, and a further 12.5% of slides, which were considered to show carcinoma by all pathologists. For the remaining 62.5% of slides there was some disagreement. However, we see that this disagreement is not random. When pathologists are ordered (by moving the corresponding axes) left to right from fewest number of overall carcinoma diagnoses to highest number, we see that generally for a slide more pathologists make a carcinoma diagnosis from left to right.

Note, in this example we do not need to scale the variables. Aside from the actual scale the values are ordered in the same way.

Landis and Koch [1977] (Table 1) allow us a closer look at this data. Pathologists evaluated the (same) scans at a five levels from 1 to 5, given as: (1) Negative, (2) Atypical Squamous Hyperplasia, (3) Carcinoma in Situ, (4) Squamous Carcinoma with Early Stromal Invasion, and (5) Invasive Carcinoma. Figure 11 gives an overview of this more detailed data. The different pathologists are drawn in the same order as in Figure 10. The results for each scan are colored by the overall average score (rounded to the closest integer). Compared to the previous figure, Figure 11 shows more variability between pathologists' evaluations, but

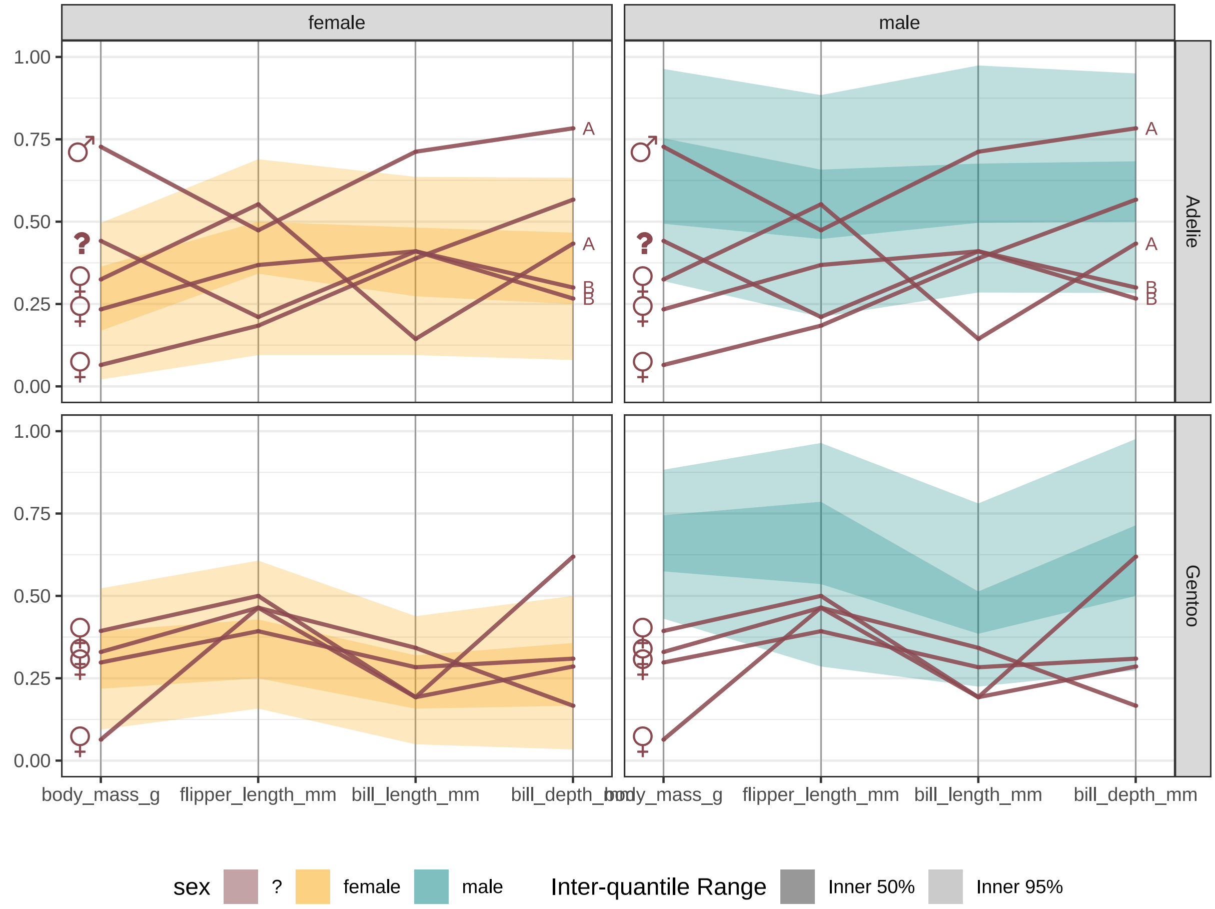


Figure 9: *Closer investigation of non-sexed Adelie and Gentoo penguins. The group_by call before pcp_scale is responsible for scaling by species while the same scale is kept across sex within species. Penguins without assigned sex (based on blood markers) are drawn on top of both sexes. The labels to the left of the ribbons are our best guess at a penguin's sex based on body measurements of other penguins of the same species. The letters on the right indicate nests – two penguins with the same letter share the same nest.*

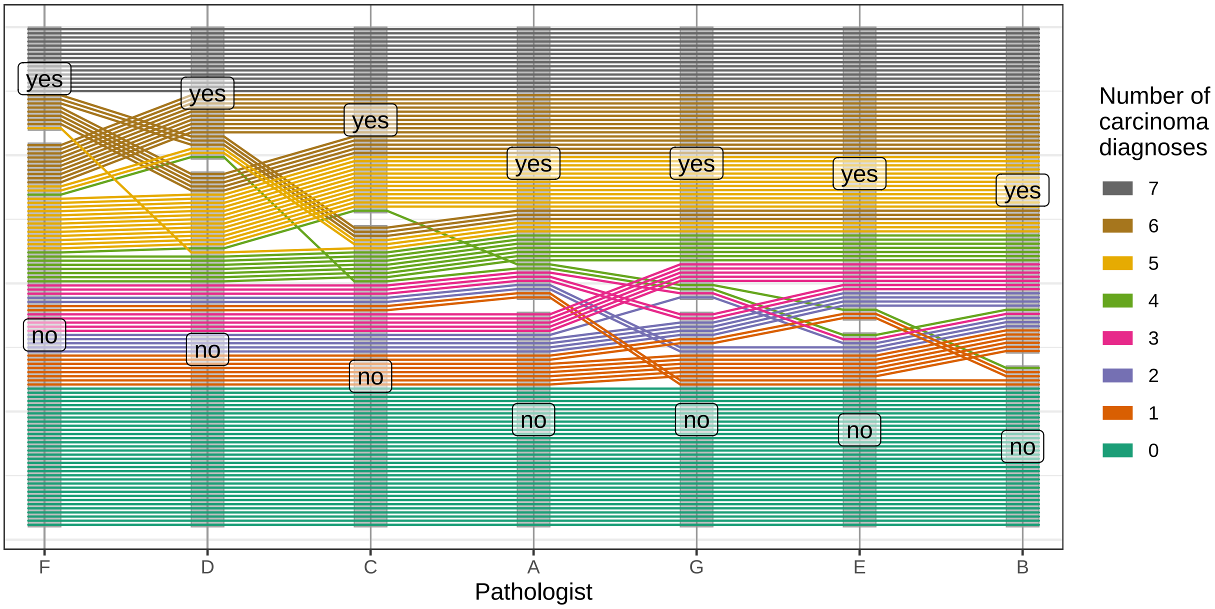


Figure 10: *Pathologists' diagnoses of absence (no) or presence (yes) of carcinoma in the uterine cervix based on 118 slides. Each slide is shown by a poly-line.*

only few scans have vastly different scores assigned to them. Pathologist C, in particular, rates two scans as negative, that all other pathologists rate as quite advanced cancer. Overall, the variability between pathologists' scores stems froma difference in applying the scores rather than an actual difference of opinions. XXX this needs to be phrased differently. What I mean is that we see a lot of agreement in the parallel lines, but the boxes are shifted from one pathologist to another. The similarity in evaluations is particularly striking between pathologists A, G, E, and B.

5.3 Clustering with PCPs

Let's revisit the penguins data for an example of working with clusters in the framework of generalized parallel coordinate plots. We use k-means clustering on all numeric body measurements and investigate which observations are generally captured in each of the clusters.

Because k-means clustering assigns cluster labels arbitrarily based on random cluster centers, in order to maintain a persistent ordering over different values of k we reorder the clusters by the value of `body_mass_g`. This helps us to compare between e.g. k and $k + 1$ clusters. Figure 12 shows the numeric measurements along with the assigned clusters, with categorical variables sex and species on the right. Each line is colored by the assigned cluster, allowing us to determine how the categorical variables relate to the quantitative variables and the resulting clusters. When $k = 2$, Figure 12a shows that the largest difference in the observed data is between Gentoo penguins and the other two species. When $k = 3$, in Figure 12b, the additional cluster separates the Adelie and Chinstrap penguins into two groups with a few misclassifications; this additional cluster is based on the length of the bill (which we can follow due to the clear connection between data values in the generalized PCP). Adding a fourth cluster, as in Figure 12c splits Adelie penguins into males and females, though again there are again some penguins who are misclassified. The addition of a fifth cluster in Figure 12d splits Chinstrap penguins into male and female. Once we add a sixth cluster in Figure 12e, we finally split the Gentoo penguins by sex as well, though again this clustering is not perfect.

What is clear from this exercise is that Adelie and Chinstrap penguins are much more similar to each other than they are to Gentoo penguins, but that there is still noticable sexual dimorphism within each species. We also see from the figure that some of separation into sexes is lost from one clustering to the next.

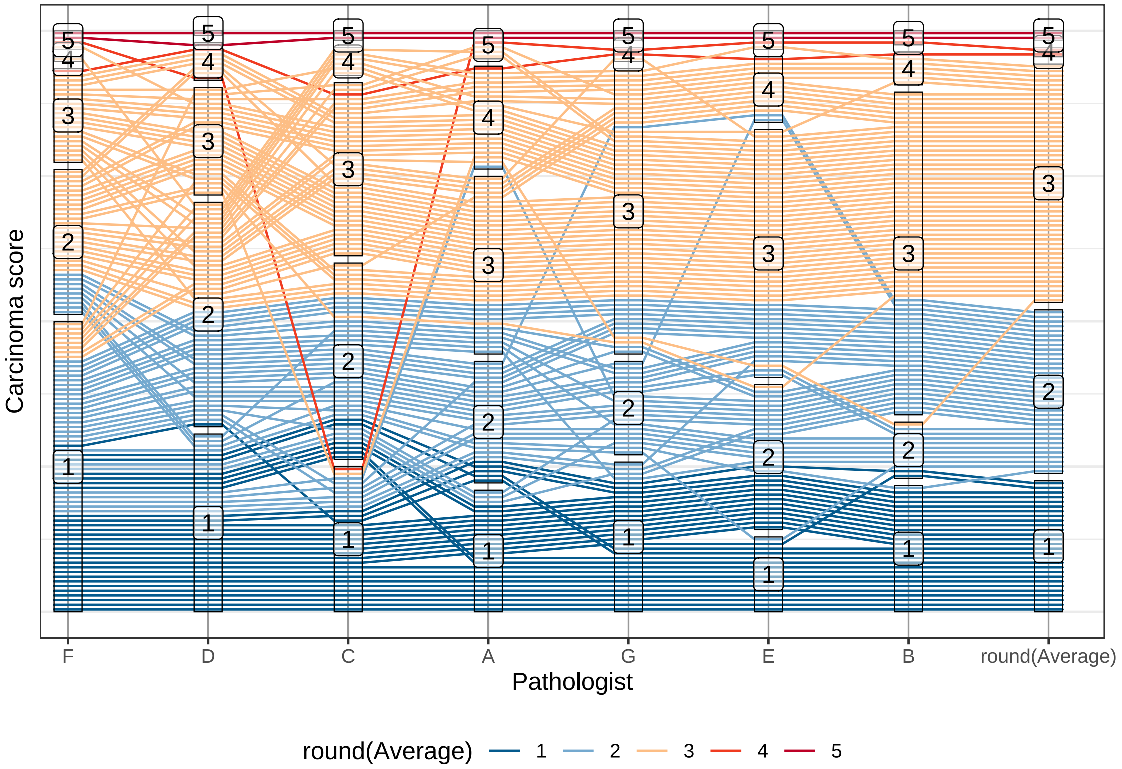


Figure 11: *Closer look at pathologists' evaluations on a more detailed scale from 1 (Negative) to 5 (Invasive Carcinoma). Rounded average scores are mapped to color to help distinguish severity of scan evaluations.*

This is typical for non-hierarchical clustering algorithms. Rather than refining a previous cluster, a switch from k clusters to $k+1$ clusters starts the clustering process anew. If the signal in the data to separate into k clusters is not strong or ambiguous, we will see this reflected in the results; observations might be quite arbitrarily put together into groups, or a group of observations might be split into multiple clusters. In the Hartigan-Wong [Hartigan and Wong, 1979] algorithm used here for the clustering, points are assigned to random clusters in the initialization. In order to assess the effect of this non-deterministic start on the results, it is good practice to investigate the cluster stability by repeating the clustering multiple times for the same number of classes k (if $k > 1$). Figure 13 shows a comparison of the results from multiple runs of the k-means algorithm for $k = 6$. The lines in this figure are colored by species and sex. We see that the splits by species are relatively stable – there are only a few cases across all results in which individuals end up in clusters with individuals from another species, and if they do, it is the same individuals across different results. Splits by sex show more variability: Chinstrap penguins rarely split into male/female clusters, while Gentoo penguins shows a relatively stable separation into males and females. The Adelie population has subsets of individuals that are separated into males only, females only, and a third, more variable subset of a combination of the two.

For the conclusion? XXX Using generalized parallel coordinate plots and item sorting allows us to assess the stability of clustering results.

6 Discussion

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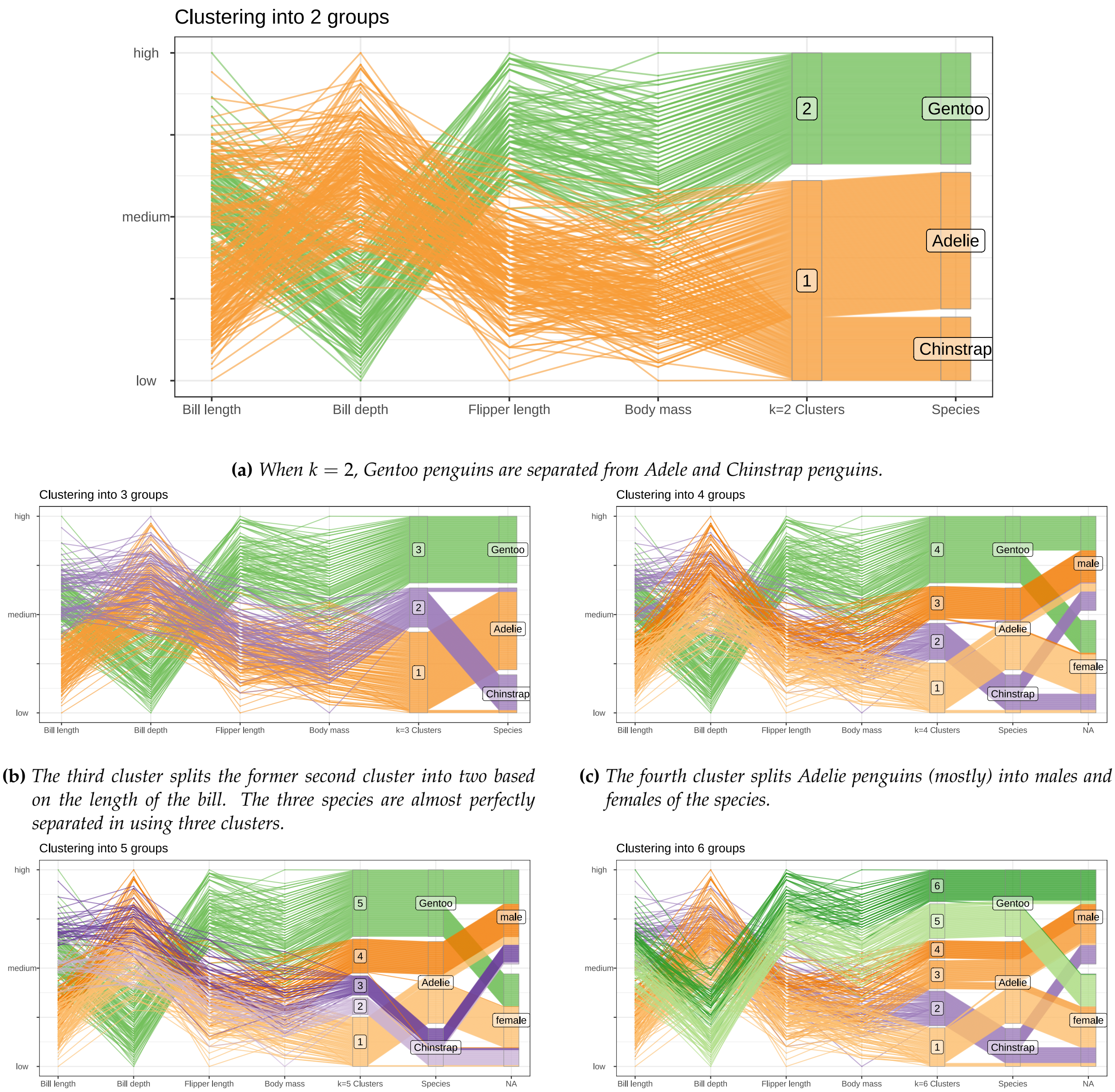

(a) *When $k = 2$, Gentoo penguins are separated from Adele and Chinstrap penguins.*

(b) *The third cluster splits the former second cluster into two based on the length of the bill. The three species are almost perfectly separated in using three clusters.*

(c) *The fourth cluster splits Adelie penguins (mostly) into males and females of the species.*

(d) *The fifth cluster splits the group of Chinstrap penguins (mostly) into females and males. Only a handful of individual penguins are grouped with the wrong species or the wrong sex.*

(e) *With the introduction of a sixth cluster, all previous clusters change: Gentoo penguins are split into males and females. The sex separation for Chinstrap penguins gets lost, but Adelie males get split into two separate clusters.*

Figure 12: *An overview of the use of parallel coordinate plots to examine which variables contribute to clustering and to identify individuals who are misclassified.*

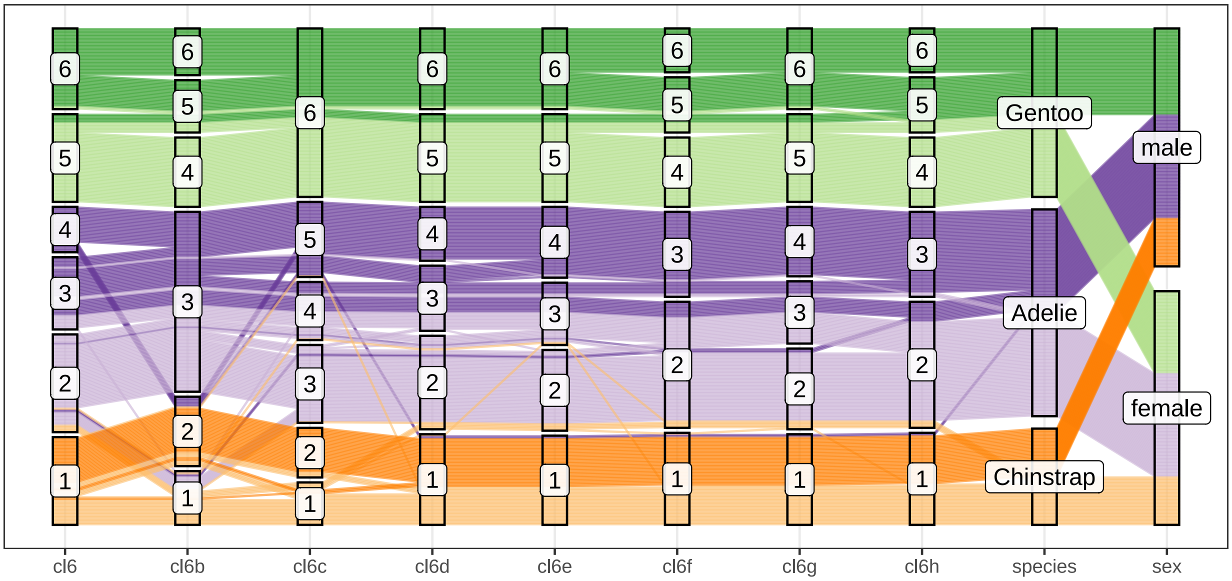

Figure 13: *Comparison of eight k-means runs for* $k = 6$*. Color of lines is given by species and sex. The differences between the clusters are introduced by the different random seeds in the inital cluster centers.*

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A Example usage

Commented code for Figure 10:

```
data(carcinoma, package = "poLCA")

# Prepping the Dataset
carcinoma$total <— rowSums(carcinoma) — 7
carcinoma <— carcinoma %>% mutate(
  across(A:G, .fns = as.factor)
)

carcinoma %>%

# Selecting and scaling variables
```

```
pcp_select(F, D, C, A, G, E, B, tot) %>%
pcp_scale(method="uniminmax") %>%
pcp_arrange() %>%

# Setting up ggplot for pcp and setting pcp display options
ggplot(aes_pcp()) +
geom_pcp_axes() +
geom_pcp_boxes(colour="black", alpha=0) +
geom_pcp(aes(colour = tot)) +
geom_pcp_labels(aes(label = pcp_level), fill="white", alpha = 1) +

# Choosing general ggplot display options
scale_colour_brewer("Number of\ncarcinoma\ndiagnoses", palette ="Dark2") +
theme_bw() +
guides(color = guide_legend(reverse=TRUE, override.aes = list(size = 5))) +
scale_x_discrete(expand = expansion(add=0.25)) +
xlab(NULL) + ylab(NULL) +
theme(axis.text.y=element_blank(), axis.ticks.y=element_blank())
```