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

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by

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Contents

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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 contribution in Chapter 3 will soon be submitted to the R journal and the accomanying R package *spinifex* will be submitted to CRAN.

Abstract

Visualizing data space is crucial to exploratory data analysis yet doing so quickly becomes difficult as the dimensionality of the data increases. Traditionally, static low dimensional embeddings are used, as in PCA and LDA. Observing one such embedding often misses a significant amount of variation, and hence, information held within the data. Touring is a method that animates many projections as the orientation in data space is varied. This maintains inter-operability the original variables, while preserving observable information.

I have implemented manual tours in the programming language R with compatibility to the other touring package while extending to new graphics paradigms to display tours. The application of manual tours to experimental high energy physics data that exists in 56-dimensional space is also presented extenting previous touring on the same data.

Next, I will conduct an experimental survey comparing manual tour perception across 4 display types: 2d desktop, 3d desktop, head-mount virtual reality, and in-person immersion in a virtual display. From the same interface using the game engine Unity.

Lastly, I'll combine existing packages in R and Unity to explore the human-computer interaction with projections and functions of high dimensional spaces.

Chapter 1

Research problem

Data and models are typically high-dimensional, with many variables or parameters. Developing new methods to visualise high dimensions have been a pursuit of statisticians, computer scientists and visualisation researchers for decades. As technology evolves examining, extending, and assessing current techniques, in new environments, for new data challenges, is an important endeavour.

This thesis focuses on tour methods for visualising high-dimensional data. Tours are a famiily of algorithms for generating paths on the space of low dimensional ($d = 1, 2, 3, ..., p$) projections of high-dimensional (p) space. The resulting projection of the data (or model) is displayed using low-dimensional techniques such as histograms, dotplots, scatterplots, or parallel coordinate plots, and the path generates a movie or animation to shows many low-dimensional projections. The method can be applied with other techniques such as machine learning techniques like discriminant analysis, neural networks, support vector machines, to open the black box, and complements dimension reduction techniques like principal component analysis (PCA), multidimensional scaling (MDS) on nonlinear embeddings (e.g. tSNE).

The primary research question is:

Does allowing the user to steer the tour, facilitate the exploration and understanding of the sensitivity of structure to the original variables or parameters? This question is reduced to four research objectives:

A **Can user controlled steering (UCS) be utlized in an environment providing only animation?**

C **What benefits does UCS provide over current common practices, such as PCA, MDS, tSNE?**

B **How do we extend UCS to 3D?**

D **Does UCS with 3D displays provide perception benefits over 2D displays?**

These questions are studied in chapters 3 thru 6 respectively.

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 rotations in p-space. These frames are then viewed in order as an animation of the lower dimensional embedding changing as the orginial variable space 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. In some views more information is hidden than in others, and complex strutures generally require more time to comphrehend the nature of the geometry.

Terminology

Terminology varies accross author and implementation. In my work, I use the following

- n, numerber of observations
- p, number of numeric variables, the dimensionality of data space,
- d, dimensionality of projection space

- $\mathbf{X}_{[n,\ p]}$, a data matrix in variable-space, $\mathbf{X} \in \mathbb{R}^p$. Typically centered, scaled, and optionally sphered.
- $B_{[p,\ d]}$, orthonormal basis vector, defining the orientation of projection from $p-$ to $d-$space
- $\mathbf{Y}_{[n,\ d]}$, projected data matrix in projection-space, $\mathbf{Y} \in \mathbb{R}^d$
- For projections down to 1- and 2-d, It's common to display the contribution and direction on it's own axis (1d) or relative to a unit circle (2d), this is sometime refered to as basis axes or a reference frame.
- Geometric objects are referred to in generalized dimensions; the use of plane isn't necessarily a 2d surface, but a hyperplane in the arbitary dimensions of the projection space.

2.1.2 History

Touring was first introduced by Asimov in 1985 with his purposed Grand Tour(Asimov, 1985) at the Stanford Linear Accelerator, 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. The original application of touring was on high energy physics on the PRIM-9 system.

Before choosing projection paths randomly, an exhaustive search of was suggested by McDonald (1982), also at the Stanford Linear Accelerator, and acknowledges Asimov and Buja.

In 1974 Friedman and Tukey purposed Projection Pursuit(Friedman and Tukey, 1974) (sometimes referred to as PP) while working at Bell Labs. Projection Pursuit involves identifying "interesting" projection, remove a single component of the data, and then iterate in this newly embedded subspace. Within each subspace the projection seeks for a local extrema via hill climbing algorithms. This formed the basis for guided tours Hurley and Buja (1990),

The grand and little tour have no input from the user aside from the starting basis. Purjection Pusuit allows for an index to be selected, but the bulk of touring development since has largely been around dynamic display, user interaction, geometric representation, and application. The extent to which will be expounded on in the following sections.

2.1.3 Path genration

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)
  - at-random
  - random-walk
  - *local tour*, a sort of grand tour on a leash, such that it goes to a nearby random projection before returning to the original position and iterating
- *guided tour*, data driven tour that optimizing some objective function via projection pursuit(Hurley and Buja, 1990), analogous to gradient descent.
  - 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).
  - convex (Laa and Cook, 2019) - the ratio of area of convex and alpha hulls.
  - skinny (Laa and Cook, 2019) - the ratio of of the perimeter distance to the area of the alpha hull.

  - stringy (Laa and Cook, 2019) - based on the minimum spanning tree (MST), the diameter of the MST over the length of the (MST).
  - dcor2D (Grimm, 2017; Laa and Cook, 2019) - distance correlation that finds linear and non-linear dependancyes between variables.
  - splines2D (Grimm, 2017; Laa and Cook, 2019) - measure of non-linear dependence by fitting spline models.
  - other user-defined objective function can be implemented with the *tourr* package 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, typically an array of basis targets to interpolate between as produced by the R function `tourr::save_history()`.

- *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.
- *dependence 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 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

Tour path evaluation

Consider $d = 2$, then each projection is called a 2-frame (each spanning a 2-plane). Mathematically we call the set of all possible unoriented 2-frames in p-space a Grassmannian, $\mathbf{Gr}(2,\ p)$. Asimov (1985) pointed out that the unique 2-frames of the grand tour approaches $\mathbf{Gr}(2,\ p)$ as time goes to infinity. We could then define the *density* of a tour as the fraction of the Grassmannian explored. Ideally a grand tour will be dense, but the time taken to become dense vastly increases as variable space increase dimensionality.

We could then also talk about the *rapidity* of a tour as how quickly a tour encompasses the Grassmannian. Due to the random selection of a grand tour it will end up visiting homomorphisms of previous 2-frames, sub-optimal rapidity.

The little tour introduced in McDonald (1982), on the the other hand is necessarily both dense and rapid, performing essentially an exhaustive search on the Grassmannian. However the path choosen is uninteresting, the pre-defined sequence rarely results in insightful observations.

Guided tours (Hurley and Buja (1990)) optimize an ojective functionm generating path will be relatively small subset of the Grassmanian, density and rapidity become poor measures, while interesting projections are quickly identified. Recently, Laa and Cook (2019), compares projection pursuit indices with the metrics: smoothness, squintability, flexibility, rotation invariance and speed. See the original work to see how the indices perform.

2.1.4 Geom display dimensionality

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 (available on Github at `https://github.com/nspyrison/tourr`)
  - $x - y$ scatterplot

- 2.5d geoms - these geoms do not perform project to 3 dimensions, but rather give persception cues into the add dimension of the manipulation space of 2d projection.
  - 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 Tour software implementations

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, tours 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.
- Explor4 (Carr and Nicholson, 1988) – Four-Dimensional Data Using Stereo-Ray Glyphs
- 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 many 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* utilizes 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

A tour is a multivariate data analysis technique in which is a sequence of orthogonal projection into a lower subspace are viewed in order. each frame of the sequence corresponds to a small change in the projection for a smooth transition.

Multivariate data analysis can be broken into 2 groups: linear and non-linear transformations. Similar to PCA and LDA, touring uses linear dimension reduction with inter-operability back to the original parameter-space. They differ from non-linear transformations such as t-SNE (t-distributed stochastic nearest neighbor embeddings), MDS (multi-dimension scaling), and LLE (local linear embedding), which distort parameter-space for more opaque interpretations

There are many ways that a tour path can be generated, we will focus on one in particular, the manual tour. 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 sequence 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 Algorithm

Creating a manual tour animation requires these steps:

1. Provided with a 2D projection, choose a variable to explore. This is called the "manip" variable.
2. Create a 3D manipulation space, where the manip variable has full contribution.
3. Generate a rotation sequence which zero's the norm of the coefficient and also increases it to 1.

These steps are described in more detail below.

3.3.1 Notation

This section describes the notation used in the algorithm description. The data to be displayed is an $n \times p$ numeric matrix.

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

and an orthonormal d-dimensional projection matrix is

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

The algorithm is primarily operating on the projection basis and utilizes the data only when making a display.

3.3.2 Toy data set

The flea data from the R package *tourr* (Wickham et al., 2011), is used to illustrat the algorithm. The data, originally from Lubischew (1962),contains 74 observations across 6 variables, which physical measurements of the insects. Each individual belonged to one of three species.

A guided tour on the flea data is conducted by optimizing on the `holes` index (Cook, Swayne, and Buja, 2007). In a guided tour the data the projection sequence is shown by optimizing an index of interest. The holes index is maximized by when the projected data has a lack of observations in the center. Figure 3.1, shows an optimal projection of this data. The left plot displays the projection basis, while the right plot shows the projected data. The display of the basis has a unit circle with lines showing the horizontal and vertical contributions of each variable in the projection. Here is is primarily tars1 and aede2 contrasting the other four variables. In the projected data it can be seen that there are three clusters, which have been colored, although not used in the optimization. The question that will be explored in the explanation of the algorithm is how important is aede2 to the separation of the clusters.

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

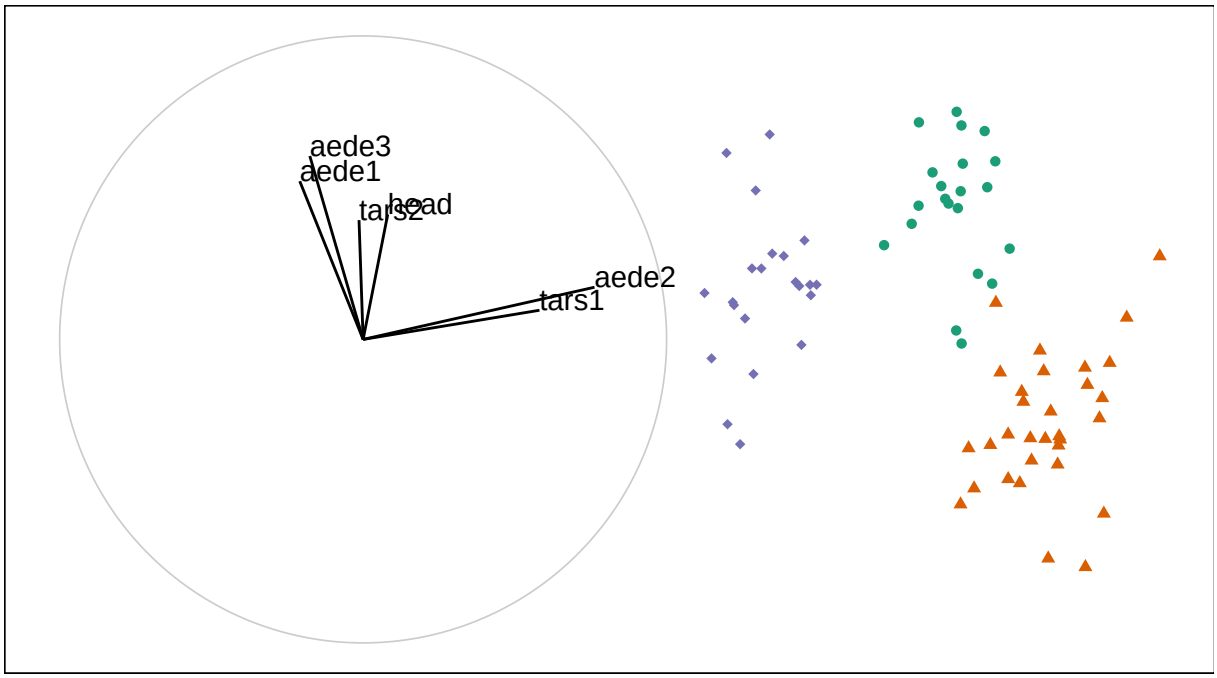


Figure 3.1: *Basis reference frame (left) and projected data (right) of standardized flea data. Basis identified by holes-index guided tour. The variables 'aede2' and 'tars1' contribute mostly in the x direction, whereas the other variables contribute mostly in the y direction. We'll select 'aede2' as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

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.

$$\mathbf{M}_{[p,\,d+1]} = Orthonormalize_{GS}(\mathbf{B}_{[p,\,d]}|\mathbf{e}_{k\ [p,\,1]})$$

$$= Orthonormalize_{GS}\left(\begin{bmatrix} B_{1,1} & \dots & B_{1,d} \\ B_{2,1} & \dots & B_{2,d} \\ \vdots & \ddots & \vdots \\ B_{k,1} & \dots & B_{k,d} \\ \vdots & \ddots & \vdots \\ B_{p,1} & \dots & B_{p,d} \end{bmatrix} \Bigg| \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix}\right)$$

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

```
e            <- rep(0, len = nrow(basis))
e[manip_var] <- 1
manip_space  <- tourr::orthonormalise(cbind(basis, e))
```

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. orthonormalizing 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 controlling the angle between

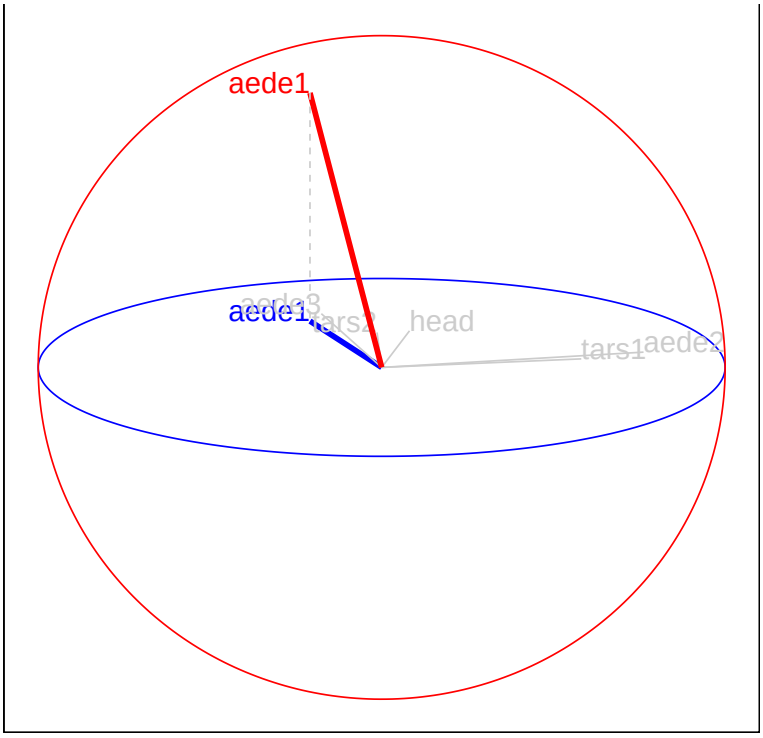


Figure 3.2: *Manipulation space for controlling the contribution of aede2 of standardized flea data. Basis was identified by holes-index guided tour. The out of plane axis, in red, shows how the manipulation variable can be rotated, while other dimensions stay embedded within the basis plane.*

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 corresponds to the angle between the red manipulation 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.

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

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

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.

```
for (phi in seq(seq_start, seq_end, phi_inc_sign)) {
  slide <- slide + 1
  tour[,, slide] <- rotate_manip_space(manip_space, theta, phi)[, 1:2]
}
```

In 3.3 we illustrate the sequence with 15 projected bases and highlight the manip variable on top, while showing the corresponding projected data points on the bottom. A dynamic version of this tour can be viewed online at https://nspyrison.netlify.com/thesis/flea_manualtour_mvar4/, will take a moment to load. This format of this figure and linking to dynamic version will be used again the 3.5 section.

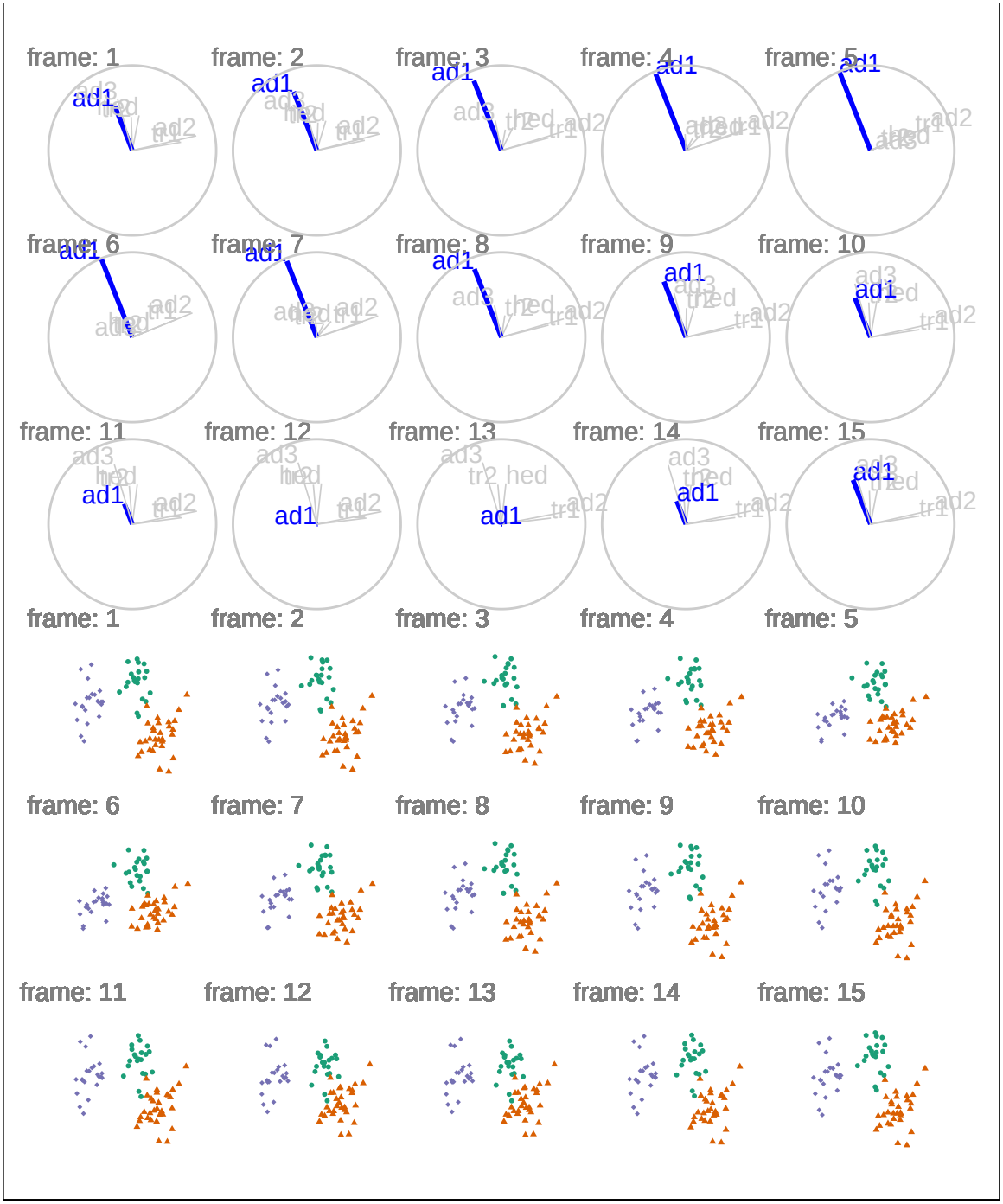


Figure 3.3: *Rotated manipulation spaces, a radial manual tour manipulating aded2 of standardized flea data. The manipulation variable, aede2, extends from it's initial contribution to a full contribution to the projection before decreasing to zero, and then returning to it's initial state. A dynamic version can be viewed at* `https://nspyrison.netlify.com/thesis/flea_manualtour_mvar4/` .

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.

$$\mathbf{P}_{d[n,\,d+1]} = \mathbf{X}_{[n,\,p]} \;*\; \mathbf{P}_{b[p,\,d+1]} \tag{3.1}$$

$$= \begin{bmatrix} X_{1,\,1} & \dots & X_{1,\,p} \\ X_{2,\,1} & \dots & X_{2,\,p} \\ \vdots & \vdots & \vdots \\ X_{n,\,1} & \dots & X_{n,\,p} \end{bmatrix}_{[n,\,p]} * \begin{bmatrix} P_{b:1,\,1} & P_{b:1,\,2} & P_{b:1,\,3} \\ P_{b:2,\,1} & P_{b:2,\,2} & P_{b:2,\,3} \\ \vdots & \vdots & \vdots \\ P_{b:p,\,1} & P_{b:p,\,2} & P_{b:p,\,3} \end{bmatrix}_{b[p,\,d+1]} \tag{3.2}$$

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 third notable 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 compatible 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 advancement 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 tool tips, 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 in between can be interpolated by supplying 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 performant storage and transferring.

3.5 Application

In a recent paper, Wang et al. (2018), the authors aggregate and visualize the sensitivity of hadronic experiments. The authors introduce a new tool, PDFSense, to aid in the visualization of parton distribution functions (PDF). The parameter-space of these experiments lies in 56 dimensions, $\delta \in \mathbb{R}^{56}$, and are presented in this work in 3-d subspaces of the 10 first principal components and non-linear embeddings.

The work in Cook, Laa, and Valencia (2018) applies touring for discern finer structure of this sensitivity. Table 1 of Cook et. al. summaries the key findings of PDFSense & TFEP (tensorflow embedded projection) and those from touring. The authors selected the 6 first principal components, containing 48% of the variation held within the full data when centered, but not sphered. This data contained 3 clusters: jet, DIS, and VBP. Below pick up from the projections used in their figures 7 and 8 (jet and DIS clusters respectively) and apply manual tours to explore the local structure with finer precision.

3.5.1 Jet cluster

The jet cluster is of particular interest as it contains the largest data sets and is found to be important in Wang et al. (2018). The jet cluster resides in a smaller dimensionality than the full set of experiments with 4 principal components explaining 95% of it's variation (Cook, Laa, and Valencia (2018)). We subset the data down to ATLAS7old and ATLAS7new to narrow in on 2 groups with a reasonable number of observations and occupy different parts of the subspace. Below, we perform radial manual tours on various principal components within the this scope. In PC3 and PC4 are manipulated in 3.4 and 3.5 respectively. Manipulating PC3, where varying the angle of rotation brings interesting features in-to and out-of the center mass of the data, is interesting than the manipulation of PC4, where features are mostly independent of the manip var.

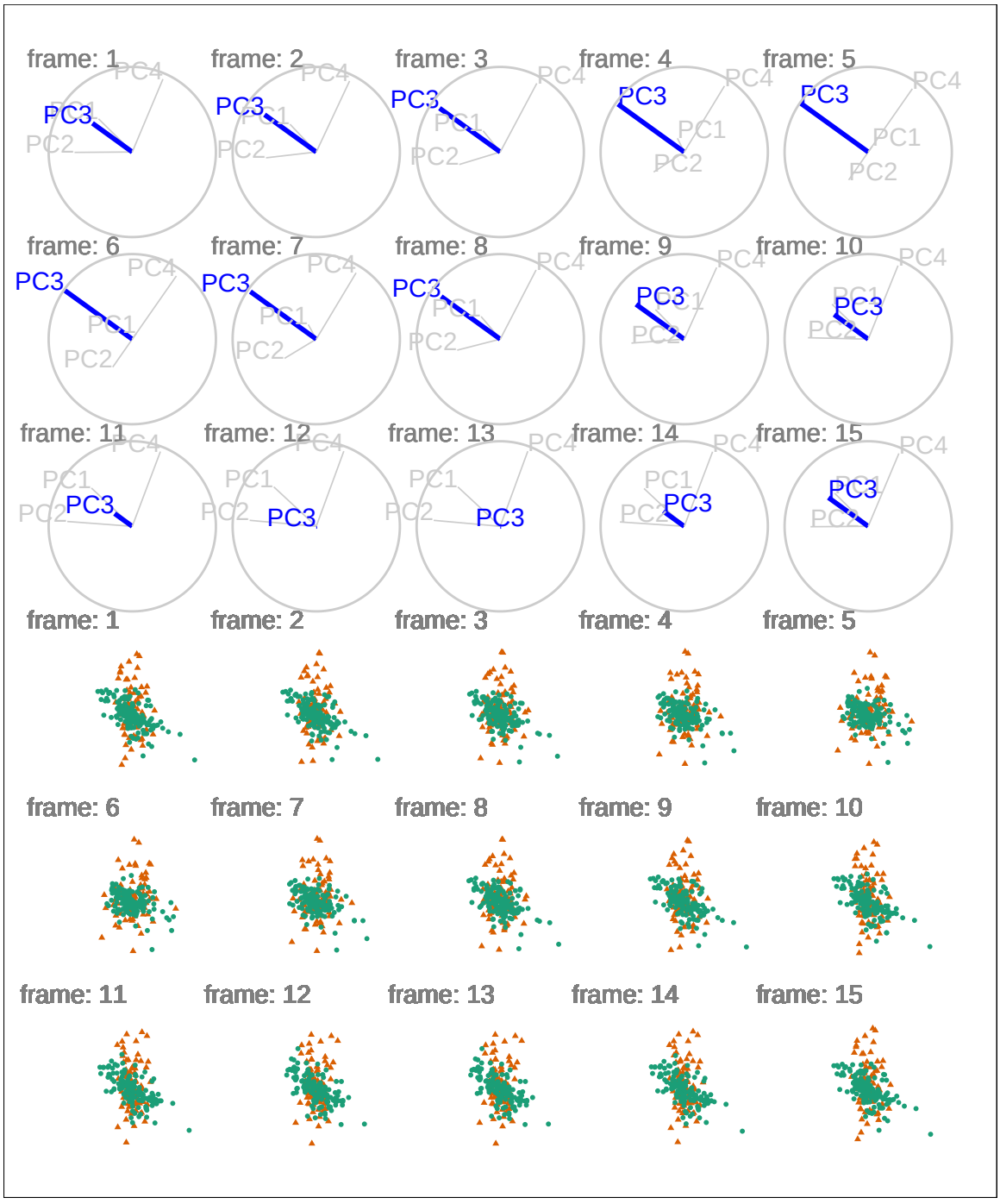


Figure 3.4: *Jet cluster, radial manual tour of PC3. Colored by experiment type: 'ATLAS7new' in green and 'ATLAS7old' in orange. When PC3 fully contributes to the projection ATLAS7new (green) occupies unique space and several outliers are identifiable. Zeroing the contribution from PC3 to the projection hides the outliers and indeed all observations with ATLAS7new are contained within ATLAS7old (orange). A dynamic version can be viewed at* `https://nspyrison.netlify.com/thesis/jetcluster_manualtour_pc3/` .

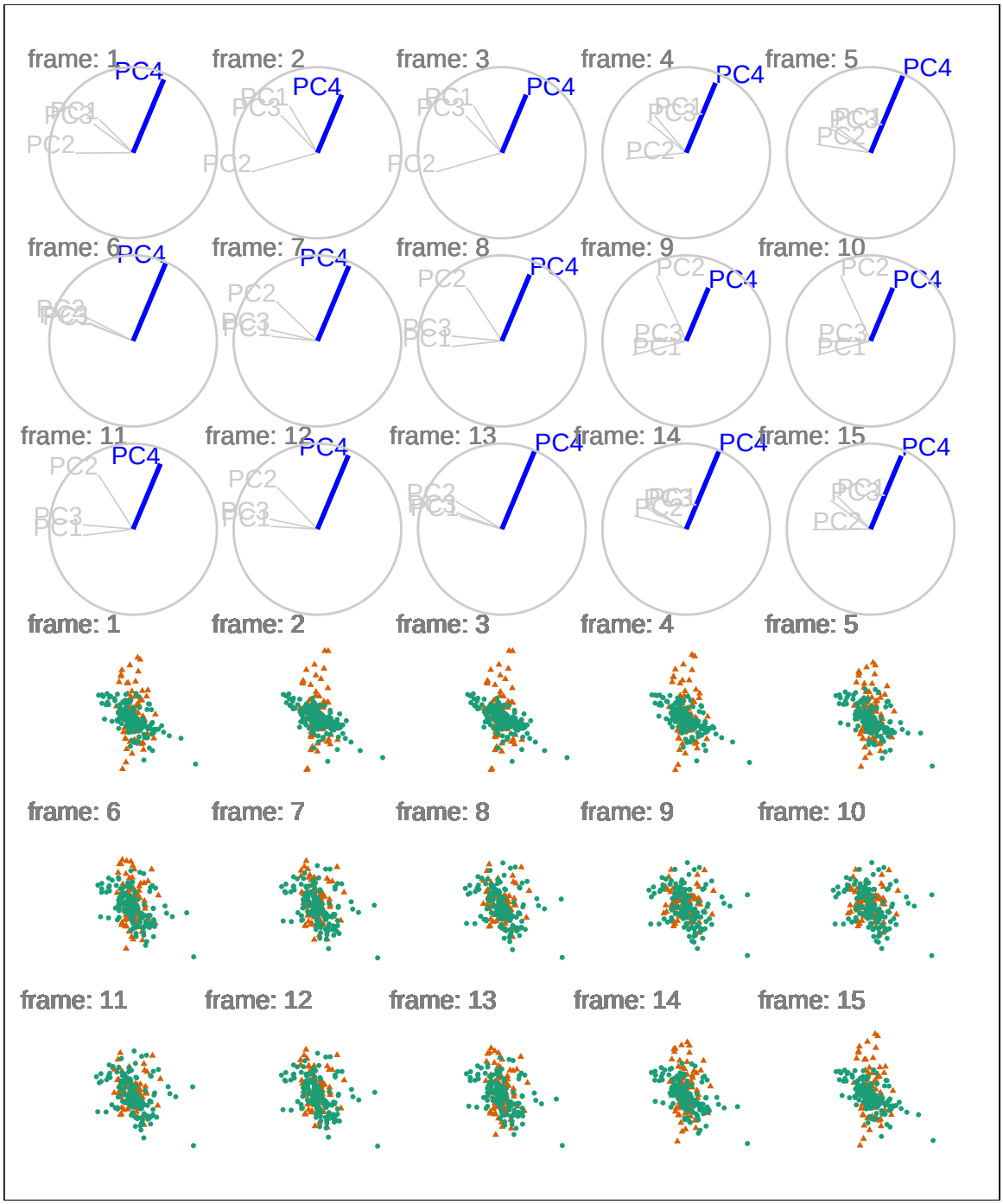


Figure 3.5: *Jet cluster, radial manual tour of PC4. Colored by experiment type: 'ATLAS7new' in green and 'ATLAS7old' in orange. This tour contain less interesting information ATLAS7new (green) has points that are right and left of ATLAS7old, while most points occupy the same projection space, regardless of the contribution of PC4. A dynamic version can be viewed at* `https://nspyrison.netlify.com/thesis/jetcluster_manualtour_pc3/` .

Jet cluster manual tours manipulating each of the principal components can be viewed from the links below:

- PC1
- PC2
- PC3
- PC4

3.5.2 DIS cluster

We perform a manual tour on this data, manipulating PC6 as depicted in 3.6. Looking at several frames we see that DIS HERA lie mostly on a plane. When PC6 has full contributions we see the dimuon SIDIS in purple is almost orthogonal to the DIS HERA (green). Yet the contribution of PC6 is zeroed the dimuon SIDIS data occupy the same space as the DIS HERA data. A dynamic version of this manual tour can be found at: `https://nspyrison.netlify.com/thesis/discluster_manualtour_pc6/`. The page take a bit to load, as the animation is several megabytes.

This is different story than if we had selected a different variable to manipulate. In 3.7 we manipulate PC2.

DIS cluster manual tours manipulating each of the principal components can be viewed from the links below:

- PC1
- PC2
- PC3
- PC4
- PC5
- PC6

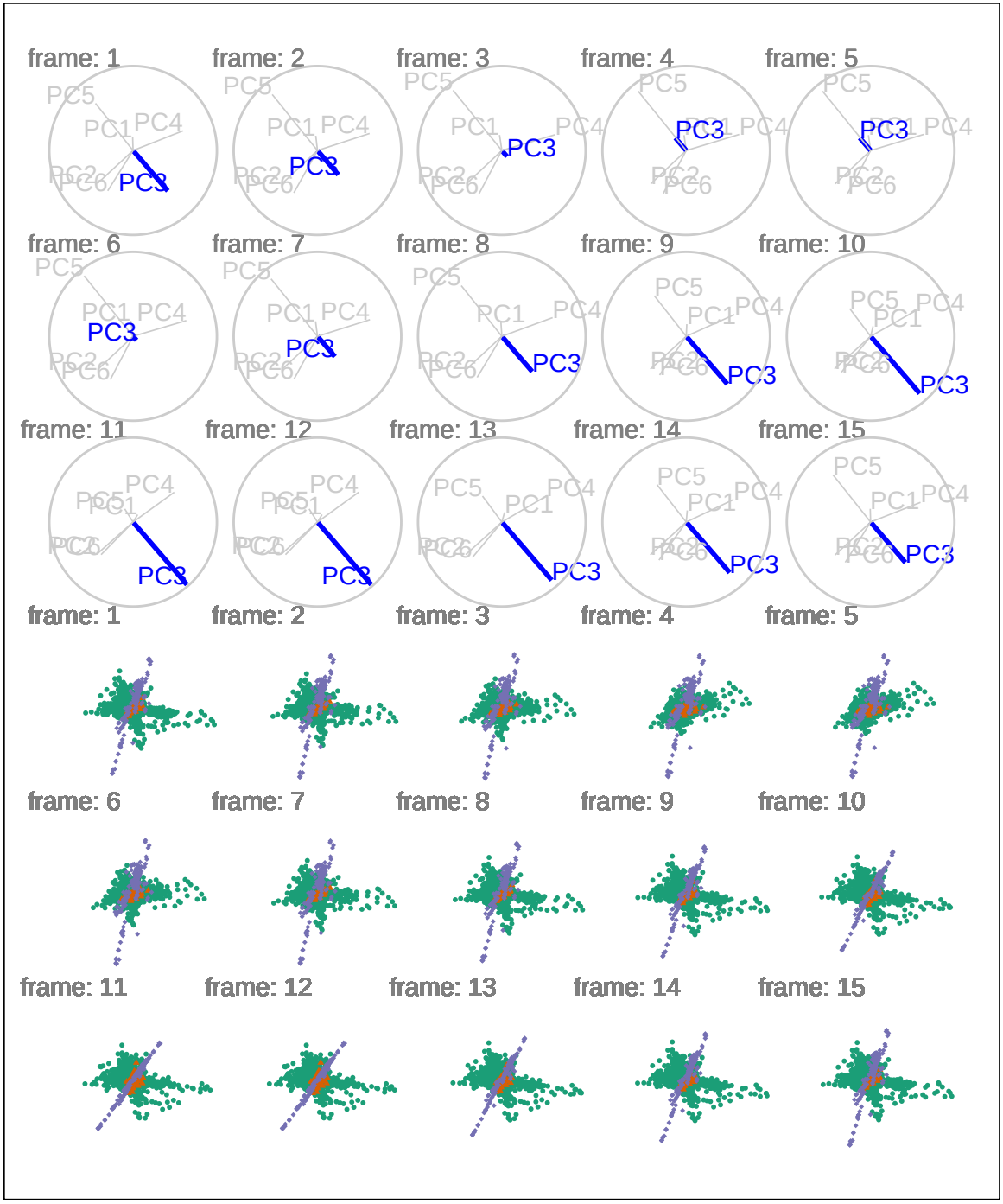


Figure 3.6: *DIS cluster, radial manual tour of PC6. colored by experiment type: 'DIS HERA1+2' in green, 'dimuon SIDIS' in purple, and 'charm SIDIS' in orange. When the contribution PC 6 is large we see that dimuon SIDIS (purple) data are nearly orthogonal to DIS HERA (green) data. As the data is rotated, we can also see that DIS HERA (green) practically lie on a plane in this 6-d subspace. When the contribution of PC6 is near zero, dimonSIDIS (purple) occupies the same space as the DIS HERA data. A dynamic version can be viewed at* `https://nspyrison.netlify.com/thesis/discluster_manualtour_pc6/` .

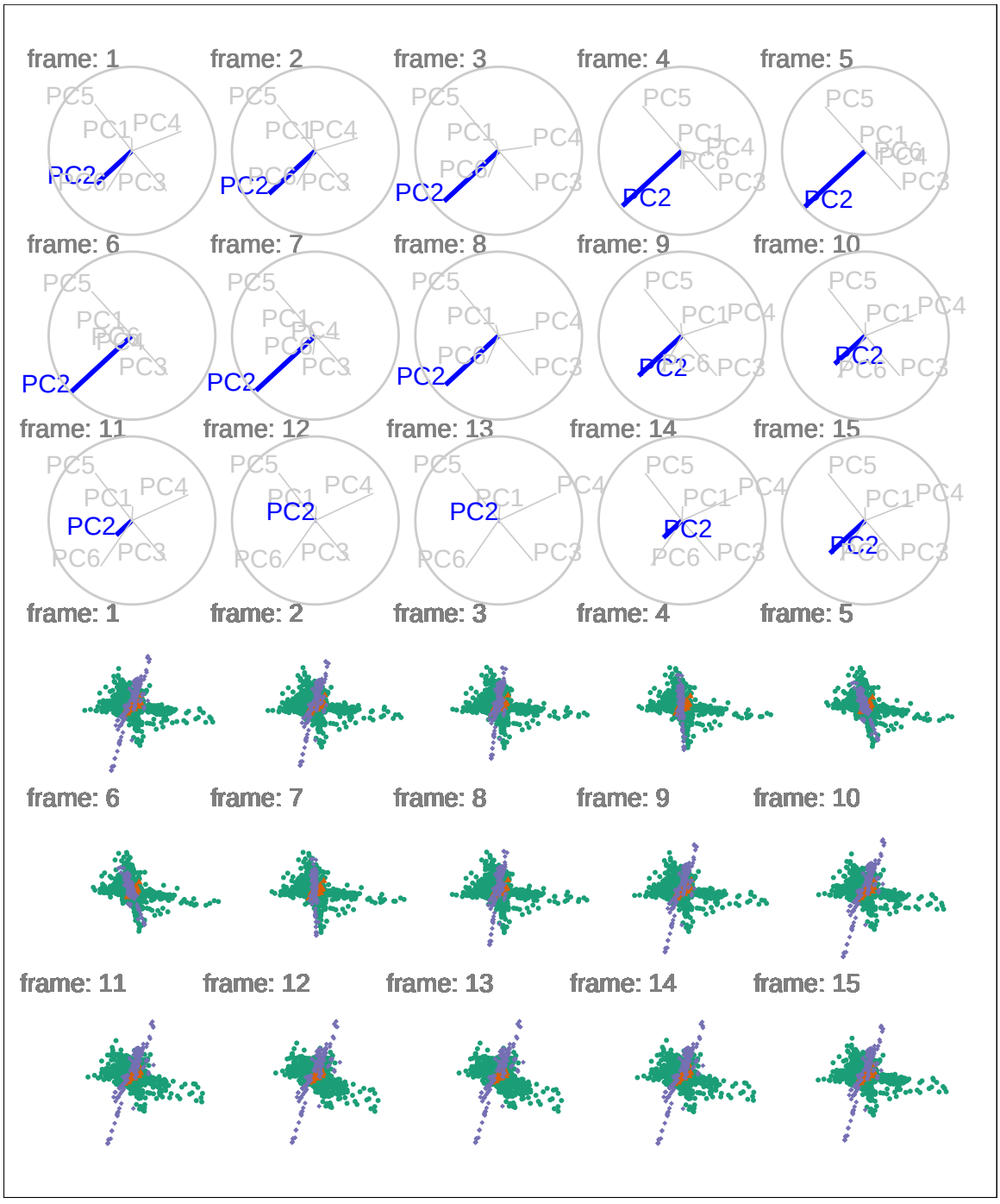


Figure 3.7: *DIS cluster, radial manual tour of PC2. Colored by experiment type: 'DIS HERA1+2' in green, 'dimuon SIDIS' in purple, and 'charm SIDIS' in orange. The structure of previously described plane of DIS HERA (green) and nearly orthogonal dimuon SIDIS (purple) is present, however the manipulating PC2 does not give a head-on view of either, a less useful manual tour than that of PC6. A dynamic version can be viewed at* https://nspyrison.netlify.com/thesis/discluster_manualtour_pc2/ .

3.6 Source code and usage

This article was created `bookdown` (Xie (2016)) using `rmarkdown` (Xie, Allaire, and Grolemund (2018)), with code generating the examples inline, and the source files can be found at github.com/nspyrison/confirmation/.

The source code for the `spinifex` package can be found at github.com/nspyrison/spinifex/. To install the package in R, run:

```
# install.package("devtools")
devtools::install_github("nspyrison/spinifex")
```

3.7 Discussion

This chapter has described an algorithm and package for exploring conducting a manual tour, from a 2D projection, to explore the sensitivity of structure to the contributions of a variable.

Future work on the algorithm and package would include developing it to work with arbitrary projection dimension, enabling the method to operate on other displays like parallel coordinates, and implementing the unconstrained manual control, called oblique in Cook and Buja (1997).

The Givens rotations and Householder reflections as outlined in Buja et al. (2005) may provide a way to conduct higher dimensional manual control. In a Givens rotations, the x and y components ($ie. \theta = 0,\ pi/2$) of the in-plane rotation are calculated separately and would be applied sequentially to produce the radial rotation. Householder reflections define reflection axes to project project points on to the axes and generate rotations.

The *tourr* package provides a number of d-dimensional graphic displays including andrews curves, chernoff faces, parallel coordinate plots, scatterplot matrix, and radial glyphs. Having manual controls available for these types of displays requires a general algorithm.

Development of a graphical user interface, e.g. *shiny* app, would make the *spinifex* package more flexible. The user could easily switch between variables to control, adjust the step

size to make smoother rotation sequences, or save any state to continue to continue to explore the contributions of other variables.

Chapter 4

UCS_benefits

High dimensional data and models are ubiquitous, but viewing them in data space is not trivial. Currently it is common practice to use Principal Component Analysis (PCA), Multi-Dimensional Scaling (MDS), or a non-linear embedding like tSNE. Unfortunately, static projections necessarily cut variation in the components not shown, while non-linear techniques lose inter-operability, back to the original data-space. Touring preserves variable inter-operability and keeps variation in tack. By providing user controlled steering of tour we should be able to provide finer structural exploration than the alternatives/

This work will be a comparison study between UCS and 3 or 4 of the leading alternatives.

Chapter 5

How can we extend the manual tour to 3d?

Wagner Filho et al. (2018) performed an $n = 30$ empirical study of PCA embedded projections, and perception error across 4 tasks and 3 display types: 2d, 3d, and immersive. Overall task error was less in 3d and immersive relative to 2d. According to user Likert-scale 2d is slightly easier to navigate and slightly more comfortable. On the flip-side 3d and immersive are slightly easier to interact and moderately easier to find information.

Info visualization in virtual spaces has been through waves of popularity since the 80's, results seems to produce conflicting results, and are regularly conflated by mismatch in user familiarity between 2d and 3d displays as discussed in Marriott et al. (2018) and others.

Immerse analytics, is becoming more and more popular. More research needing to be conducted to shed light onto previous mixed results. However, the results of Wagner Filho et al. (2018), Nelson, Cook, and Cruz-Neira (1998) and, Arms, Cook, and Cruz-Neira (1999) point positive light on 3d and immerse spaces improving perception of project high dim data. The Immerse Analytics group at Monash University have been programming packages in C#, for use with the Unity game engine for such uses (Cordeil et al. (2017), Cordeil (2019)). I will extend Cordeil's Immersive Analytics Toolkit (IATK) framework and implement dynamic communication with R scripts to apply 2d, 3d and

touring in virtual spaces, and leave room to implement other dimensionality reduction methods in Unity.

Chapter 6

Does 3d UCS provide benefits over UCS in 2d?

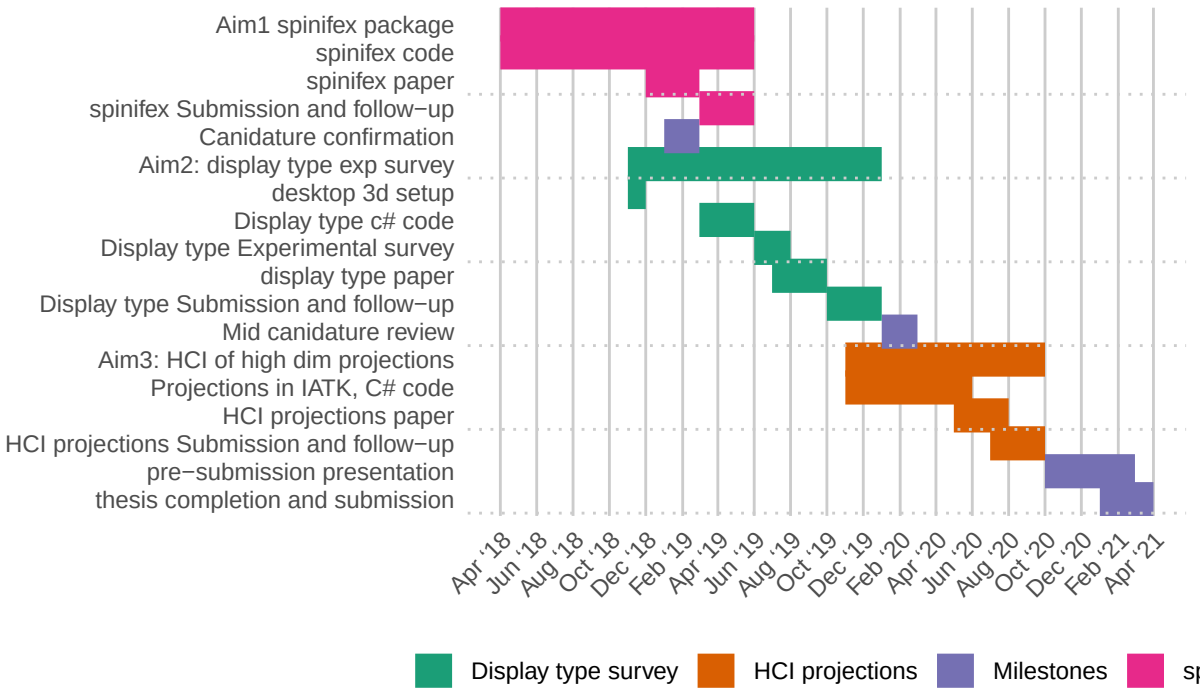
The bulk of previous work embeds in 2-space, for display on traditional monitors. Nelson, Cook, and Cruz-Neira (1998) performed a small ($n = 15$) experimental study comparing tasks performed across 2d and 3d touring displays. The XGobi interface was used on a standard 2d monitor while VR-Gobi (on the C2 setup) was used VR display without head tracking. The accuracy 3 tasks: clustering, intrinsic data dimensionality and radial sparseness was recorded along with the speed of a data brushing task. Accuracy was the same for the dimensionality task, while the d3 display out performed 2d on clustering, and even more so on the radial sparsity. However, time taken to brush a cluster was less than half the time in 2d display as compared with 3d.

I purpose an experimental study comparing touring across display dimension in 4 instances: standard 2d monitor, stereoscopic 3d monitor (on a zSpace 200), and head-mounted VR goggle (HTC Vive), and immersion in a CAVE environment. Implementation in the game engine Unity will allow for a standardized user interface. 3 tasks of structure perception will be conducted across 2 data sets of high energy physics data already in publication (Wang et al., 2018; Cook, Laa, and Valencia, 2018). Task order will be randomly assigned to minimize learning bias. Participants will perform the 3 tasks, on each of the display devices, for each of the data sets. Time, and accuracy will be tracked, and

participants will be asked to fill out a small survey with demographics data and subjective experience on a 5-point Likert scale. The design space of this study includes display type, task type, familiarity with 3d, familiarity with linear projections.

Chapter 7

PhD timeline



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