SHORT TECHNICAL NOTE

New and simplified manual controls for projection and slice tours, with application to exploring classification boundaries in high dimensions

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ABSTRACT
Something here

1. Introduction

From a statistical perspective it is rare to have data that are strictly 3D, and so unlike in most computer graphics applications, the more useful methods for data analysis show projections from an arbitrary dimensional space. These are dynamic data visualizations methods and are collected under the term *tours*. Tours involve views of high-dimensional (p) data with low-dimensional (d) projections. In his original paper on the grand tour, Asimov (1985) provided several algorithms for tour paths that could theoretically show the viewer the data *from all sides*. Prior to Asimov's work, there were numerous preparatory developments including Fisherkeller, Friedman, and Tukey (1974)'s PRIM-9. PRIM-9 had user-controlled rotations on coordinate axes, allowing one to manually tour through low-dimensional projections. (A video illustrating the capabilities is available through video library of ASA Statistical Graphics Section (2022).) Steering through all possible projections is impossible, unlike Asimov's tours which allows one to quickly see many, many different projections. After Asimov there have been many, many tour developments, which are summarized in Lee et al. (2021).

One such direction of work develops the ideas from PRIM-9, to provide manual control of a tour. Cook and Buja (1997) describe controls for 1D (or 2D) projections, respectively in a 2D (or 3D) manipulation space, allowing the user to select any variable axis, and rotate it into, or out of, or around the projection through horizontal, vertical, oblique, radial or angular changes in value. Spyrison and Cook (2020) refined this algorithm and implements them to generate animation sequences.

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Manual controls are especially useful for assessing sensitivity of structure to particular elements of the projection. There are many places where it is useful. In exploratory data analysis, where one sees clusters in a projection, can some variables be removed from the projection without affecting the clustering. For interpreting models, one can reduce or increase a variable's contribution to examine the variable importance. These controls can also be used to interactively generate faceted plots (**?**), or spatiotemporal glyphmaps (**?**). Having the user interact with a projection is extremely valuable for understanding high-dimensional data. However, these algorithms have two problems: (1) the pre-processing of creating a manipulation space overly complicates the algorithm, (2) extending to higher dimensional control is difficult.

Through experiments with the relatively new interactive graphics capabilities in mathematica(?), we have realized that there is a simpler approach, which is more direct, and extensible for generating user interaction. This paper explains this, and is organized as follows. The next section describes the new algorithm for manual control. This is followed by details on implementation. The applications section illustrate how these can be used.

2. How to construct a manual tour

A manual tour allows the user to alter the coefficients of one (or more) variables contributing to a $d - D$ projection. The initial ingredients are an orthonormal basis ($A_{p \times d}$) defining the projection of the data, and a variable id ($m \in \{1, ..., p\}$) specifying which coefficient will be changed. A method to update the values of the component of the controlled variable V_m is then needed.

2.1. *Existing methods*

The method for updating component values in Cook and Buja (1997) (and utilised in Spyrison and Cook (2020)) are prescribed primarily for a 2D projection, to take advantage of (then) newly developed 3D trackball controls made available for computer gaming. The first step was to construct a 3D manipulation space from a 2D projection, as illustrated in Figure 1. In this space the coefficient of the controlled variable ranges between -1 and 1. Movements of a cursor are recorded and converted into changes in the values of V_m thus changing the displayed 2D projection. The algorithm also provided constraints to horizontal, vertical, radial or angular motions only.

2.2. *A new simpler and broadly applicable approach*

The new approach emerged from experiments in mathematica. The components corresponding to V_m are directly controlled by cursor movement, which updates row m of A. The updated matrix is then orthonormalised.

2.2.1. Algorithm

1. Provide A, and m. (Note that m could also be automatically chosen as the component that is closest to the cursor position.)
2. Change values in row m, giving A^*. A large change in these values would correspond to making a large jump from the current projection. Small changes would correspond to tracking a cursor, making small jumps from the current projection.
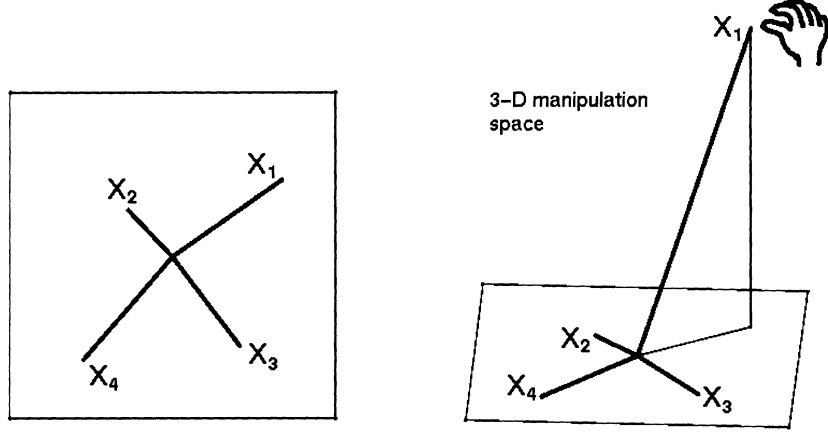
Figure 1. Original contruction of the manual tour designed for 2D projections and created a 3D space from which to utilise track ball controls to change it's contribution. (Figure 3 from Cook and Buja (1997).)

3. Orthonormalise A^*, using Gram-Schmidt. For $d = 2$, and $A^* = [a_{.1} \, a_{.2}]$, the steps are:

    i. Normalise $a_{.1}$, and $a_{.2}$.
    ii. $a_{.2}^* = a_{.2} - a_{.1}^T a_{.2} a_{.1}$.
    iii. Normalise $a_{.2}^*$.

This algorithm will produce the changes to a projection as illustrated in Figure 2 (top row). The controlled variable, V_m, corresponds to the black line, and sequential changes to row m of A can be seen to roughly follow a specified position (orange dot). Changes in the other components happen as a result of the orthonormalisation, but are uncontrolled.

2.3. *Refinements to enforce exact position*

The problem with new simple method (Algorithm 1) is that the precise values for V_m cannot be specified because the orthonormalisation will change them.

2.3.1. *Adjustment method 1*

A small modification to algorithm 1 will maintain the components of V_m precisely (Figure 2 (bottom row)). It is as follows:

1. Provide A, and m.
2. Change values in row m, giving A^*.
3. Store row m separately, and zero the values of row m in A^*, giving A^{*0}.
4. Orthonormalise A^{*0}, using Gram-Schmidt.
5. Replace row m with the original values, giving A^{**}.
6. For $d = 2$, adjust the values of $a_{.2}^{**}$ using

$$a_{j2}^{**} + \frac{a_{m1}a_{m2}}{p-1}, j = 1, ..., p, j \neq m$$
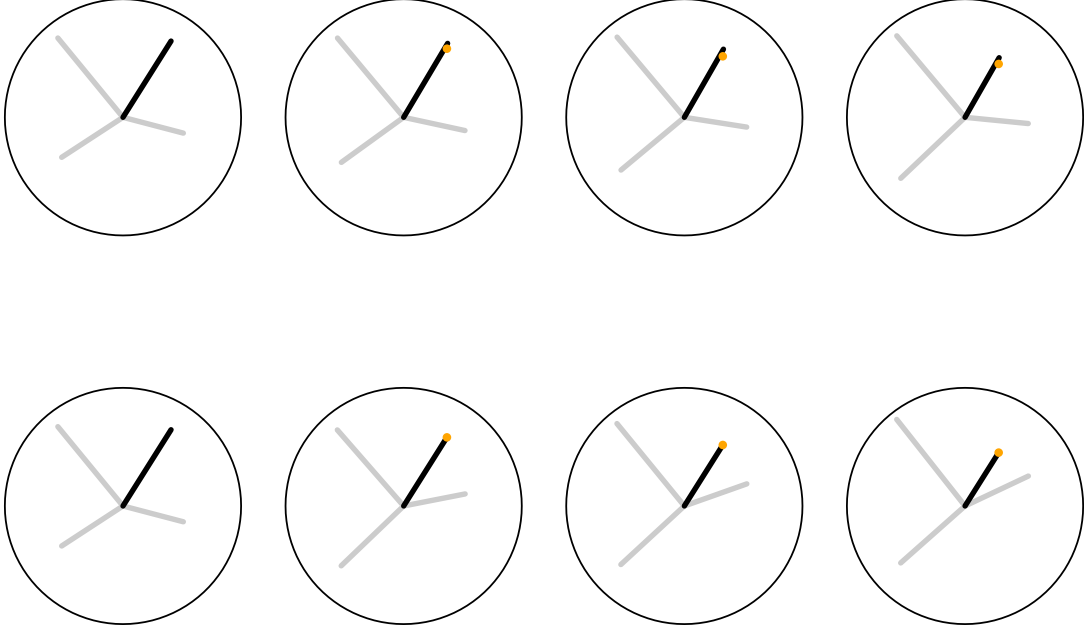
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Figure 2. Sequence of projections where contribution of one variable is controlled (black) is changed: (top) unconstrained orthonormalisation, (bottom) constrained as specified. The dot (orange) indicates the chosen values for the controlled variable. For the constrained orthonormalisation it can be seen to precisely match the axis, but not so for the unconstrained orthonormalisation.

which ensures that

$$\sum_{j=1,j\neq m}^{p} a_{j1}^{**} a_{j2}^{**} + a_{m1} a_{m2} = 0$$

.

If $d > 2$ the process would be sequentially repeated in the same manner that Gram-Schmidt is applied sequentially to orthormalise the columns of a matrix. If $d = 1$ no orthonormalisation is needed, and the projection vector would simply need to be normalized after each adjustment.

2.3.2. Adjustment method 2

For $d = 2$ projections, the projection matrix is the sub-matrix of A formed by its first two columns. Whereas orthonormality of the basis for the p-dimensional space is given by $e_i \cdot e_j = \delta_{ij}, i, j, = 1, \cdots ,$, orthonormality of the projection matrix is expressed as $P_i \cdot P_j = \delta_{ij}, i, j = 1, 2$. Movement of the cursor takes the two components x_{m1}, x_{m2} into a selected new value a, b. Although the motion is constrained by $a^2 + b^2 \leq 1$, this is not sufficient to guarantee orthonormality of the new projection matrix. One possible algorithm to achieve this is

(1) Cursor movement takes $x_{m1}, x_{m2} \to a, b$
(2) The freedom to change the components $A_{i3} \cdots A_{ip}$ (the columns of A not corresponding to the projection matrix) is used to select a new orthonormal basis as follows:
  (a) For row m one chooses $A_{m3} = \sqrt{1 - a^2 - b^2}$, $A_{m,k>3} = 0$

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(b) For other rows, $A_{i \neq m, j \geq 3}$ random selections in the range $(-1, 1)$ are made.

(c) The Gram-Schmidt algorithm is then used to obtain an orthonormal basis taking e_m as the first vector (which is already normalized), and then proceeding as usual $e_1 \to e_1 - (e_1 \cdot e_m)e_m$, $e_1 \to e_1/(e_1 \cdot e_1)$, etc.

(3) this results in the orthonormal basis A^* and a new projection matrix with $P_{m1} = a$, $P_{m2} = b$.

The random choice for the components of A not in the projection matrix allows the exploration of dimensions perpendicular to the projection plane.

$$
A = \begin{array}{c} e_1 \to \\ e_2 \to \\ \vdots \\ e_m \to \\ \vdots \\ e_p \to \end{array} \begin{pmatrix} x_{11} & x_{12} & x_{13} & \cdots & x_{1p} \\ x_{21} & x_{22} & \cdot & \cdots & x_{2p} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ x_{m1} & x_{m2} & \cdot & \cdots & x_{mp} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ x_{p1} & x_{p2} & \cdot & \cdots & x_{pp} \end{pmatrix}, \quad (x_{m1}, x_{m2}) \to (a, b) \tag{1}
$$

with P_1 above column 1 and P_2 above column 2.

2.3.3. *Adjustment method 3*

For now just sketching the idea:

- first step is to click on the axis display to change the contribution of one variable m
- capture that position and replace the corresponding row in the projection matrix
- for 2D projection this gives components m_1 along "x" direction and m_2 along y direction
- next step: rotate basis such that direction of row m now corresponds to the first basis vector, this means we apply 2x2 rotation matrix to each row of the projection matrix, where the rotation angle is $tan(\theta) = m_2/m_1$ (that matrix can be written just in terms of that ratio, $x = m_2/m_1$, when $m_1 < 0$ I think we just need to translate $\theta \to \theta + \pi$)
- take the rotated basis, apply Gram-Schmidt, now the direction of m will not change (but the length will change during normalization)
- rotated back to the original xy basis to update the plots

XXX need to check calculation of angle when $m_1 < 0$

3. Experimenting with new techniques using Mathematica

- **Why is this a good sandbox**
- **Explain the functionality available in the notebooks**

The following functions are implemented in the Mathematica package `mmtour.wl`:

- `ProjectionPlot[data, projmat, xRange(=Automatic), yRange(=Automatic), colour(=Automatic)]` with arguments
  - `data`: A list of data matrices (they must all have the same dimensionality)

- ○ 'projmat: A projection matrix which describes the projection plane. This is the initial projection and does not need to be orthonormal (XXX is this right?).
- ○ 'xRange: A list which details the range of the horizontal axis.
- ○ 'yRange: A list which details the range of the vertical axis.
- ○ 'colour: A list of graphics directives to be applied to each data matrix.

There are problems with the default values for x and y ranges and colour. It would be better to fix the ranges and colour based on the data as well as the origin of axes and the size of the points.

It would be good if the initial projection matrix (and maybe the center) had default values. Perhaps a random matrix with the correct dimensions read from the data? Fix 1

The format for the printed projection matrix can be improved also. Maybe fix the number of digits and the position of the label.

- • SlicePlot[data, projmat, centrePoint, height, heightRange, ptSize1(=0.005), ptSize2(=0.004), minDist(=0)] with arguments (used to be called SliceDynamic in Alex's first version, the name SliceDynamic was taken by something else below)
  - ○ data: A data matrix
  - ○ projmat: The inital projection matrix
  - ○ centrepoint: The initial position of the slice
  - ○ height: The initial height of the slice
  - ○ heightRange: The range of heights
  - ○ ptSize1: The size of the points that exist within the slice
  - ○ ptSize2: The size of the points that exist outside of the slice

This function requires some auxiliary functions. It does not accept more than one data set.

It would be good if the initial projection matrix (and maybe the center) had default values. Perhaps a random matrix with the correct dimensions read from the data?

It may be good to fix the size of the points, the center of the axes and the scales of the axes rather than allow them to change as the projection and slicing changes

- • SliceDynamic[data, projmat, centrePoint, height, heightRange, ptSize1 : 0.005, ptSize2 : 0.004] with arguments
- • data: A data matrix with an extra grouping or clustering column (numerical)
- • projmat: The initial projection matrix
- • centrepoint: The initial position of the slice
- • height: The initial height of the slice
- • heightRange: The range of heights
- • ptSize1: The size of the points that exist within the slice
- • ptSize2: The size of the points that exist outside of the slice

Does this need to be a separate function from SlicePlot? Fix 2

It would be good if the initial projection matrix (and maybe the center) had default values. Perhaps a random matrix with the correct dimensions read from the data? Fix 3

It may be good to fix the size of the points, the center of the axes and

the scales of the axes rather than allow them to change as the projection and slicing changes. Fix 4

I have found it useful to input different data sets rather than have this function sort them automatically using the last column. One data set with a flag column at the end, is best! Is the code too complicated? Fix 5

- `Projected2DSliderPlot[]`

This function uses a different display for the projection that I find very useful. However as it stands it is specific to one data set. Needs to be generalised to arbitrary data if we want to keep it.

For Alex to do

- **We would need a screenshot (and video) for each of these.**
- **Fix 1, 2, 3, 4, 5**
- **Code consistent for applications to work - see slice_tour_compare_sets.nb. See below**
    - **We need to make sure the drawing range is fixed (no resizing of the axis when changing projection or slicing). It could be nice if there was a manual zoom in/zoom out to change scale occasionally.**
    - **Should also make sure the size of the points is fixed (maybe this will be automatic if the drawing range is fixed?), bigger points would be preferred, currently the size is sometimes really tiny and it becomes difficult to see anything.**
    - **Can we have some heuristic to decide the range for the slice thickness slider? In the second graph there is a tiny part of the slider where the changes are interesting, difficult to navigate since this makes it super sensitive to any small movement, while most of the options are not interesting. My suggestion would be to keep (as I understand is the case now) the maximum thickness (all points in) as the upper bound, but instead of zero use a thickness below which slices tend to be empty as the lower bound.**
    - **For the olives example I think the relation between x2 and the blue region could be interesting.**
    - **pdfsense data: can we use random samples instead of the first 10k rows? Then we should still be able to see the bigger picture (with picking the first ones we get some artificial structure from how the data was sampled initially).**
    - **I was playing around with this today. Looks like the axes are fixed when changing slice thickness, but not when rotating?**
    - **Anyways, some observations that might be useful, but all of this seems difficult for including in a paper:**
    - **In the first example we can show how the yellow group is associated with the first variable (x1, I guess this is C9?) - when slicing through the center it only appears when x1 has a bigger component on the projection, it is associated with low values of x1. Since they are not near the average value of x1 the points do not get captured in a slice where x1 is not important in the projection. We can move the center point to -1 in the first component to then explore how the yellow group relates to the other three**

variables. Much less clear, maybe some indication of smaller x2 and larger x3 for this.

- ○ The second example is too busy for manual exploration I would say (too many axes to move around separately).
- ○ Third example could be similar to the first: blue region requires small values of x2, can be understood from the exploration, then move center point to -0.5 in x2 to explore further. Now interpretation becomes tricky. Sometimes blue and yellow seem just randomly everywhere, sometimes blue more contained in an ellipsoid around the center (indicating some correlation between variables). For example try zeroing out components 2 and 3 to see this slice in x1 vs x4.
- ○ For the last example x4 seems to be the one to work with. I feel like this is again very similar, maybe better to instead explore other examples (maybe something without slicing?)

4. Application

To illustrate the usefulness of the manual tour we use the 4D penguins data (Horst, Hill, and Gorman 2020). We will show how classification boundaries can be explored and better understood using a manual tour, on projections and slices through 4D space. Figure 3 shows a scatterplot matrix of this data. There are four variables (`bl = bill_length_mm, bd = bill_depth_mm, fl = flipper_length_mm, bm = body_mass_g`) measuring the size of the penguins from three species (Adelie, Chinstrap and Gentoo). The scatterplot matrix shows that the three species appear to be likely separable, and that at least the Gentoo can be distinguished from the other two species when `bd` is paired with `fl` or `bm`. The steps for exploring boundaries are as follows:

1. Build classification model, here we use a random forest and linear discriminant analysis.
2. Predict the class for a dense grid of values covering the data space.
3. Examine projections, using a manual tour so that the contribution of any variable is controlled.
4. Slice through the center, to explore where the boundaries will likely meet.
5. Move the slice by changing the center in the direction of a single variable to explore the extent of a boundary for a single group relative to a variable.

4.1. Constructing the 4D prediction regions

We use the `classifly` package (Wickham 2022) to generate predictions across the 4D cube spanned by the data, with two classification models: linear discriminant analysis (LDA) and random forest(RF).

4.2. Exploring projections manually

We start by first exploring the projections of the model prediction. Through manual rotation of the view we can get a feeling for where in the space we primarily predict each
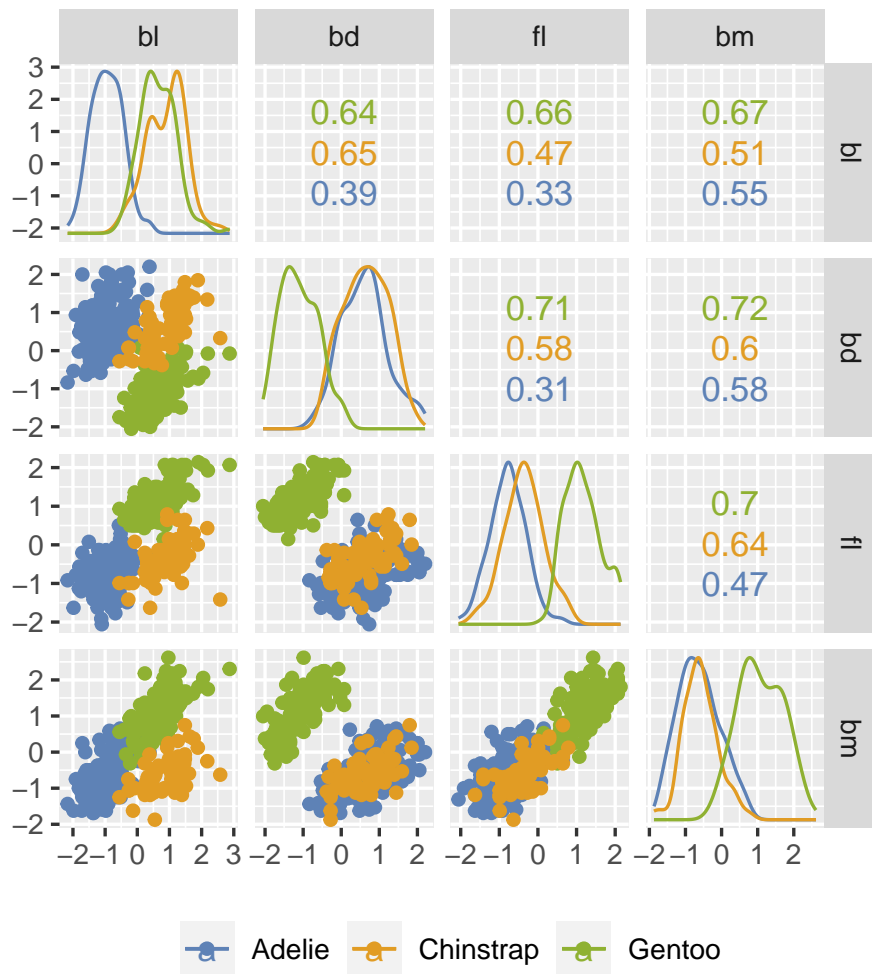
Figure 3. Scatterplot matrix of the (standardised) penguins data. The three species are reasonably different in size, with Gentoo distinguised from the other two on body depth relative to flipper length and body mass.

of the three species, and we also get a sense of the difference between the two models. To illustrate this difference we have rotated the projection view from the RF model to identify a projection that shows the non-linear, block-type structure introduced by the model, see Fig. 4. We then export the corresponding matrix A_1 to look at the same projection for the LDA model and the original data. Here we notice that while the overall picture is similar, the linearity of the LDA leads to a big difference in how two of the three species overlap across the projection (blue vs green, i.e. Adelie vs Gentoo penguins). Interestingly that same projection leads to almost perfect separation of the three species when looking at the data points, the overlap between the models is driven by what is happening in the orthogonal space to the plane.
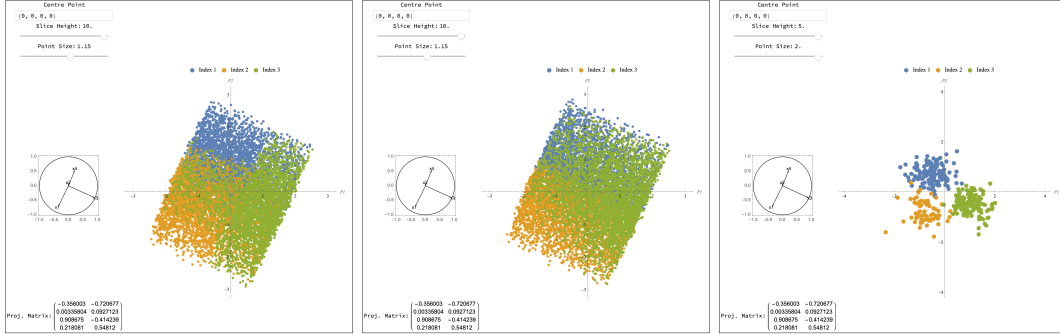

Figure 4. Projection identified using the manual tour, because it reveals an interesting structure in the predictions from the RF model (left). We can clearly see the block structure, while the LDA model (middle) produces linear boundaries instead. The three groups are separated in this projection of the data (right)
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4.3. *Slicing through the center*

XXXX currently in the notebook A_1 is called A5, and A_2 is called A6

We continue the investigation by now slicing based on the projection A_1. For both models we look at a thin ($h = 0.5$) slice through the center, S_1^0. As a first option we explore how manually changing the projection away from A_1 can help with understanding the boundary better. For our example we notice that A_1 does not contain any contribution from the second variable (`bd`), and in our illustration we will first rotate this variable into the view.

We again start by looking at the RF model, the slice S_1^0 shows the block structure of the model, with the third group (green, Gentoo penguins) overlapping with both of the other groups (Fig. 5, top-left). This is similar for the LDA model (Fig. 5, top-right), but again the linearity results in different boundaries and thus differences in how the classes overlap.

By rotating in the second variable we can find a view that shows three neatly separated blocks for the RF model, and we export the corresponding projection matrix A_2 to see the same views for the LDA model which also shows a neater separation of the classes along the boundary (see bottom row of Fig. 5).

Finally we look at the data projection based on A_2 and find that the third group (green, Gentoo penguins) is further away from the other two groups (compared to A_1), see Fig. 6.
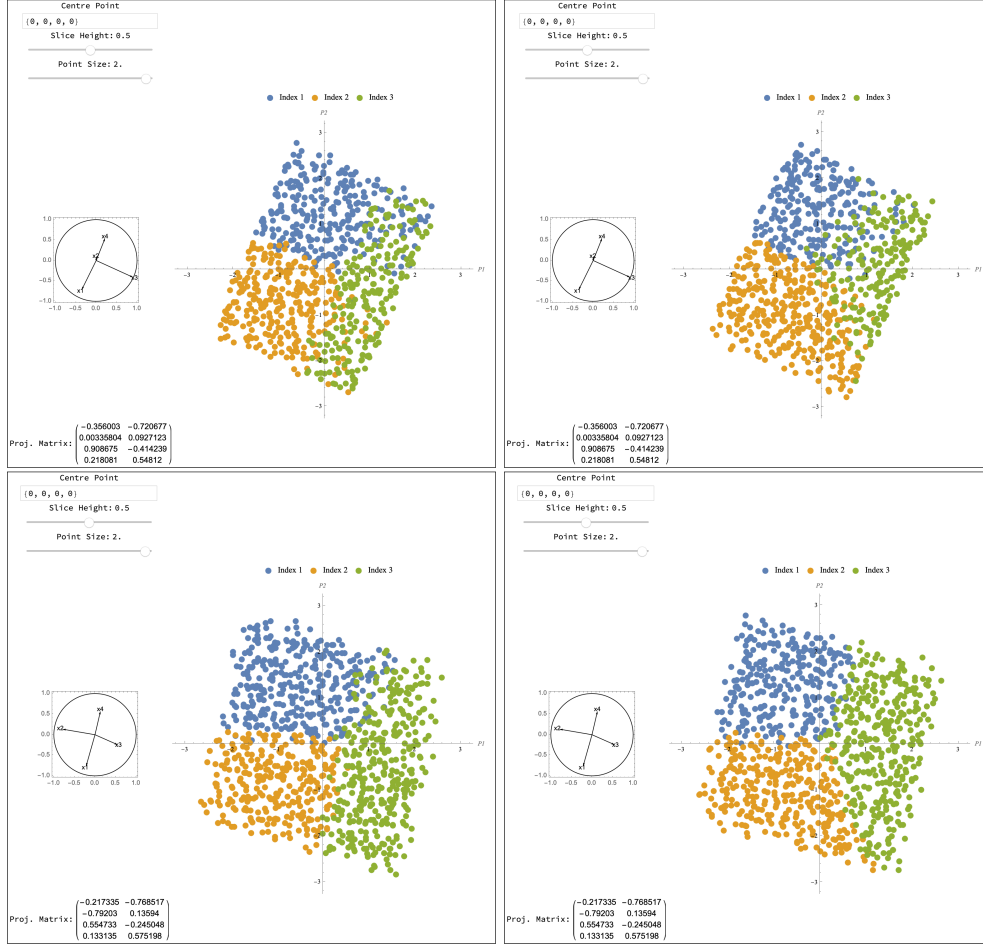
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Figure 5. Comparing slices based on A_1 (top row) and A_2 (bottom row), for the two models RF (left) and LDA (right). With the starting projection A_1 we see one group overlapping (green, Gentoo), while A_2 results in clear boundaries inside the slice. The block vs linear structure of the two models is clearly visible in both slices.

4.4. *Shifting the slice center*

We have seen that starting from A_1 using the manual controls to change the contribution of the second variable we could find a clear separation boundary indicating the relation between this variable (bill depth) and the Gentoo penguin species. Instead of rotating to a different projection, we might also change the view by moving the slice along one direction in the 4D space. Here we will continue our exploration of the dependence on `bd` and move the slice defined by A_1 to either large or small values of the bill depth (± 1.5 after centering and scaling). We will label these slices as $S_1^{\pm}$. Here we will also look at slices of the observed data points, using a thicker slice ($h = 1.5$) to capture enough points in a given view.

We start by a comparison of the two models and the data distribution in S_1^+, thus the slice is localized towards high values of bill depth in Fig. 7. We can see that all three slices (the two models and the data) contain almost no points from the third class (green, Gentoo), and that the decision boundary between the two models is very similar.

A more interesting comparison is found for S_1^-, thus the slice localized towards low values of bill depth, shown in Fig. 8. The RF model (left) predicts all three species
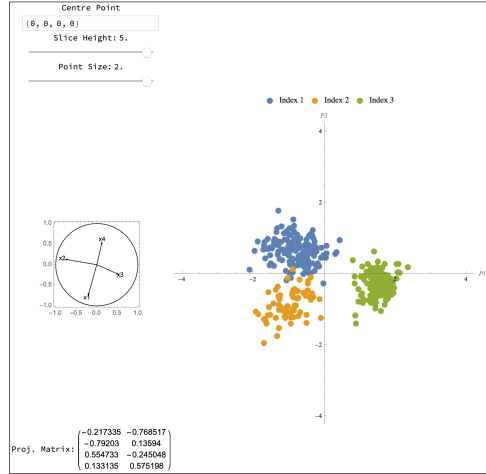
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Figure 6. Projection of the data based on A_2. Compared to projecting onto A_1 we see that the green observations (Gentoo) are more separated from the other two species.
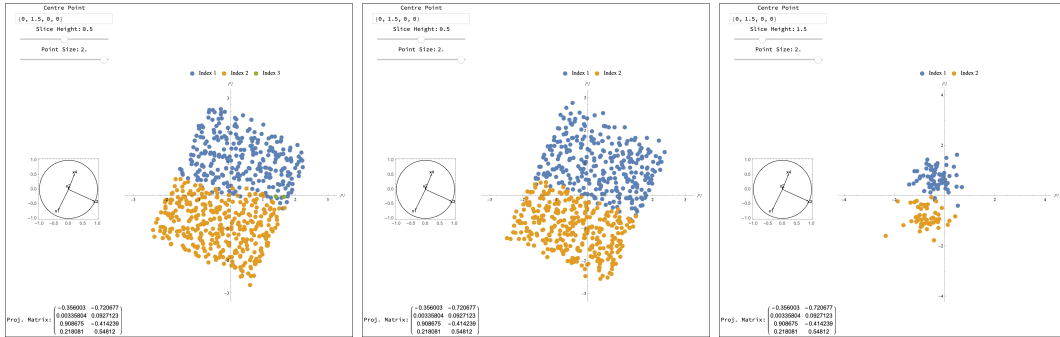

Figure 7. ...

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within this slice, with an interesting boundary for the third class (green, Gentoo). On the other hand the LDA model (middle) predominantly predicts the third class within the slice, this appears to be enforced through the linear structure of the model. Looking finally at the thick slice through the data we see that there are primarily observations from this class within the slice we can conclude that the two models have filled in the "empty" space (where we do not have any training observations) in very different ways and according to what we might expect given the model structure.

Finally it is interesting to compare the slice views to the projection of the models seen in Fig. 4 to better understand how the boundaries change along the `bd` direction and where the differences in the projections come from.

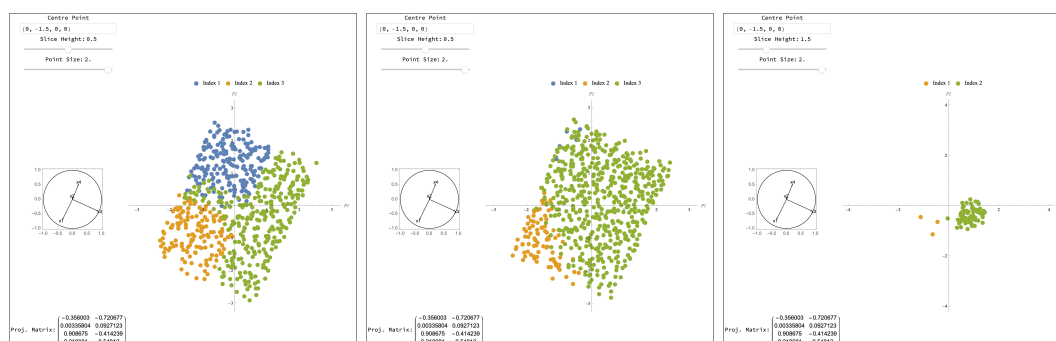## 5. Extension added in the R package `tourr`

Explain `radial_tour`

Figure 8. ...

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6. What would be desirable for implementations in R?

7. Discussion

Acknowledgements

Supplementary material

The source material and animated gifs for this paper are available at

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