spinifex: An R Package for Creating a Manual Tour of Low-dimensional Projections of Multivariate Data

by Nicholas Spyrison, Dianne Cook

Abstract Dynamic low-dimensional linear projections of multivariate data collectively known as **tours** provide an important tool for exploring mulitvariate data and models. The R package **tourr** provides functions for several types of tours: grand, guided, little, local and frozen. Each of these can be viewed dynamically, or saved into a data object for animation. This paper describes a new package, **spinifex**, to provide a manual tour, that allows the coefficient for a single variable to be controlled. The variable is rotated fully into the projection with a coefficient of 1 or -1, or completely out of the projection with a coefficient of 0. The resulting sequence of projections can be displayed using animation, with functions from either the **plotly** and **gganimate** packages. By varying the coefficient of a single variable, it is possible to explore the sensitivity of structure in the projection to that variable. It is particularly useful when used with a projection pursuit guided tour to simplify and understand the solution. The use of the manual tour is illustrated using a problem from particle physics.

Introduction

Exploring multivariate spaces is a challenging task, increasingly so as dimensionality increases. Traditionally, static low-dimensional projections are used to display multivariate data in two dimensions, such as principal component analysis, linear discriminant spaces or projection pursuit. These are useful for finding relationships between multiple variables, but they are limited because they show only a glimpse of the high-dimensional space. An alternative approach, is to use a tour of dynamic linear projections, to look at many different low-dimensional proections. Tours can be considered to extend the dimensionality of visualization, which is important as data and models exist in more than 3D. The package **tourr** (Wickham et al. 2011) provides a platform for generating tours. It has many types of tours available, and many types of displays possible. A user can make a grand, guided, little, local or frozen tour, and display the resulting projected data as a scatterplot, density plot, histogram, or even as Chernoff faces if the projection dimension is more than 3.

This work adds a manual tour to the collection. The manual tour was described in Cook and Buja (1997) and allows a user to control the projection coefficients of a selected variable in a 2D projection. The manipulation of these coefficients allows the analyst to explore their sensitivity to the structure within the projection. As manual tours operate on only one variable at a time, they are particularly useful once a feature of interest has been identified.

One way to identify "interesting" features is with the use of a guided tour (Cook et al. 1995). Guided tours select a very specific path, that which approaches a projection that optimizes an objective-function. The optimization is conducted in a manner similar to simulated annealing (Kirkpatrick, Gelatt, and Vecchi 1983). The direct optimization of a function allows guided tours to rapidly identify interesting projection features given the relatively large parameter-space. After a projection of interest is identified an analyst can then use the "finer brush" of the manual tour, by controlling the contributions of individual variables to explore the sensitivity they have on the structure visible in the projection.

The paper is organized as follows. Section 2.2 describes the algorithm used to perform a radial manual tour as implemented in the package **spinifex**. Section 2.3 explains how to generate an animation of the manual tour using the animation frameworks offered by **plotly** (Sievert 2018) and **gganimate** (Pedersen and Robinson 2019). Package functionality and code usage following the order applied in the algorithm follows in section 2.4. Section 2.5 illustrates how this can be used for sensitivity analysis applied to multivariate data collected on high energy physics experiments (Wang et al. 2018). Section 2.5.3 summarizes this paper and discusses potential future directions.

Algorithm

This section describes the algorithm for performing a 2D radial manual tour, containing these steps:

1. Provided with a 2D projection, choose a variable to manipulate. This is called the "manip var".
2. Create a 3D manipulation space, where the manip variable has the full contribution.

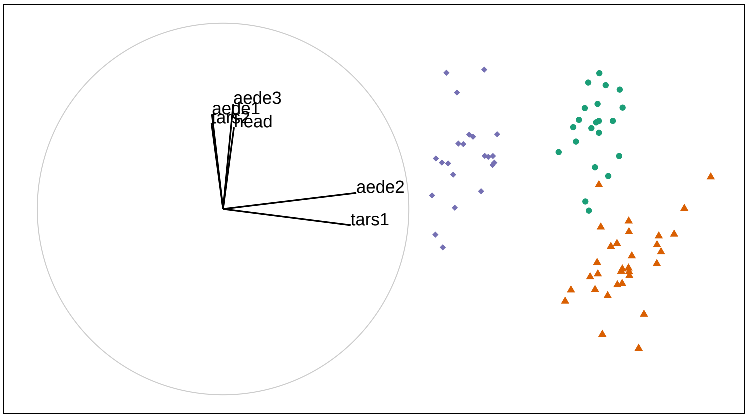

Figure 1: Initial 2D projection: representation of the basis (left) and resulting data projection (right) of standardized flea data. The color and shape of data points are mapped to beetle species. The basis was identified using a projection pursuit guided tour, with the holes index. The contribution of the variables aede2 and tars1 approximately contrasts the other variables. The visible structure in the projection are the three clusters corresponding to the three species.

3. Generate a rotation sequence which increases the norm of the coefficient to 1 and zeros it.

More detail is provided in the following sections. Function names are provided, but code structure and usage is discussed in section 2.4.

Notation

This section describes the notation used in the algorithm for a 2D radial manual tour.

- $\mathbf{X}$, the data, an $n \times p$ numeric matrix to be projected to 2D.
- $\mathbf{B} = (B_1,\ B_2)$, any 2D orthonormal projection basis, $p \times 2$ matrix, describing the projection from p to two dimensions
- $\mathbf{e}$, a 1D coordinate basis vector of length p with the $k-$th element set to one, where k is the index of the variable to manipulate, called the "manip var".
- θ_i, the sequence of angles of in-projection-plane rotation, for example, on the reference axes.
- ϕ_i, the sequence of angles of out-of-projection-plane rotation, coming into the manipulation space.

The algorithm primarily operates on projection bases and utilizes the data only when making a display. The projection space can be viewed at any point in the process by pre-multiplying the data and plotting the first two variables.

Set up

The flea data, originally from Lubischew (1962), made available in **tourr** is used to illustrate the algorithm. The data contains 74 observations across 6 variables, which are physical measurements of the flea beetles. Each observation belongs to one of three species.

An initial 2D projection basis set must be provided. One way to identify a projection containing interesting features is to apply a guided tour. In a guided tour, the projection sequence is selected by optimizing an index function via hill-climbing on the projection space. In this case, the holes index is selected and applied to standardized flea data. The holes index is maximized when the projected observations are furthest from the center. Figure 1 shows a locally optimized projection of the data. The left panel displays the reference axes of the projection basis, a visual indication of the magnitude and direction each variable contributes to the projection. The right panel shows the data as projected through the basis set described by the reference axes (left). Data points are colored and given shape according to the species.

Call `view_basis()` on a basis to produce a **ggplot2** (Wickham 2016) graphic similar to Figure 1. The projected data is always available for display via matrix multiplication $\mathbf{X}_{[n,\ p]}\ *\ \mathbf{B}_{[p,\ d]}\ =\ \mathbf{P}_{[n,\ d]}$.

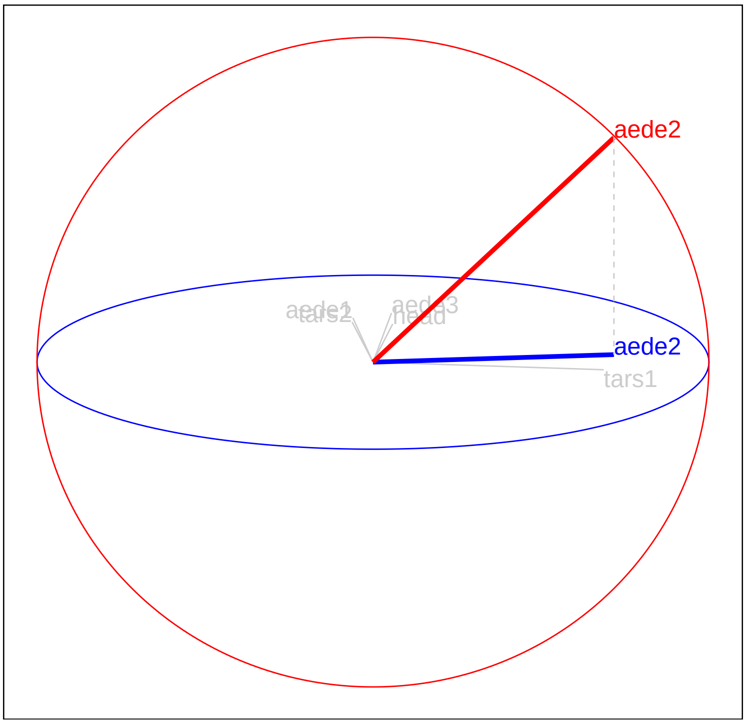

Figure 2: Manipulation space for controlling the contribution of aede2 of standardized flea data. The basis was selected by a holes-index optimized guided tour lies on the horizontal projection plane, shown in blue. The manip var axis, in red, extends into the vertical manipulation space, allowing the coefficients of the manip var to be changed by rotation around the origin.

Step 1) Choose variable of interest

In figure 1 the contributions of the variables tars1 and aede2 are mostly orthogonal to the contributions of the other four variables. These two variables explain the variation of the data distinguishing the purple cluster from the rest of the sample. Select aede2 as the manip var, the variable to be manipulated, as it has a larger contribution to the projection. The question that will be explored is how important the variable aede2 is to the separation of the clusters.

Step 2) Create the manip space

Initialize a zero vector $\mathbf{e}$ of length p. Set the fifth element to one, as aede2 is the fifth variable in the data, giving the manip var a full contribution in this dimension. Use the Gram-Schmidt process to orthonormalize the zero vector onto the basis yielding the 3D manipulation space, $\mathbf{M}$.

$$\begin{aligned}
\mathbf{e}_k &\leftarrow 1 \\
\mathbf{e} &\leftarrow \mathbf{e} - \langle \mathbf{e}, \mathbf{B}_1 \rangle \mathbf{B}_1 - \langle \mathbf{e}, \mathbf{B}_2 \rangle \mathbf{B}_2 \\
\mathbf{M}_{[p,\,3]} &= (\mathbf{B}_1, \mathbf{B}_2, \mathbf{e})
\end{aligned}$$

Adding this new dimension to our projection space allows for the coefficients of the manip var to be changed via rotation about the origin. For example, the ability to lift a piece of paper, rather than being constrained to a 2D plane. Orthonormalizing rescales the new vector, while the projection down to 2D remains as the original basis. Place the projection plane horizontally, with the new dimension extending vertically, with axes projecting back onto the reference axes. Figure 2 illustrates this 3D manipulation space with the manip var highlighted (height of the other variables are not depicted). This representation is produced by calling the `view_manip_space()` function. Functionally, the manipulation space is more of a mathematical construct that needn't be visualized but does help to digest what is happening mathematically.

Step 3) Generate rotation

Imagine holding the manip var, the red axis, one end fixed to the origin. As it is controlled the manipulation space rotates about the origin, the projection onto the horizontal projection plane correspondingly moves. This is what happens in a manual tour. Generating a sequence of values for the horizontal and vertical, angles produces a path for the rotation of the manipulation space. This defines the (orthonormally-constrained) rotation on the coefficients of the variables.

For a radial tour fix the (horizontal) angle within the projection plane, θ, and define a sequence for the (vertical) angle coming out of the projection plane, ϕ, bringing the initial XY contributions of the manip var to a maximum and then to zero before returning to the initial position. For an oblique manual tour, capture the user manipulation directly on the XY of the projection plane.

Post-multiply the manipulation space by the pre-defined rotation matrix producing **RM**, the rotated manip space. This is one frame of basis values, repeat this process for each value in the sequences of θ and ϕ for the complete animation.

Let:

c_θ be the cosine of θ_i

c_ϕ be the cosine of ϕ_i

s_θ be the sine of θ_i

s_ϕ be the sine of ϕ_i

For each value of i :

$$\begin{aligned}
\mathbf{RM}_{[p,\,3,\,i]} &= \mathbf{M}_{[p,\,3]} \ * \ \mathbf{R}_{[3,\,3,\,i]} \\
&= \mathbf{M}_{[p,\,3]} \ * \ \begin{bmatrix} c_\theta^2 c_\phi s_\theta^2 & -c_\theta s_\theta (1 - c_\phi) & -c_\theta s_\phi \\ -c_\theta s_\theta (1 - c_\phi) & s_\theta^2 c_\phi + c_\theta^2 & -s_\theta s_\phi \\ c_\theta s_\phi & s_\theta s_\phi & c_\phi \end{bmatrix}_{[3,\,3,\,i]}
\end{aligned}$$

A note on application: ϕ is the angle relative to the initial value of ϕ, we find the transformation ϕ_i - ϕ_1 useful to think about ϕ relative to the basis plane. Additionally, the value of ϕ may be out of phase by a factor of pi. If the manip variable doesn't move as expected these are the first places to check.

Figure 3 illustrates a sequence with 15 projected bases, showing the reference axes on the top half with the corresponding projected data points below. Changes in the basis coefficients of the manip var correspond to the distance separating the purple cluster and the remaining sample, aede2 is crucial in distinguishing the variation of species. Tours are typically viewed as an animation. The animation of this tour can be viewed online at `https://nspyrison.netlify.com/thesis/flea_manualtour_mvar5/`. The page may take a moment to load. Animations can be produced using the function `play_manual_tour()`.

Data in projection-space

In an appeal to performance, the operations of a tour are performed on the bases while the larger datasets are not operated on until the display of data points are needed. After the bases are brought into the projection-space, however, it is helpful to observe them with projected data in the same space. Pre-multiply the data by basis frame bringing the data into the projection space.

$$\mathbf{P}_{[n,\,3]} = \mathbf{X}_{[n,\,p]} \ * \ \mathbf{RM}_{[p,\,3]}$$

For a 2D scatterplot, plot the first two variables within each frame. Show each frame in sequence to form an animation. The remaining manipulation space variable can be linked to point aesthetic (such as size or color) to produce depth cues used in conjunction with the XY scatterplot.

Package structure and functionality

This section discusses the functions and code usage of the package before delving into a domain-specific application of the manual tour.

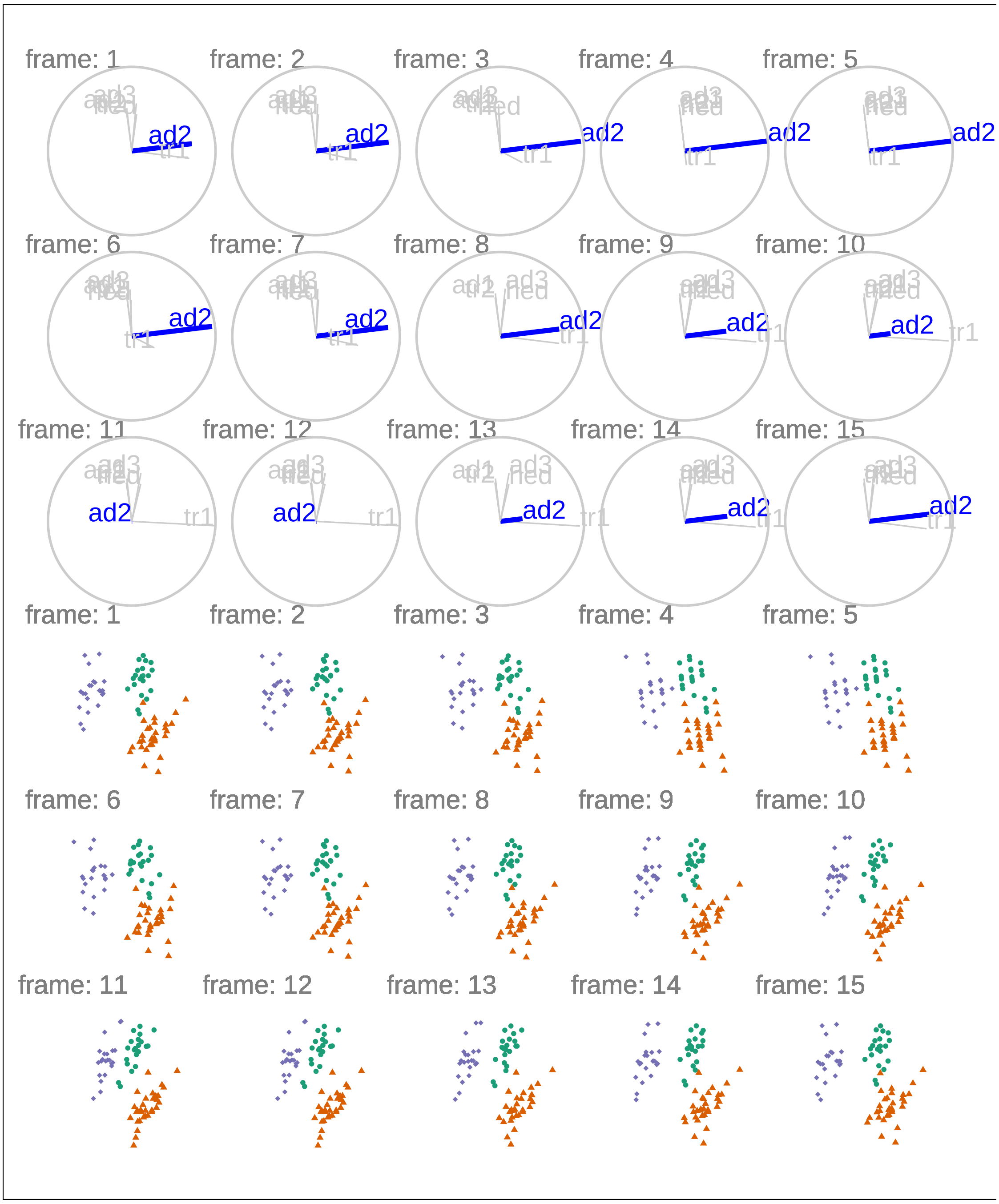

Figure 3: Radial manual tour manipulating aede2 of standardized flea data. The contributions increase from its initial contribution to a full contribution to the projection before decreasing to zero and then returning to its initial value. Manipulating the coefficeients of aede2 changes the distance separating the purple cluster. This shows that aede2 is important for distinguishing this species from the ramaining data. An animated version can be viewed at https://nspyrison.netlify.com/thesis/flea_manualtour_mvar5/.

Table 1: Primary functions

Class	Function	Description
tour preparation	view_basis	displays the reference frame of the basis
tour preparation	view_manip_space	displays the manipulation space
tour animation	play_tour_path	animates given tour path
tour animation	play_manual_tour	animates the manual tour algorithm
utility	render_gganimate	uses gganimate to render the animation
utility	render_plotly	uses plotly to render the animation

Installation

```
# remotes::install_github("nspyrison/spinifex") # Development version
install.package("spinifex")
library("spinifex")

# Also see the vignette:
vignette("spinifex_vignette")
```

Primary package functions

The primary functions that will aid users in performing their own manual tours are broken into the following groupings: tour preparation, tour animation, and utility.

In the following section describes and demonstrates usage of the above functions following the order in the algorithm. The utility functions are called by the tour animation functions, passed to the arguments `render_type`. Usage is demonstrated below and in the example documentation.

Algorithm code

We'll start by initializing values including a standardized data set (numeric columns only), a starting basis, a categorical variable for point aesthetics (optional), and a manip var. To get bearings on the projection, start by observing the reference axes of the basis with `view_basis()` producing figure 1.

```
f_data  <- tourr::rescale(flea[, 1:6])                 ## standardize data
f_path  <- save_history(f_data, guided_tour(holes()))    ## produce guided tour
f_basis <- matrix(f_path[,, max(dim(f_path)[3])], ncol=2) ## end of guided tour
f_cat   <- factor(flea$species)                          ## categorical var

view_basis(basis = f_basis,
           data = f_data,
           labels = colnames(f_data))
```

After becoming familiar with this space, select a manip var, the variable to change the contributions of. Use `view_manip_space()` to view the new space with a dimension orthogonal to the projection plane where the manip var has a full contribution. This illustrates how the manip var is manipulated with the addition of the manipulation space as shown in figure 2.

```
f_mvar  <- 5  ## manip var number

view_manip_space(basis = f_basis,
                 manip_var = f_mvar,
                 labels = colnames(f_data))
```

Now we are ready to perform a manual tour on the selected variable. Use `play_manual_tour()` to perform the algorithm as discussed above, in section 2.2. This is the animated equivalent of figure 3.

```
angle_speed <- .26

play_manual_tour(data = f_data,
                 basis = f_basis,
                 manip_var = f_mvar,
```

```
              angle = angle_speed,
              col = f_cat,
              pch = f_cat)
```

This concludes the content of the algorithm section, however, lets cover animating paths generated in **tourr**. Animate the previously generated guided tour path via `play_tour_path()`. Utility functions can also be passed as arguments into either of the tour animation function to change the resulting graphics object, set `render_type = render_gganimate` to view the animation as a GIF.

```
play_tour_path(tour_path = f_path,
               data = f_data,
               render_type = render_gganimate,
               angle = angle_speed
)
```

Rendering and sharing

The **tourr** package utilizes **base** graphics for the display of tours. **spinifex** allows tours to be rendered in **plotly** as an HTML5 object or **gganimate** as GIF or MP4 files. Both of which build off **ggplot2** objects in internal functions. Sharing of animations is not trivial especially in print and static file formats such as PDF. Even with the use of computers and dynamic file formats capturing the correct resolution, aspect, and display is challenging and many formats quickly bloat file sizes. Keep in mind hosting options and exporting functions from **plotly**, **gganimate** and **tourr**.

Storage

Storing each data point for every frame of the animation is redundant. Just as operations are performed on the bases, so too should tour paths be stored as bases and a single instance of the data. Consider a radial manual tour, we can store the salient features in 3 bases, where ϕ is at its starting, minimum, and maximum values. The frames in between can be interpolated by supplying angular speed. With the use of the `tourr::save_history()` function, the target bases can be saved. From there geodesic interpolation can be used to populate the intermittent frames. This type of interpolation should not be used on manual tours, which have already been initialized into a 3D manipulation space where direct linear interpolation is appropriate.

Application

In a recent paper, Wang et al. (2018), the authors aggregate and visualize the sensitivity of hadronic experiments to nucleon structure. 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 visualized as 3D subspaces of the 10 first principal components in linear (PCA) and non-linear (t-SNE) embeddings.

Using the same data, another study, Cook, Laa, and Valencia (2018), applied grand tours (Asimov 1985) to the same subspaces. Grand tours are dynamic linear projections of high dimensional spaces where basis sets are selected at random and animated with geodesic interpolation of the intermediate frames. Because of the change in the basis, or orientation to the subspace, tours are able to better resolve the distribution shape of clusters, intra-cluster detail, and better outlier detection than the use of PDFSense & TFEP (TensorFlow embedded projections) or traditional static embeddings. Before applying manual tours let's discuss the structure of the data.

The data has a hierarchical structure with top-level clusters; DIS, VBP, and jet. Each cluster is a particular class of experiments, each with many experimental datasets which, in turn, have many observations. In consideration of data density, we conduct manual tours on subsets of the DIS and jet clusters. This explores the sensitivity of the structure to each of the variables in turn and we present the subjectively best and worst variable to manipulate for identifying dimensionality of the clusters and describing the span of the clusters.

Jet cluster

The jet cluster resides in a smaller dimensionality than the full set of experiments with four principal components explaining 95% of the variation in the cluster (Cook, Laa, and Valencia 2018). The data within this 4D embedding is subset down to ATLAS7old and ATLAS7new to focus in on two groups with a reasonable number of observations that occupy different parts of the subspace. Radial manual tours controlling contributions from PC4 and PC3 are shown in figure 4 and figure 5 respectively. These variables are selected to contrast the difference of information conveyed by touring different variables. Links to dynamic HTML5 animations controlling each of the four variables are also provided.

When manipulating PC4, there is a clear difference in the parameter space spanned by the experiment types ATLAS7new and ATLAS7old. Specifically, the variation of ATLAS7new becomes more singular. The experiments are probing different parameter space and PC4 is important to demonstrate this. Yet, when PC3 is manipulated there is no clear indication that the different experiments probe different parameter space. Performing a radial manual tour on PC4 is more insightful than for PC3. Radial manual tours manipulating each of the principal components in the jet cluster can be viewed by following the links: PC1, PC2, PC3, and PC4.

DIS cluster

A different space is used to explore the DIS cluster; specifically the first six principal components, which explains 48% of the variation contained within the aggregated data (Cook, Laa, and Valencia 2018). Radial manual tours are performed on PC6 and PC2 in figure 6 and figure 7 respectively.

The selection of the manip variable is important, as the manipulation spaces convey substantially different information. The manual tour of PC6 offers information about the dimensionality, shape, and orientations of the different experiment classes. PC6 is particularly important to describe the variations of DIS HERA1+2 and charm SIDIS observations, Whereas manipulating the contributions of PC2 only shows a subset of the dimensionality and shape information. Manipulating the contributions of PC6 turned out to be much more insightful than that of PC2. This result might seem counter-intuitive at first as PC2 should explain much more of the variation in the data. However, features and structures in the data regularly reside in smaller dimensionality. The details finer resolution of these features can be lost when looking only at static projections. DIS cluster manual tours manipulating each of the principal components can be viewed from the links: PC1, PC2, PC3, PC4, PC5, and PC6.

Discussion

Tours, which are a dynamic linear projection of multivariate data, play an important role in data visualization; they extend the dimensionality of visuals while data- and parameter-spaces become ever larger. This research has modified the algorithm producing manual tours which and has made this functionality available in package **spinifex**. The package adds to **tourr**, extending the graphics offerings that can be used to display tours.

Radial manual tours were applied to a dataset across different experiments of hadronic collisions. The importance of selecting the correct variable to manipulate is demonstrated by comparing tours of varying quality. The manual tours convey a better picture of the structure of the clustering than static linear or non-linear projections. Giving the full contribution of the manipulation space to the manip var enables analysts to explore the sensitivity of the structure with the selected variable. This information can be used by physicists to identify which experiments are probing which parameter spaces, which can be indispensable for smarter planning of effort and funding.

Future research on the algorithm would include extending it for use in 3D projections. The addition of another dimension theoretically allows for improved perception. This could explore interactions in immersive virtual reality or mixed reality, which may further allow for a better perception of structure and aid in higher-dimensional function visualization. Functions with many parameters suffer from the same dimensionality problem as data while their possible values lie on a plane of values rather than discrete points. Occulation, or the closer surface blocking further surfaces, will likely be an issue that may be alleviated by the use of wire mesh, changing opacity, or looking at sections of the projections (Furnas and Buja 1994).

The **tourr** package provides many other geometric displays with the `tourr::display_*()` family. These geometric options could be integrated into the **ggplot2** framework for display on **plotly** and **gganimate**. Additionally, the **animation** package Xie et al. (2018) could be implemented for another graphics framework. However, **animation** builds from **base** graphics while **spinifex** utilizes **ggplot2** graphics, a significant paradigm shift.

The Givens rotations and Householder reflections as outlined in Buja et al. (2005) could also be added. Currently, Gram-Schmidt is the only form of frame interpolation used (not used in manual tours). In a Givens rotation, the x and y components (for example $\theta\ = 0,\ pi/2$) 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 points on to the axes and generate rotations.

Having a script only interaction with tours causes a significant barrier to entry. To a lesser extent, **plotly** offers some static interactions with the contained object, such as tooltips, brushing, and linking

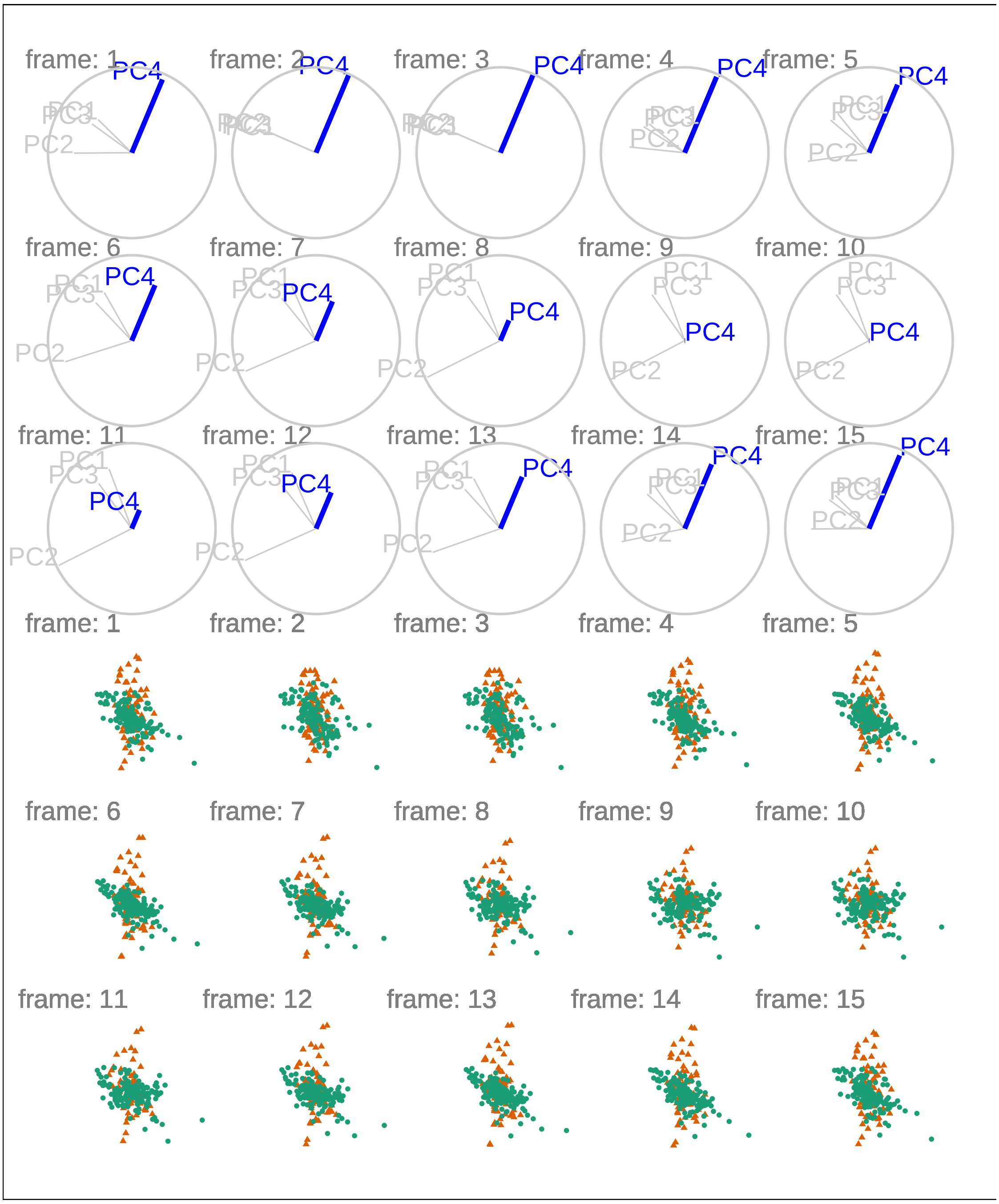

Figure 4: A radial manual tour of PC4 within the jet cluster. Colored by experiment type: ATLAS7new in green and ATLAS7old in orange. When PC4 fully/negligibly contributes to the projection ATLAS7new (green) spans the same space as the orange points. During the intermediate frames, the ATLAS7new is compressed in the direction radial to PC4. The difference in distribution shape demonstrates the experiments probe different phase-space, which has a linear mapping back to the original dimensions. An HTML5 version can be viewed at https://nspyrison.netlify.com/thesis/jetcluster_manualtour_pc4/.

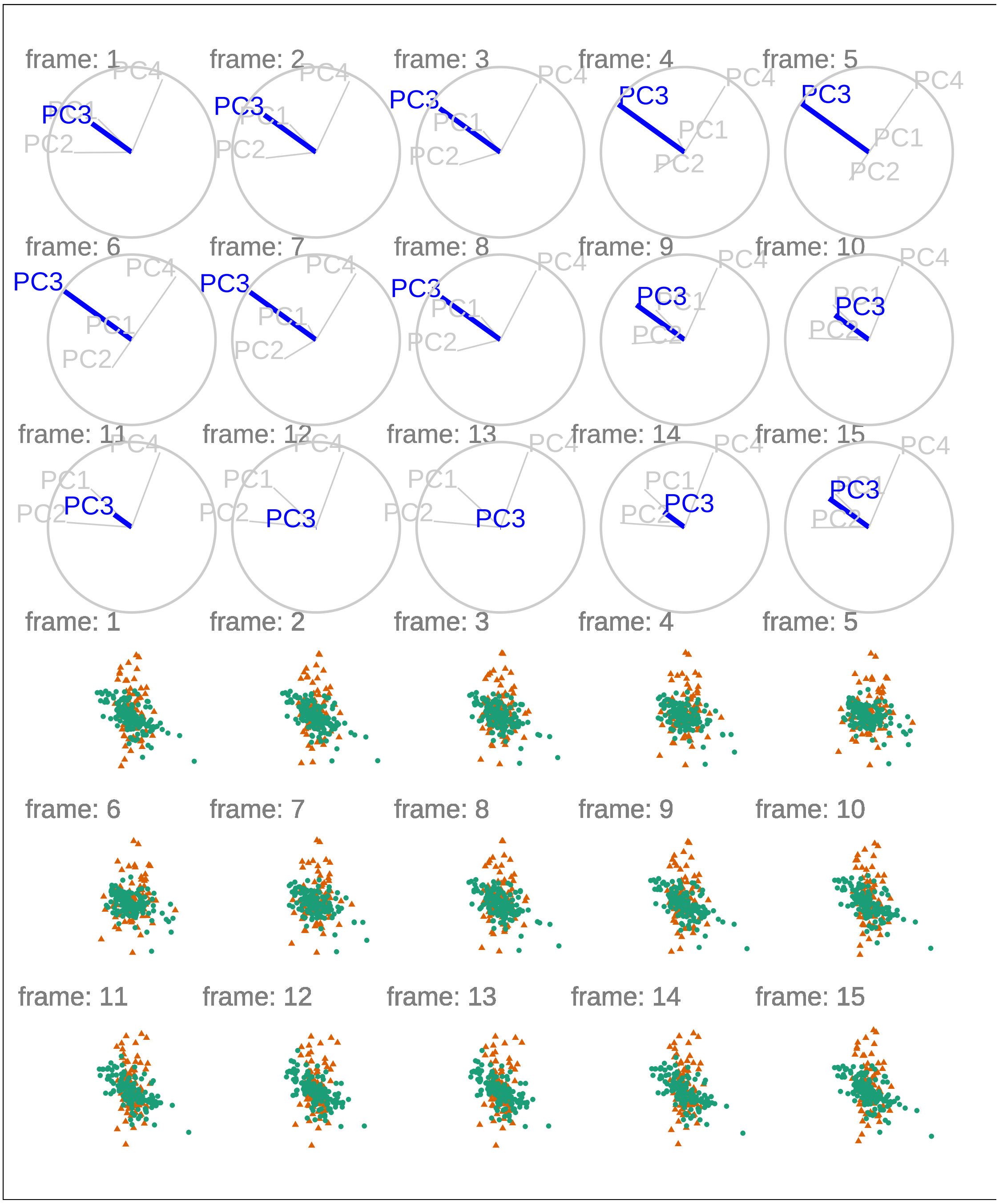

Figure 5: A radial manual tour of PC4 within the jet cluster. Colored by experiment type: ATLAS7new in green and ATLAS7old in orange. Data from ATLAS7new (green) spans mostly the same space as ALTLAS7old (orange) with no evident difference in cluster structure across varying contributions of PC3. An HTML5 version can be viewed at https://nspyrison.netlify.com/thesis/jetcluster_manualtour_pc3/.

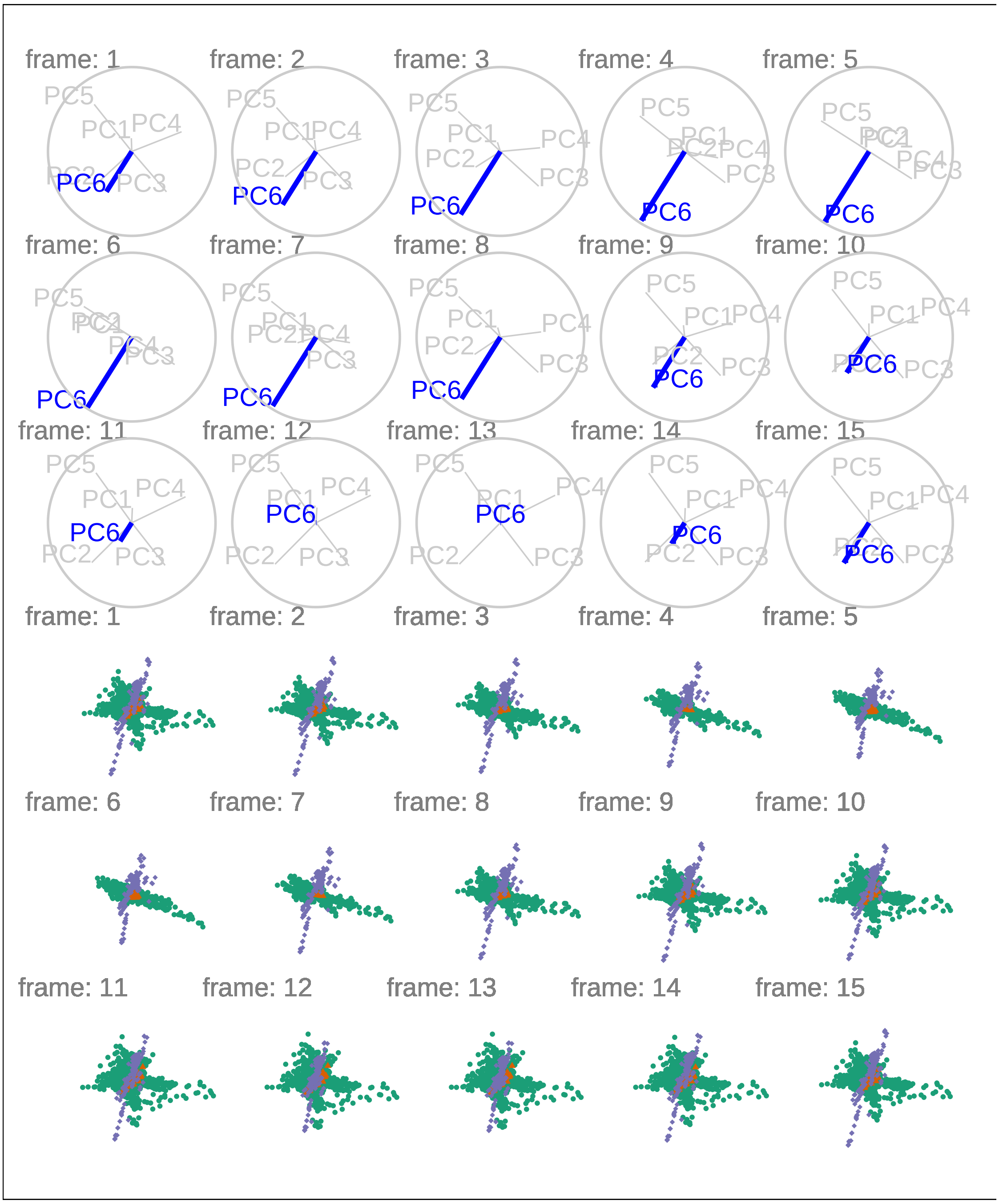

Figure 6: A radial manual tour manipulating the contribution of PC6 within the DIS cluster. Points are colored by experiment type: DIS HERA1+2 in green, dimuon SIDIS in purple, and charm SIDIS in orange. The cluster DIS HERA1+2 (green) is distributed in a cross-shaped plane, charm SIDIS (orange) occupies the center space of this cross. As the contribution of PC6 becomes whole the distributions of DIS HERA1+2 (green) and charm SIDIS (orange) become singular but offset by a small angle. Less evident is the linear dimuon SIDIS (purple) observations approaching the line of view for intermediate values of PC6. An HTML5 version can be viewed at https://nspyrison.netlify.com/thesis/discluster_manualtour_pc6/.

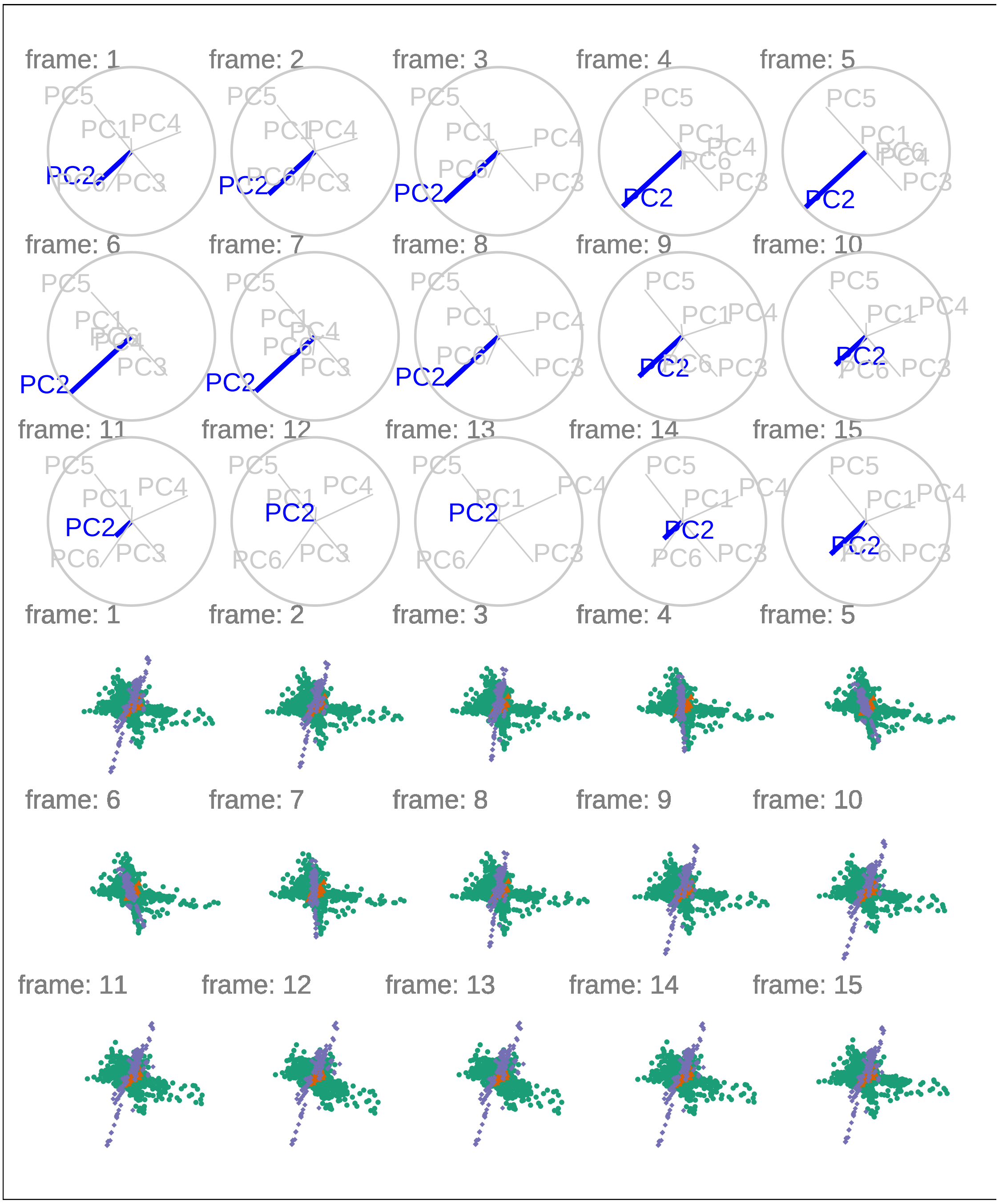

Figure 7: A radial manual tour manipulating the contribution of PC2 within the DIS cluster. Points are colored by experiment type: DIS HERA1+2 in green, dimuon SIDIS in purple, and charm SIDIS in orange. The plane of cross distributed DIS HERA data (green) and a nearly orthogonal jet of dimuon SIDIS (purple) is present. This jet does extend more in the plane of view when the contribution of PC2 is full, giving insight to its orientation. However, less information about the shape of DIS HERA (green) and charm SIDIS (orange) is available. An HTML5 version can be viewed at https://nspyrison.netlify.com/thesis/discluster_manualtour_pc2/.

without communicating back to the R console. The development of a dynamic graphical user interface, perhaps with the use of a **shiny** (Chang et al. 2018) application, would mitigate the barrier to entry, allow for more rapid analysis, and offer an approachable demo tool. The user could easily switch between variables to control, adjust interpolation step angle, or flag/save specific frame basis sets.

Acknowledgments

This article was created in R (R Core Team 2018), using **knitr** (Xie 2014) and **rmarkdown** (Xie, Allaire, and Grolemund 2018), with code generating the examples inline. The source files for this article be found at github.com/nspyrison/spinifex_paper/. The source code for the **spinifex** package can be found at github.com/nspyrison/spinifex/.

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