Dynamic visualization of high-dimensional data via low-dimension projections and sectioning across 2D and 3D display devices

A thesis submitted for the degree of

Doctor of Philosophy

by

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Contents

Acknowledgements

I would like to thank …

Declaration

I hereby declare that this thesis contains no material which has been accepted for the award of any other degree or diploma in any university or equivalent institution, and that, to the best of my knowledge and belief, this thesis contains no material previously published or written by another person, except where due reference is made in the text of the thesis.

Nicholas S Spyrison

Preface

The material in Chapter 1 has been submitted to *Something interesting jornal* for possible publication.

The contribution in Chapter 3 of this thesis was presented in the super awesome confrence held in Dublin, Ireland, in July 2015.

Abstract

This thesis is about . . .

Chapter 1

Introduction

This is where you introduce the main ideas of your thesis, and an overview of the context and background.

In a PhD, Chapter 2 would normally contain a literature review. Typically, Chapters 3–5 would contain your own contributions. Think of each of these as potential papers to be submitted to journals. Finally, Chapter 6 provides some concluding remarks, discussion, ideas for future research, and so on. Appendixes can contain additional material that don't fit into any chapters, but that you want to put on record. For example, additional tables, output, etc.

Chapter 2

Literature review

2.1 Touring

2.1.1 Overview

In univariate data sets histograms, or smoothed density curves are employed to visualize data. In bivariate data scatterplots and contour plots (2-d density) can be employed. In three dimensions the two most common techniques are: 2-d scatter plot with the 3rd variable as an aesthetic (such as, color, size, height, *etc*.) or rendering the data in a 3-d volume using some perceptive cues giving information describing the seeming depth of the image [1]. When there are 4 variables: 3 variables as spatial-dimensions and a 4th as aesthetic, or a scatterplot matrix consisting of 4 histograms, and 6 unique combinations of bivariate scatterplots.

Let p be the number of numeric variables; how do we visualize data for even modest values of p (say 6 or 12)? It's far too common that visualizing in data-space is dropped altogether in favor of modeling parameter-space, model-space, or worse: long tables of statistics without visuals (Wickham, Cook, and Hofmann, 2015). Yet, we all know of the risks inherent in relying too heavily on parameters alone (Anscombe, 1973; Matejka and Fitzmaurice, 2017). So why do we move away from visualizing in data-space? Scalability,

[1] Graphs of data depicting 3 dimension are typically printed on paper, or rendered on a 2-d monitor, they are intrinsically 2-d images. They are sometimes referred to as 2.5-d, or more frequently erroneously referred to as 3-d, more on this later.

in a word, we are not familiar with methods that allow us to concisely depict and digest $p \geq 5$ or so dimensions. This is where dimensionality reduction comes in. Specifically, we will be focusing on a specific group called touring. In the interest of time I will not belabor the diversity of dimensionality reduction, (see [Grinstein, Trutschl, and Cvek (2002); Carreira-Perpinán (1997); heer_tour_2010] for a quick summary). Suffice it to say that touring has a couple of salient features: linear transformations such that we can interpolate back to the original variable space and does not discard dimensions, something that is common to other linear techniques. By employing the breadth of tours we are able to preserve the visualization of data-space, and with it, the intrinsic understanding of structure and distribution of data that is more succinct or beyond the reach of statistic values alone.

Touring is a linear dimensionality reduction technique that orthogonally projects p-space down to $d(\leq p)$ dimensions. Many such projections are interpolated, each making local rotations in p-space. These frames are then viewed in order to the effect of watching an animation of the lower dimensional embedding changing as p-space is manipulated. Shadow puppets offer a useful analogy to aid in conceptualizing touring. Imagine a fixed light source facing a wall. When a hand or puppet is introduced the 3-dimensional object projects a 2-dimensional shadow onto the wall. This is a physical representation of a simple projection, that from $p = 3$ down to $d = 2$. If the object rotates then the shadow correspondingly changes. Observers watching only the shadow are functionally watching a 2-dimensional tour as the 3-dimensional object is manipulated.

Terminology

n, p (sometimes called d by Wegman, or n), d (sometimes called k by wegman, or d in tourr)

2.1.2 History

Touring was first introduced by Asimov in 1985 with his purposed Grand Tour(Asimov, 1985) at Stanford University. In which, Asimov suggested three types of Grand Tours:

torus, at-random, and random-walk. The specifics of which will be discussed below in the Typology section.

TALK ABOUT maths Here::

Note that the the above methods have no input from the user aside from the starting basis. The bulk of touring development since has largely been around dynamic display, user interaction, geometric representation, and application.

This works well when the number of dimensions being toured is small (in the neighborhood of 5-10), yet the number of view, or 2-frames and we can produce from p-space suffers from the so called blessing/curse of dimensionality. In which the plethora of degrees of freedom either offer many (non-unique) solutions to a problem or something that becomes ever increasing unlikely,

2.1.3 Tour path

A fundamental aspect of touring is the path of rotation. Of which there are four primary distinctions(Buja et al., 2005): random choice, precomputed choice, data driven, and manual control.

- *grand tour*, a constrained random choice p-space. Paths are constrained for changes in direction small enough to maintain continuity and aid in user comprehension
  - torus-surface (Asimov, 1985)
  - Geodesic
  - at-random
  - random-walk
  - *local tour*, a sort of grand tour on leash, such that it goes to a nearby random projection before returning to the original position and iterating
- *guided tour*, data driven tour optimizing some objective function via (stochastic) gradient descent (Hurley and Buja, 1990).
  - holes (Cook, Buja, and Cabrera, 1993) - iterates projections that add more white space to the center of the projection.

  - cmass (Cook, Buja, and Cabrera, 1993) - find the projection with the most density or mass in the center.
  - lda (Lee et al., 2005) - linear discriminant analysis, seeks a projection where 2 or more classes are most separated.
  - pda - principal component analysis finding where the data is most spread (1d only).
  - other user-defined objective function (Wickham et al., 2011).

- *planned tour*, Precomputed choice, In which the path has already been generated or defined.

  - *little tour* (McDonald, 1982), where every permutation of variables is stepped through in order, analogous to a brute-force or exhaustive search.
  - a saved path of any other tour

- *manual tour* - Manual control, a constrained rotation on selected manipulation variable and magnitude(Cook and Buja, 1997). Typically used to explore the local area after identifying an interesting feature from another tour.

- *dependance tour*, combination of n independent 1d tours. A vector describes the axis each variable will be displayed on. **ie** $c(1, 1, 2, 2)$ is a 4 to 2d tour with the first 2 variables on on the first axis, and the remaining on the second.

  - *correlation tour* (Buja, Hurley, and McDonald, 1987), a special case of the dependence tour, analogous to canonical correlation analysis

2.1.4 Geometrics and display dimension

Up to this point we have been talking about 2d scatterplots, which offer the first and a simple case for viewing lower-dimensional embeddings of p-space. However, other geometrics (or geoms) offer perfectly valid orthonormal projections as well.

- 1d geoms

  - 1-d densities: such as histogram, average shifted histograms(**scott85**), and kernel density(**scott95**).
  - image: (**Wegman**)
  - time series: where multivariate values are independently lagged to view peak and trough alignment. Currently no package implementation, but use case is discussed in (Cook and Buja, 1997).

- 2d geoms
  - 2-d density (**NS**)
  - scatterplot
  -

- 2.5d, 3d geoms {ADD FOOTNOTE ABOUT 2.5d vs 3d}
  - Anaglyphs, sometimes called stereo, where (typically) red images are positioned for the left channel and cyan for the right, when viewed with corresponding filter glasses give the depth perception of the image.
  - Depth, which use some subset of depth cues, most commonly size and/or color of data points.

- *d*-dim geoms
  - Andrews curves (Andrews, 1972), smoothed variant of parallel coordinate plots, discussed below.
  - Chernoff faces (Chernoff, 1973), variables linked to size of facial features for rapid cursory like-ness comparison of observations.
  - Parallel coordinate plots (Ocagne, 1885), where any number of variables are plotted in parallel with observations linked to their corresponding variable value by polylines.
  - Scatterplot matrix (Becker and Cleveland, 1987), showing a triangle matrix of bivariate scatterplots with 1-d density on the diagonal.
  - Radial glyphs, radial variants of parallel coordinates including radar, spider, and star glyphs (Siegel et al., 1972).

2.1.5 Aplication

Below is a non-exhaustive list of software implementing touring in some degree, ordered by descending year:

- Spinifex (**spinifex**) – for Linux, Unix, and Windows.
- Tourr (Wickham et al., 2011) – for Linux, Unix, and Windows. R package.
- CyrstalVision (Wegman, 2003) – for Windows.
- GGobi (Swayne et al., 2003) – for Linux and Windows.
- DAVIS (Huh and Song, 2002) – Java based, with GUI.
- VRGobi (Nelson, Cook, and Cruz-Neira, 1998) – for use with the C2 in stereoscopic 3d displays.
- ExplorN (Carr, Wegman, and Luo, 1996) – for SGI Unix.
- XGobi (Swayne, Cook, and Buja, 1991) – for Linux, Unix, and Windows (via emulation).
- XLispStat (Tierney, 1990) – for Unix, and Windows.
- Prim-9 (Asimov, 1985; Fisherkeller, Friedman, and Tukey, 1974) – on an internal operating system.

Support and maintenance of such implementations give them a particularly short life span, while conceptual abstraction and technically heavier implementations have hampered user growth. There have been notable efforts to diminish the barriers to entry and make touring more approachable as a data exploration tool [Huh and Song (2002); Swayne et al. (2003); Wegman (2003); Wickham et al. (2011); huang_tourrgui:_2012].

2.2 Virtual reality

Chapter 3

spinifex: An R package that provides manual rotations in high-dimensions

3.1 Abstract

The tour algorithm, and its various versions provide a systematic approach to viewing low-dimensional projections of high-dimensional data. It is particularly useful for understanding multivariate data, and useful in association with techniques for dimension reduction, supervised and unsupervised classification. The *R* package *tourr* provides manhy methods for conducting tours on multivariate data. This paper discusses an extension package which adds support for the manual tour, called *spinifex*. It is particularly usefully for exploring the sensitivity of structure discovered in a projection by a guided tour, to the contribution of a variable. *Spinifex* utlizes the animation packages *plotly* and *gganimation* to allow users to rotate a variable into and our of a chosen projection.

Keywords: grand tour, projection pursuit, manual tour, high dimensional data, multivariate data, data visualization, statistical graphics, data science, data mining.

3.2 Introduction

The manual tour was described in Cook and Buja (1997), and allows a user to rotate a variable into and out of a 2D projection of high-dimensional space. The primary purpose is to determine the sensitivity of structure visible in a projection to the contributions of a variable. Manual touring can also be useful for exploring the local structure once a feature of interest has been identified, for example, by a guided tour (Cook et al., 1995). The algorithm for a manual tour allows rotations in horizontal, vertical, oblique, angular and radial directions. Rotation in a radial direction, would pull a variable into and out of the projection, which allows for examining the sensitivity of structure in the projection to the contribution of this variable. This type of manual rotation is the focus of this paper.

A manual tour relies on user input, and thus has been difficult to program in R. Ideally, the mouse movements of the user are captured, and passed to the computations, driving the rotation interactively. However, this type of interactivity is not simple in R. This has been the reason that the algorithm was not incorporated into the *tourr* package. Spinifex utilizes two new packages for conducting animations, *plotly* (Sievert, 2018) and *gganimate* (Pedersen and Robinson, 2019), to conduct a manual tour. From a given projection, the user can choose which variable to control, and the animation equence is generated to remove the variable from the projection, and then extend its contribution to be the sole variable in one direction. This allows the viewer to assess the change in structure induced in the projection by the variable contribution.

The paper is organized as follows. Section 3.3 explains the algorithm using a toy dataset. Section 3.5 illustrates how this can be used for sensitivity analysis. The last section summarizes the work and discusses future research.

3.3 Manual tour algorithm

The algorithm contains several steps:

1. Choose a variable to explore, called the manip variable

2. Create a 3D manipulation space, where the variable to be explored has full contribution.
3. Generate the rotation which zero's the coefficient and also increases it to 1

3.3.1 Notation

Given:

$\mathbf{X}_{[n,\ p]}$ A data set containing n observations of p numeric variables.

$\mathbf{B}_{[p,\ d]}$ An orthonormal [1] basis describing the current orientation projecting p down to d dimension.

$$\mathbf{X}_{[n,\ p]} = \begin{bmatrix} X_{1,\ 1} & \dots & X_{1,\ p} \\ X_{2,\ 1} & \dots & X_{2,\ p} \\ \vdots & \ddots & \vdots \\ X_{n,\ 1} & \dots & X_{n,\ p} \end{bmatrix}$$

$$\mathbf{B}_{[p,\ d]} = \begin{bmatrix} B_{1,\ 1} & \dots & B_{1,\ d} \\ B_{2,\ 1} & \dots & B_{2,\ d} \\ \vdots & \ddots & \vdots \\ B_{p,\ 1} & \dots & B_{p,\ d} \end{bmatrix}$$

For ease of computation we will be working mostly with the basis and not the data, once basis manipulation is done post multiply the data by the basis to get back to data-space.

3.3.2 Flea data set

We'll illustrate with the flea data set from the R package *tourr* (Wickham et al., 2011), which contains different tours on the same data. The data comes from Lubischew (1962). The

[1]Where each variable is both: orthogonal, at right angles (dot product is 0) to the other variables, and unit vectors, a norm = 1

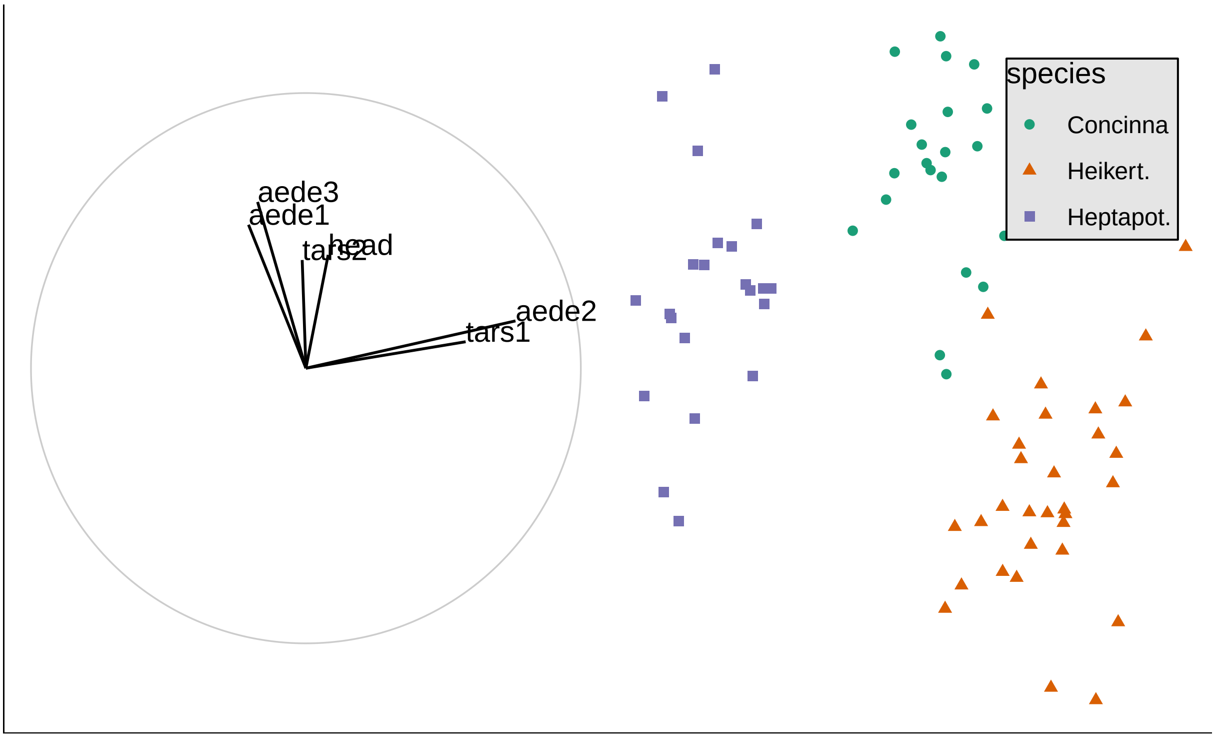


Figure 3.1: *Basis reference frame (left) and projected data (right) of standardized flea data. Basis indentified by holes-index guided tour. The variables* `aede2` *and* `tars1` *cotribute mostly in the x direction, whereas the other variables contribute mostly in the y direction. We'll select* `aede2` *as our manipulation variable to see how the structure of the projection changes as we rotate* `aede2` *into and out of the projection.*

flea data contains 74 observations across 6 variables, physical measurements of each flea beetle. Each individual belonged to one of three species being observed.

We'll perform a guided tour on the flea data optimizing on the `holes` index (Cook, Swayne, and Buja, 2007). In a guided tour the data is projected rated against the the selected index, and looks around in the local area for a projection that outperforms the current best index. A basis that spreads the projected data furthest from the center is sought after in the case of the `holes` index. In figure 3.1, below, the left frame depicted the final basis of the `holes` tour. a unit circle with lines showing the x and y contributions of each variable in the projection space. The right frame projects the data through that basis and colors the points according to the observed species.

The left frame of 3.1 shows the reference frame for the basis. It describes the X and Y contributions of the basis as it projects from the 6 variable dimensions down to 2. Call `view_basis()` on a basis to produce a similar image as a `ggplot2` object. The right side shows how the data looks projected through this basis. You can project a single basis at any time through the matrix multiplication $\mathbf{X}_{[n,\ p]} \ * \ \mathbf{B}_{[p,\ d]} \ = \ \mathbf{P}_{d[n,\ d]}$ to such effect.

3.3.3 Step 1 Choose variable of interest

Select a manipulation variable, k. Initialize a zero vector e, and set the k-th element set to 1.

$$\mathbf{e}_{k\ [p,\ 1]} \ = \ \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix}_{[p,\ 1]}$$

In figure 3.1, above, notice that the variables `tars1` and `aede2` are almost orthogonal to the other 4 variables and control almost all of the variation in the x axis of the projection. `Aede2` has a larger contribution in this basis, so we'll select it

3.3.4 Step 2 Create the manip space

Use the Gram-Schmidt process to orthonormalize the concatenation of the basis and e yielding the manipulation space.

$$\begin{aligned} \mathbf{M}_{[p,\ d+1]} &= Orthonormalize_{GS}(\mathbf{B}_{[p,\ d]}|\mathbf{e}_{k\ [p,\ 1]}) \\ &= Orthonormalize_{GS}\left(\begin{bmatrix} B_{1,\ 1} & \dots & B_{1,\ d} \\ B_{2,\ 1} & \dots & B_{2,\ d} \\ \vdots & \ddots & \vdots \\ B_{k,\ 1} & \dots & B_{k,\ d} \\ \vdots & \ddots & \vdots \\ B_{p,\ 1} & \dots & B_{p,\ d} \end{bmatrix} \ | \ \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix} \right) \end{aligned}$$

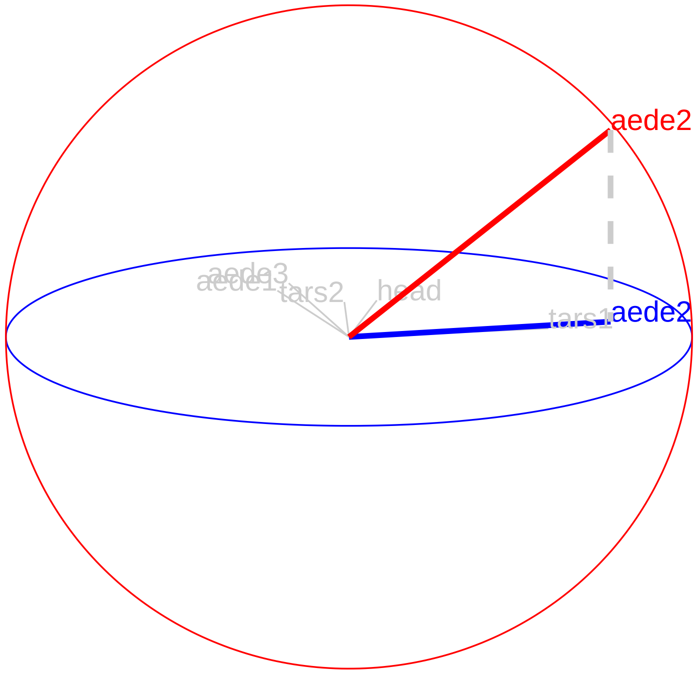


Figure 3.2: *Manipulation space for controling the contribution of aede2 of standardized flea data. Basis was identified by holes-index guided tour. The out of plane axis, in red, shows how the manipulation variable can be rotated, while other dimensions stay embeded within the basis plane.*

In R it looks like the below chunk. `tourr::orthonormalise()` uses the Gram Schimidt process (rather than Housholder reflection) to orthonormalise.

Adding an extra dimension to our basis plane allows for the manipulation of the specified variable while the others are kept fully within the basis plane. Orthonormalising rescales the matrix without bringing the other variables into this new axis. An illustration of such can been seen below in 3.2.

Imagine being able to grab hold of the red axis and rotate it changing the projection onto the basis plane. This is what happens in a manual tour. By controling the angle between the axis and the basis plane we change the contribution of the manipulation variable on the projection.

3.3.5 Step 3 Generate rotation

Define a set of values for ϕ_i, the angle of out-of plane rotation, orthogonal to the projection plane. This corisponds to the angle between the red axis and the blue plane in 3.2. **For** i **in 1 to n_slides:**

For each ϕ_i, post multiply the manipulation space by a rotation matrix, producing as many basis-projections.

$$\mathbf{P}_{b[p,\ d+1,\ i]} = \mathbf{M}_{[p,\ d+1]} \ * \ \mathbf{R}_{[d+1,\ d+1]} \qquad \text{For the } d = 2 \text{ case:}$$

$$= \begin{bmatrix} M_{1,\ 1} & M_{1,\ 2} & M_{1,\ 3} \\ M_{2,\ 1} & M_{2,\ 2} & M_{2,\ 3} \\ \vdots & \vdots & \vdots \\ M_{p,\ 1} & M_{p,\ 2} & M_{p,\ 3} \end{bmatrix}_{[p,\ d+1]} * \begin{bmatrix} c_\theta^2 c_\phi s_\theta^2 & -c_\theta s_\theta(1-c_\phi) & -c_\theta s_\phi \\ -c_\theta s_\theta(1-c_\phi) & s_\theta^2 c_\phi + c_\theta^2 & -s_\theta s_\phi \\ c_\theta s_\phi & s_\theta s_\phi & c_\phi \end{bmatrix}_{[3,\ 3]}$$

Where:

θ is the angle that lies on the projection plane (*ie*. on the XY plane)

ϕ is the angle orthogonal to the projection plane (*ie*. in the Z direction)

c_θ is the cosine of θ

c_ϕ is the cosine of ϕ

s_θ is the sine of θ

s_ϕ is the sine of ϕ

In application: compile the sequence of ϕ_i and create an array (or long table) for each rotated manipulation space. ϕ is actually the angle relative to the ϕ_1, we find the transformation ϕ_i - ϕ_1 useful to discuss ϕ relative to the basis plane.

```
## Warning: Removed 1 rows containing missing values (geom_path).
```

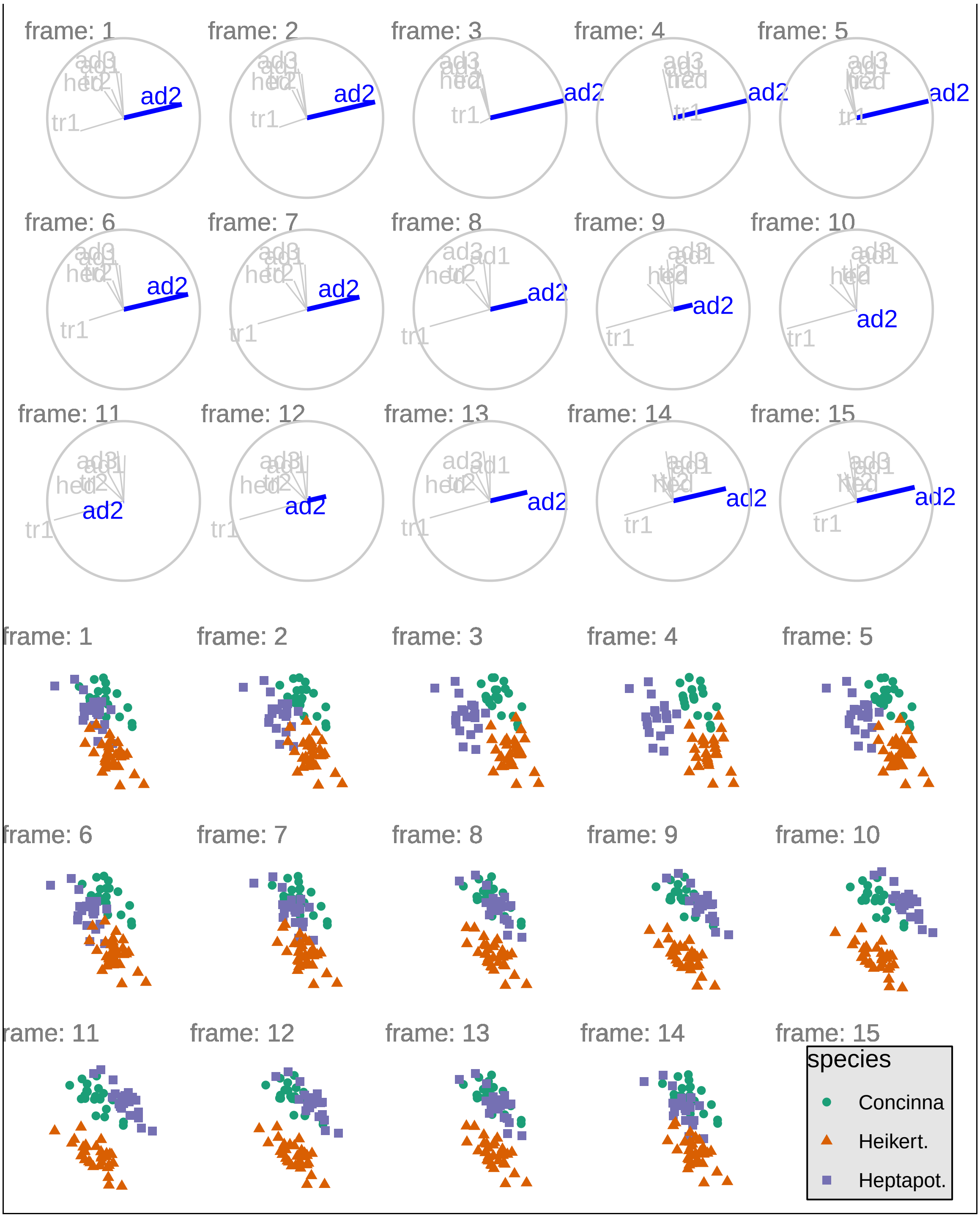


Figure 3.3: *rotated manipulation spaces, a radial manual tour manipulating aded2 of standardized flea data. The manipulation variable, aede2, extends from it's initial contribution to a full contribution to the projection before decreasing to zero, and then retruning to it's inital state.*

3.4 Display projection sequence

To get back to data-space pre multiply each projection basis by the data for the projection in data-space.

$$
\begin{aligned}
\mathbf{P}_{d[n,\ d+1]} &= \mathbf{X}_{[n,\ p]} * \mathbf{P}_{b[p,\ d+1]} && (3.1)\\
&= \begin{bmatrix} X_{1,\ 1} & \dots & X_{1,\ p} \\ X_{2,\ 1} & \dots & X_{2,\ p} \\ \vdots & \vdots & \vdots \\ X_{n,\ 1} & \dots & X_{n,\ p} \end{bmatrix}_{[n,\ p]} * \begin{bmatrix} P_{b:1,\ 1} & P_{b:1,\ 2} & P_{b:1,\ 3} \\ P_{b:2,\ 1} & P_{b:2,\ 2} & P_{b:2,\ 3} \\ \vdots & \vdots & \vdots \\ P_{b:p,\ 1} & P_{b:p,\ 2} & P_{b:p,\ 3} \end{bmatrix}_{b[p,\ d+1]} && (3.2)
\end{aligned}
$$

Plot the first 2 variables from each projection in sequence for an XY scatterplot. The remaining variable is sometimes linked to a data point aesthetic to produce depth cues used in conjunction with the XY scatterplot.

tourr utilizes R's base graphics for the display of tours. Use `render_plotly()` to display as an dynamic `plotly` Sievert (2018) object or `render_gganimate()` for a `gganimate` Pedersen and Robinson (2019) graphic. A thrid noteable animation related package is `animation` Xie et al. (2018). It's not yet implemented in `spinifex` as it uses base graphics, whereas the former two are compatiable with `ggplot2`.

Interaction with graphics in R is limited. Traditionally, all commands are passed to the R via calls to the console, conflicting with user engagement. Some recent packages have made advancment into this direction such as with the use of the R package `shinny`, which custom-made applications can be hosted either locally or remotely and interact with the R console, allowing for developers to code dynamic content interaction. To a lesser extent `plotly` offers static interactions with contained object, such as tooltips, brushing, and linking without communicating back to the R console.

Storing the each data point and all of the overhead though goes into dynamic graphics if very inefficient. In the same way that we performed math the bases, that is the same approach storage and sharing tours. Consider the manual tour, we can store the salient features in 3 basis, where ϕ is at it's starting, minimum, and maximum values. The frames inbetween can be interpolated by suppling angular speed or number of desired frames. By using the `tourr::save_history()` we can do just that. Save such tour path history and a single set of the data offers a perfomant store and tranfer.

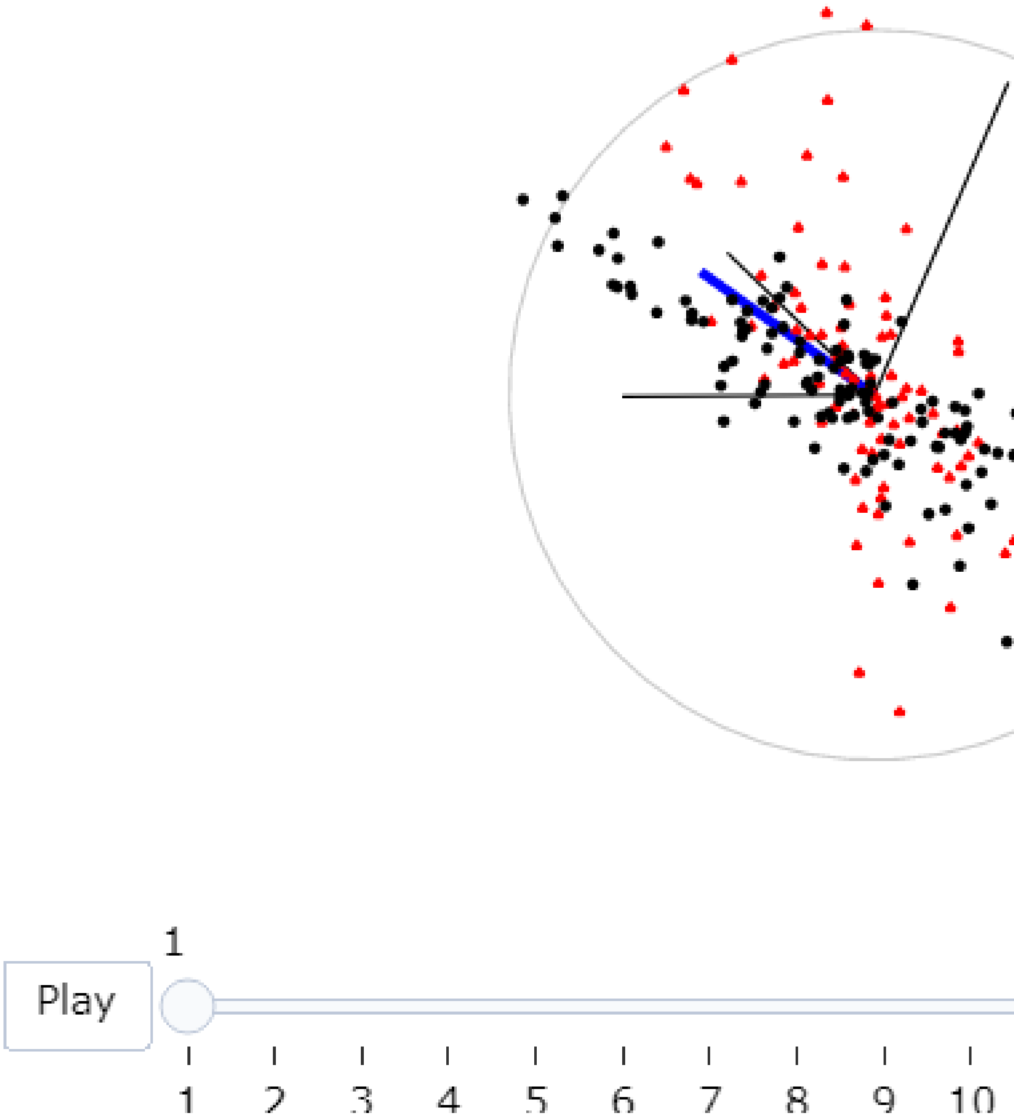
3.5 Application

NOTE: Examples from https://arxiv.org/abs/1806.09742 Cook, Laa, and Valencia (2018)

3.5.1 Subset of figure 7

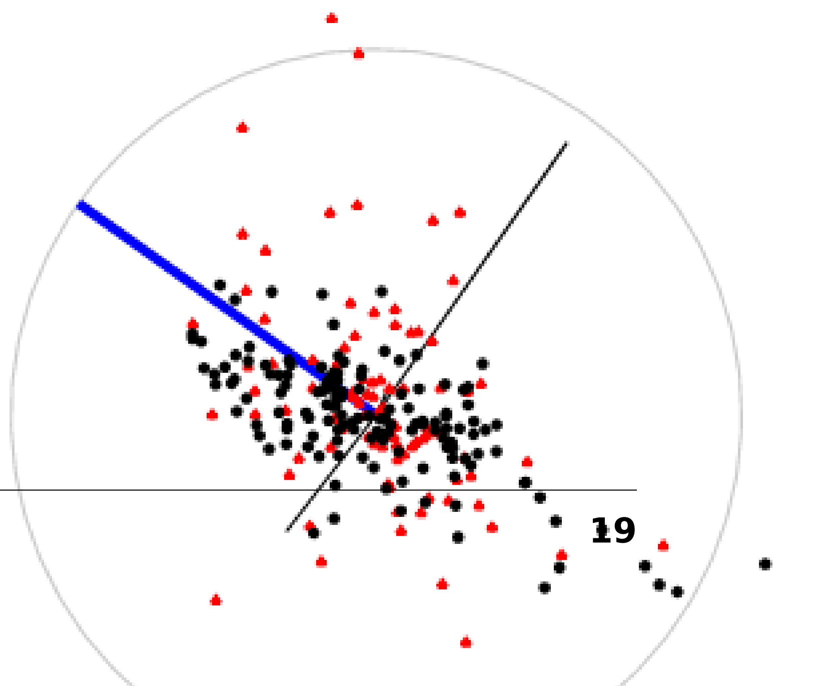
Manual tour of the first 4 principle components for experiments of ATLAS7old and ATLAS7new.

Manual tour on the PC3:



ϕ in the starting position

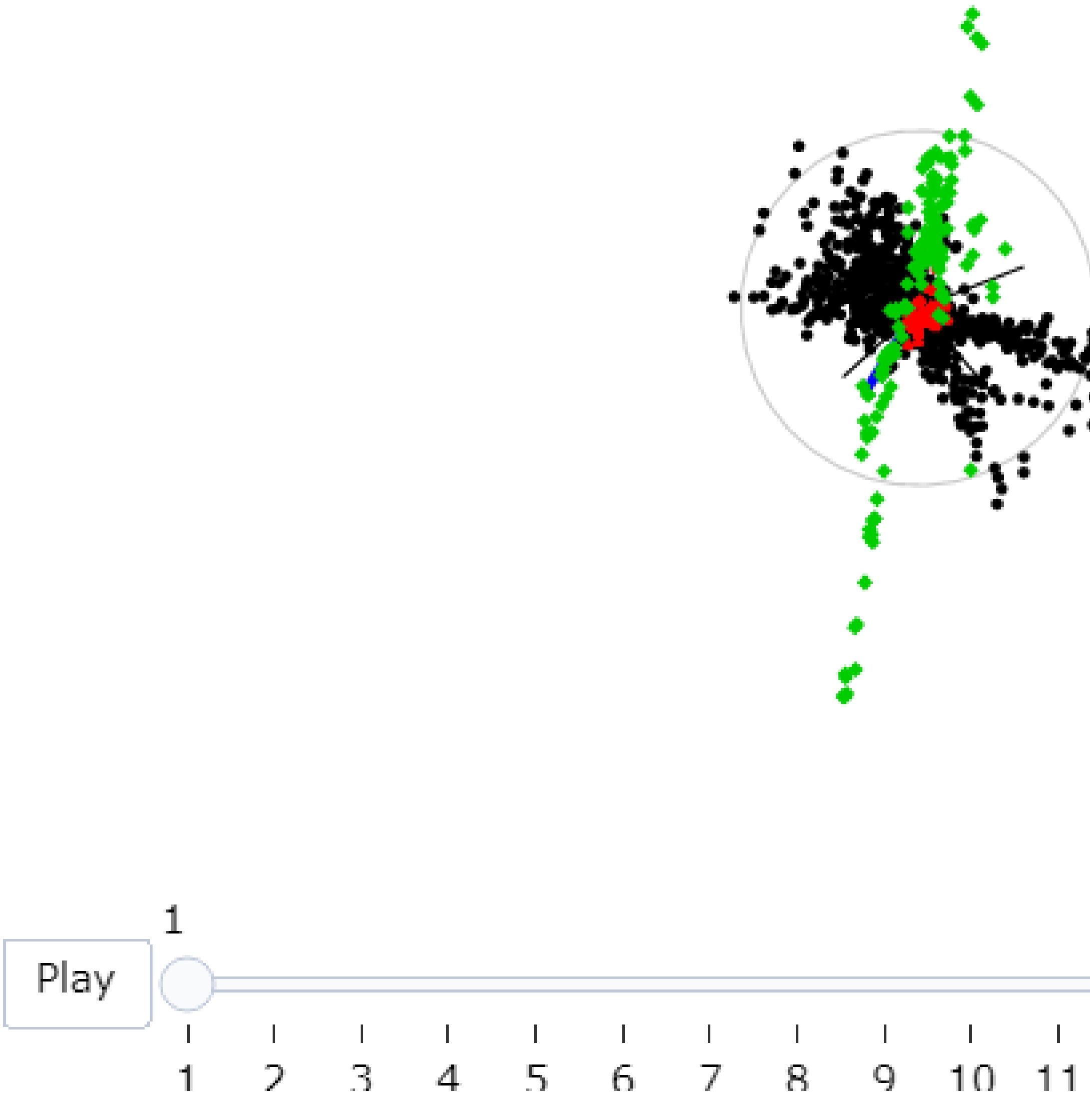
ϕ zeroed, maximizing the contribution from the 3rd principle component



3.5.2 Figure 8

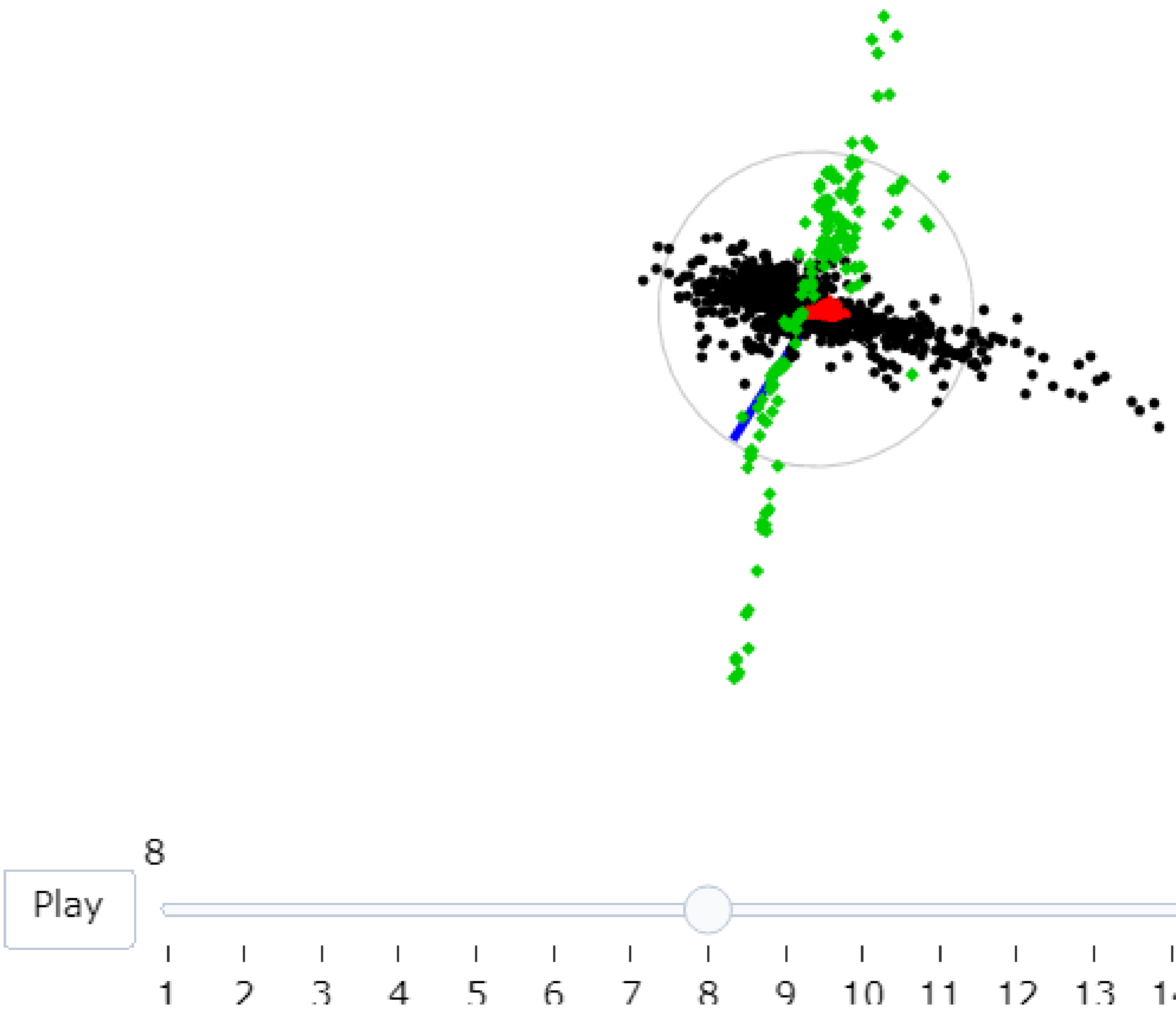
'dimuonSIDIS' experiements (green points), 'DIS HERA1+2' experiments in black.

Manual tour on PC6:

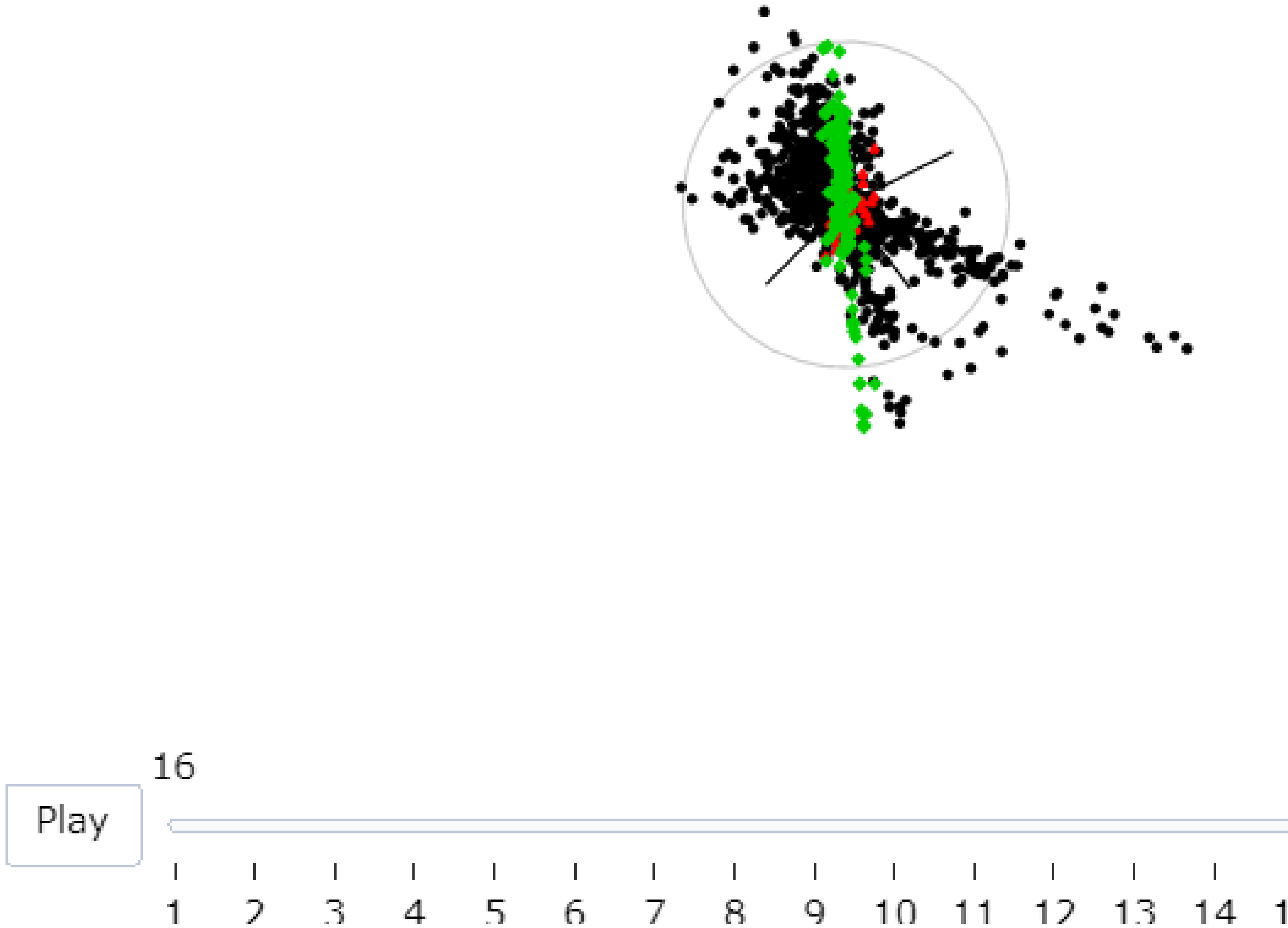


ϕ in the starting position

ϕ zeroed, maximizing the contribution from the 6th principle component


8
Play
1
2
3
4
5
6
7
8
9
10
11
12
13

ϕ at 90 degrees, minimizing the contribution from the 6th principle component



Dynamic versions of the manual tour can be found at: nspyrison.netlify.com

3.6 Source

The code used to generate this writing can be found at this GitHub.com/nspyrison/Confirmation.

3.7 Discussion

Future work:

- other rotation mechanisms like Givens and Householder
- oblique should be defined.
- other display types, would work for 1D displays, but others would need redefinition difference dimensions
- shiny app, for choosing manip variable, providing different starting projections

Chapter 4

Display dimensionality

- XGobbi vs the C2

Chapter 5

Human-computer interaction of 3d projections

- Tour in 3D
- ImAxes / IATK

Appendix A

Additional stuff

You might put some computer output here, or maybe additional tables.

Note that line 5 must appear before your first appendix. But other appendices can just start like any other chapter.

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