

spinifex: manual control of dynamic linear projections of high-dimensional data

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Abstract

The set of dynamic linear projections of multivariate data collectively known as **tours** provide a unique dynamic visualization as the dimensionality of the data increase. Tours are particularly useful for understanding the structure held within multivariate data, and in association with techniques for dimension reduction, supervised, and unsupervised classification. The R package **tourr** offers a variety of path generators and geometric displays for conducting tours. This paper discusses an extension package, **spinifex**, that adds support for the path generation of manual tours and extends the display of tours to use with the contemporary animation packages, **plotly** and **gganimate**. Manual tours are used to explore the sensitivity of structure as the contributions of a manipulation variable are changed. This is particularly useful after identifying a feature of interest. A recent paper {Wang et al. (2018)} visualizes the sensitivity of the hadronic experiments to nucleon structure. Sensitivity was characterized in non-linear 3D embeddings of the first 10 principal components. This research applies manual tours to this data showing that manual tours resolve more structural information that is orthogonal to the original viewing plane.

0.1 Introduction

A tour is a multivariate data analysis technique in which a sequence of linear (orthogonal) projections are viewed as an animation while the orientation of the projection basis is rotated across time. Each frame of the sequence corresponds to a small change in the projection for a smooth transition that perseveres continuity. This is a crucial tool extending the dimensionality of visualization which is a large boon as datasets and models exist in increasing cardinality.

While there are numerous methods that generate tour paths, this research focuses on the manual tour. The manual tour was described in Cook and Buja (1997) and allows a user to control the projection coefficients of a select variable has in a 2D projection. The manipulation of these coefficients allows the analyst to explore how sensitive the projections structure is to these changes. This makes manual tours particularly useful once a feature of interest has been identified, for example, with the use of a guided tour (Cook et al. 1995). The path of a guided tour is selected via projection pursuit, the optimization of an index function on the projection via a hill climbing algorithm. This allows guided tours to identify interesting projection features rapidly given the relatively large parameter-space. Once the given projection has been provided, it is time to define the path of rotation.

Ideally, the path would be intuitively user-generated from physical movement, be it through mouse or motion capture. Unfortunately, this type of dynamic control has proven difficult to capture for in R. Because of this, manual tours were not implemented in **tourr** (Wickham et al. 2011). This research allows for the consumption, but not the generation, of such dynamic input. After the capture of an oblique user motion, the rotation needs to be applied to step 3 (rotation sequence) of the algorithm discussed below. In the section below we stick with a radial rotation where, θ , the angle of in-projection-plane rotation is held constant.

Spinifex utilizes two new animation packages, **plotly** (Sievert 2018) and **gganimate** (Pedersen and Robinson 2019), to display tours, manual or other saved tours. 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's contribution.

The paper is organized as follows. Section 0.2 explains the algorithm using a toy dataset. Section 0.3 discussed the display of the animation after the path has been generated. Section 0.4 illustrates how this can be used

for sensitivity analysis applied to contemporary high energy physics. The last section, 0.7 summarizes the work and discusses future research.

0.2 Algorithm

The section below describes the algorithm for performing a 2D radial manual tour:

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

The steps are described in more detail below. The R functions used below mentioned briefly, but more complete code example can be found in section 0.6

0.2.1 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 embedded in two dimensions.
- $\mathbf{B} = (B_1, B_2)$, any orthonormal projection basis set, $p \times 2$ matrix, describing the projection from p to two dimensions
- \mathbf{e} , a zero column vector of length p with the k -th element set to one, where k is the number of the variable to manipulate.
- θ , the angle of in-projection-plane rotation, for example, on the reference axes.
- ϕ , the angle 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.

0.2.2 Toy data set

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, physical measurements of the flea beetles. Each observation belonging to one of three species.

The data is defined. A basis set (ideally orienting to an interesting feature) must be provided as an initial orientation. One way to identify a projection containing interesting features is to apply a guided tour (Cook, Swayne, and Buja 2007). 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 @ref{fig:step0} shows a locally optimized projection of the data. The left side displays the reference axes of the projection basis, a visual indication of the magnitude and direction each variable contributed to the projection. The right side 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 (while the guided tour was unsupervised with this information).

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

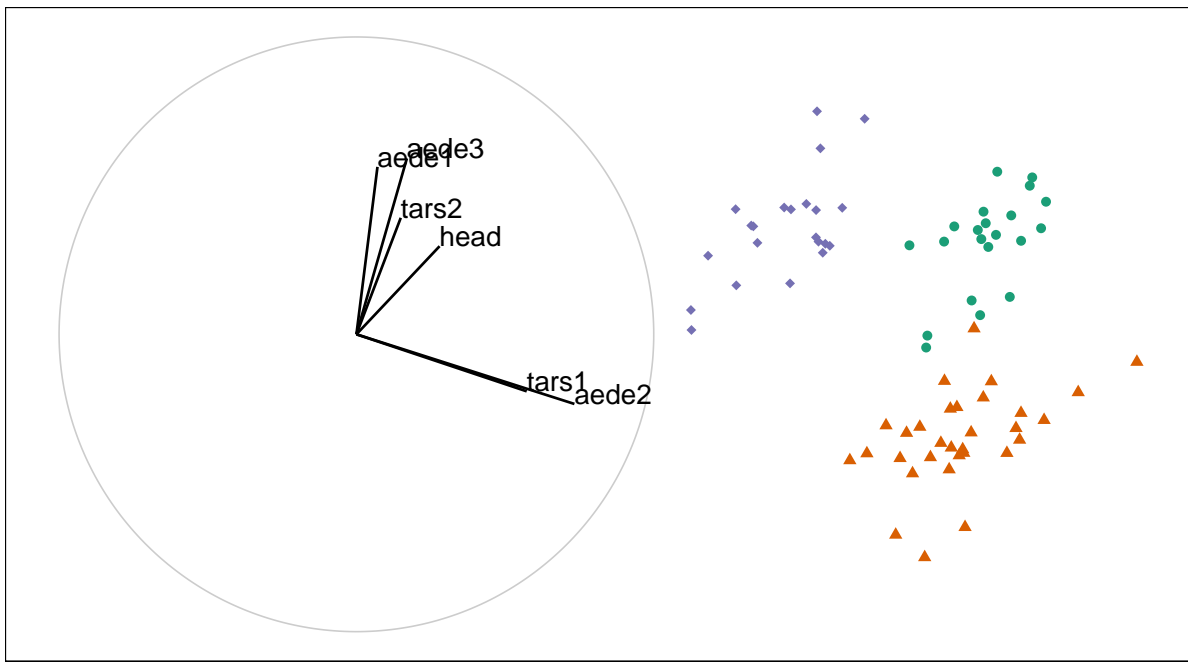


Figure 1: Basis reference axes (left) and projected data (right) of standardized flea data. Data points color and shape are mapped to beetle species. Basis identified by a holes-index guided tour. The variables **aede2** and **tars1** contribute mostly orthogonal to the other variables.

0.2.3 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 group 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.

0.2.4 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} .

$$\begin{aligned}\mathbf{e} &\leftarrow \text{Orthonormalize}_{GS}(\mathbf{e}) \quad w.r.t.the basis \\ &= \mathbf{e} - \langle \mathbf{e}, \mathbf{B}_1 \rangle \mathbf{B}_1 - \langle \mathbf{e}, \mathbf{B}_2 \rangle \mathbf{B}_2\end{aligned}$$

$$\mathbf{M}_{[p, 3]} = (\mathbf{B}_1, \mathbf{B}_2, \mathbf{e})$$

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 the original basis. Place the 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.)

The representation in figure 2 can be produced by calling the function `view_manip_space()`.

0.2.5 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. Dynamic capture of user manipulation is typically performed directly on the projection plane (without depiction of the manipulation space.)

For i in 1 to n_slides :

Post-multiply the manipulation space by the pre-defined rotation matrix producing \mathbf{RM} , the rotated manip space.

Let:

c_θ be the cosine of θ

c_ϕ be the cosine of ϕ

s_θ be the sine of θ

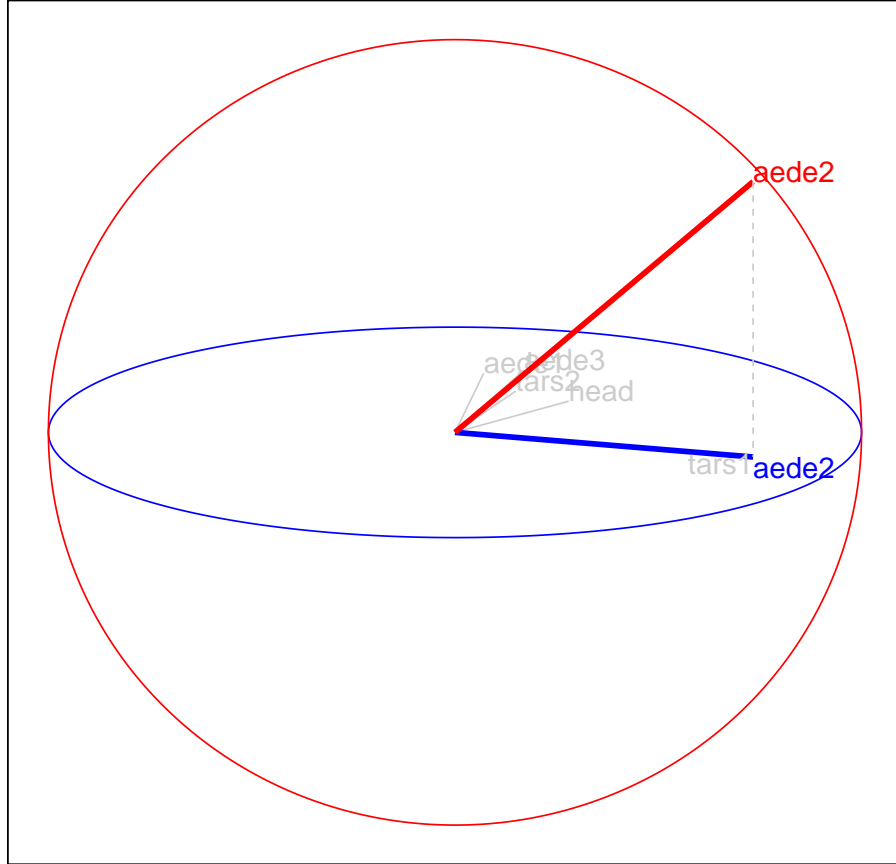


Figure 2: Manipulation space for controlling the contribution of **aede2** of standardized flea data. Basis selected by a holes-index optimized guided tour lies on the horizontal projection plane, shown in blue. The manip var axis, in red, extends into the vertical manipulation space, allowing the coefficients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

s_ϕ be the sine of ϕ

then

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

A note on application: ϕ is the angle relative to the initial value of ϕ , we find the transformation $\phi_i - \phi_1$ 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 top the corresponding projected data points on the below. As a result, we can see that changes in the manip var controlled the distance between the purple cluster and the remaining sample, **aede2** is crucial in distinguishing this species. Tours are typically viewed as an animation such a dynamic version 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()`. This function defaults to an HTML5 widget produced from **plotly**. The `render_type` argument can be changed to `render_gganimate` for exporting to .gif or .mp4 files.

0.3 Data in projection-space

In light of performance, the above operations are performed on the bases without the use of the larger datasets. After the bases are brought into the projection-space, however, it is helpful to observe them with data in the same space. Pre-multiply the data by basis frame bringing the data into the projection space.

$$\mathbf{P}_{[n, 3]} = \mathbf{X}_{[n, p]} * \mathbf{RM}_{[p, 3]} \quad (1)$$

$$= \begin{bmatrix} X_{1, 1} & \cdots & X_{1, p} \\ X_{2, 1} & \cdots & X_{2, p} \\ \vdots & \vdots & \vdots \\ X_{n, 1} & \cdots & X_{n, p} \end{bmatrix}_{[n, p]} * \begin{bmatrix} RM_{1, 1} & RM_{1, 2} & RM_{1, 3} \\ RM_{2, 1} & RM_{2, 2} & RM_{2, 3} \\ \vdots & \vdots & \vdots \\ RM_{p, 1} & RM_{p, 2} & RM_{p, 3} \end{bmatrix}_{[p, 3]} \quad (2)$$

For a 2D scatterplot, plot the first two variables from each frame statically as in the previous figure, or in sequence, producing an animated scatterplot. The remaining variable is sometimes linked to a data point aesthetic (such as size or color) to produce depth cues used in conjunction with the XY scatterplot.

0.3.1 Rendering and sharing

The **tourr** package utilizes R's base graphics for the display of tours. **spinifex** allows tours to be used in rendered in **plotly** Sievert (2018) as an HTML5 object or **gganimate** Pedersen and Robinson (2019) as .gif or .mp4 objects. Both of which build off **ggplot2** objects in internal functions. Sharing of animations is not trivial especially in print and static 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**.

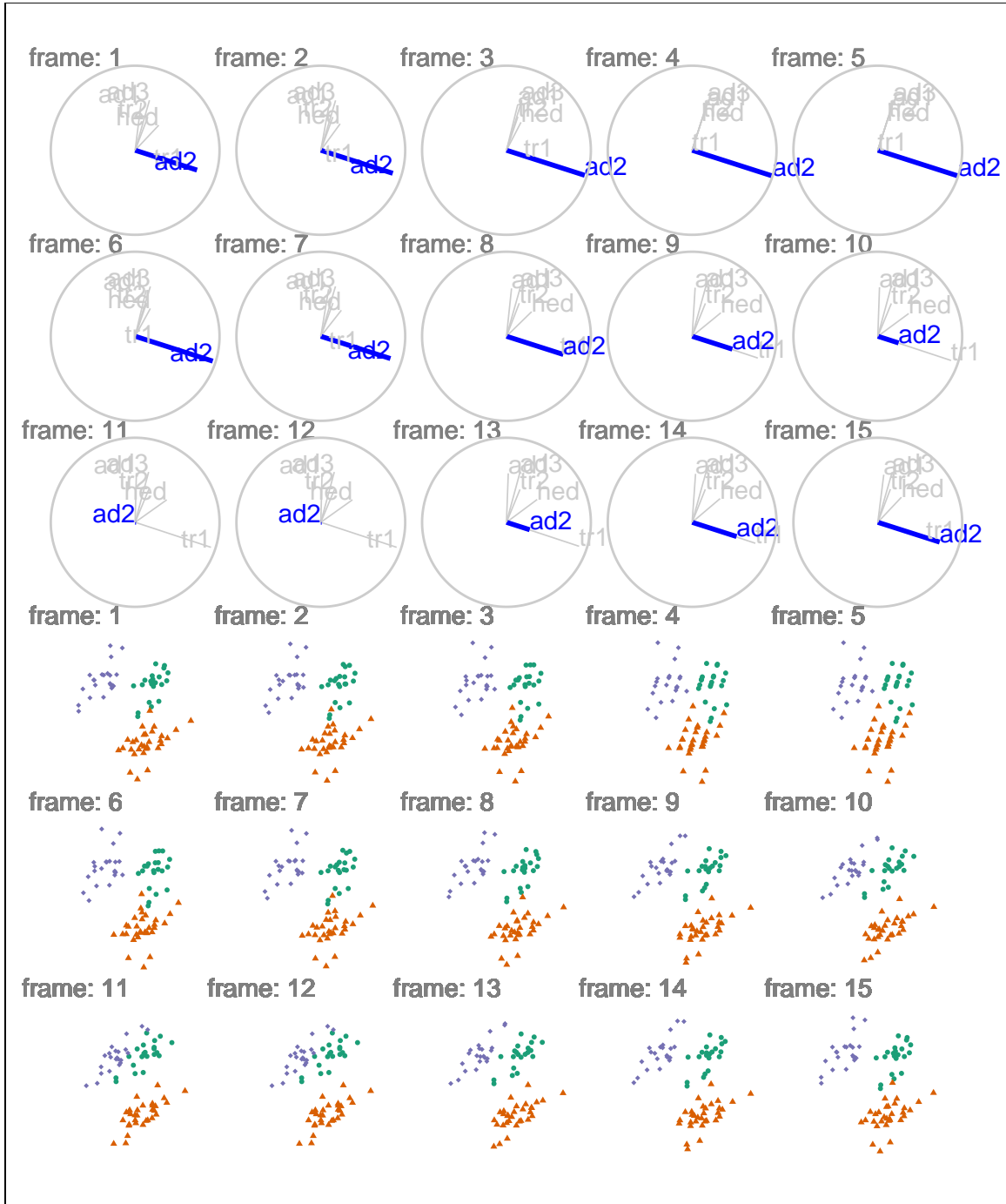


Figure 3: Radial manual tour manipulating **aede2** of standardized flea data. The contributions increase from its initial contribution to a full contribution to the projection before decreasing to zero and then returning to its initial value. The change in the projected data shows that **aede2** is important for distinguishing between the purple species. An animated version can be viewed at https://nspyrison.netlify.com/thesis/flea_manualtour_mvar5/.

0.3.2 Storage

Storing each data point for every frame of the animation is very inefficient. Just as operations are performed on the bases, so too should tour paths be stored as bases. 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.

0.4 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), applies grand tours to the same subspaces. Grand tours are able to better resolve the distribution shape of clusters, intra-cluster detail, better outlier detection, and challenges a claim presented from TFEP (TensorFlow embedded projections). Table 1 of Cook *et al.* summarizes the key findings of observations made with PDFSense & TFEP and those from grand tours.

Without getting too domain-specific the data has three primary groupings; **DIS**, **VBP**, and **jet**. Each group is a particular class of experiments and each with many experimental datasets which, in turn, have many observations. In the 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 structure and outliers.

0.4.1 Jet cluster

The **jet** cluster is of 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 the variation in the jet 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. Below, we perform radial manual tours all four principal components within this scope. Visualizing PC3 and PC4 in figure 4 (more structurally insightful) and figure 5 (less structurally insightful) respectively, and list links to dynamic animation of all variables.

0.5 TODO: edit application, Grammarly and word checks.

Manipulating PC3, where varying the angle of rotation brings interesting features into and out of the center mass of the data, is more interesting than the manipulation of PC4, where the features are mostly independent of the contribution of PC4.

Jet cluster manual tours manipulating each of the principal components can be viewed from the links: PC1, PC2, PC3, and PC4.

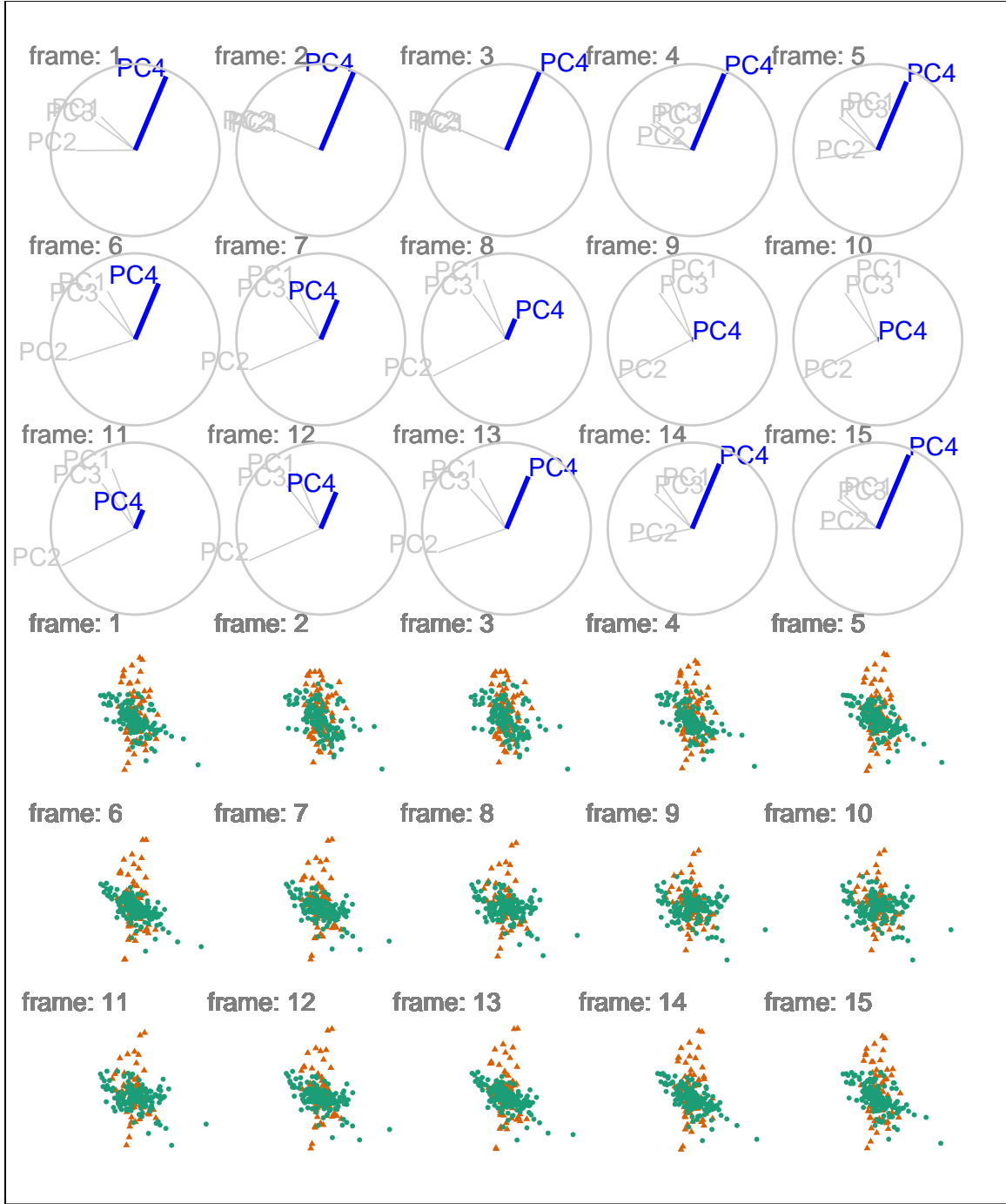


Figure 4: **Jet** cluster, a radial manual tour of PC3. Colored by experiment type: **ATLAS7new** in green and **ATLAS7old** in orange. When PC3 fully contributes to the projection **ATLAS7new** (green) occupies unique space and several outliers are identifiable. Zeroing the contribution from PC3 to the projection hides the outliers and all observations with **ATLAS7new** are contained within the area spanned by **ATLAS7old** (orange). A dynamic version can be viewed at https://nspyison.netlify.com/thesis/jetcluster_manualtour_pc3/.

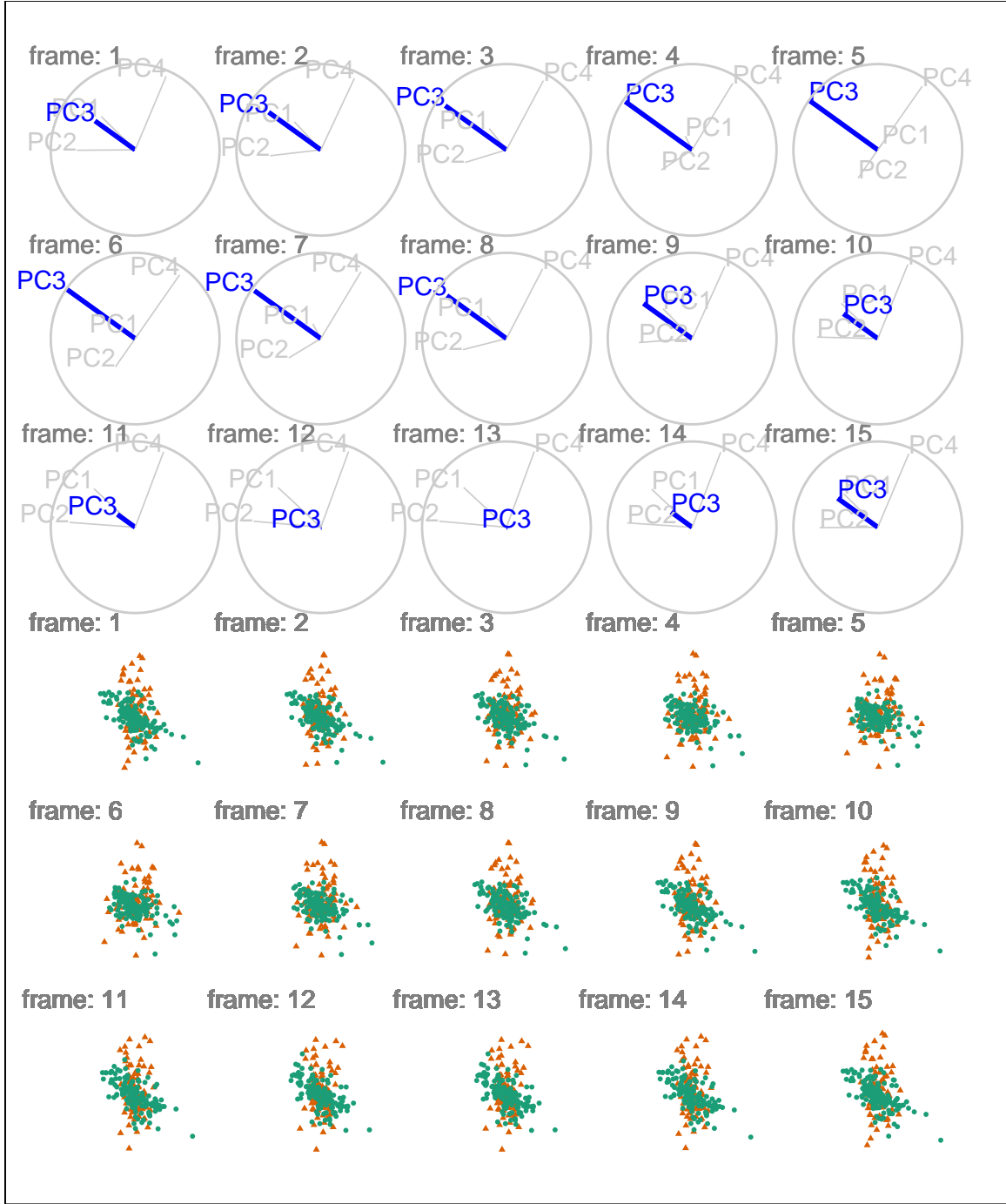


Figure 5: Jet cluster, a radial manual tour of PC4. Colored by experiment type: ATLAS7new in green and ATLAS7old in orange. This manual tour contains less interesting information ATLAS7new (green) has points that are right and left of ATLAS7old, while most points occupy the same projection space, regardless of the contribution of PC4. A dynamic version can be viewed at https://nspyrison.netlify.com/thesis/jetcluster_manualtour_pc3/.

0.5.1 DIS cluster

We perform a manual tour on this data, manipulating PC6 as depicted in figure 6. Looking at several frames we see that DIS HERA data lies 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 has 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 may some time to load, as the animation is several megabytes.

The selection of the correct manip variable is important as the manipulation spaces convey different information. For example, in figure 7 we select PC2 as the manip variable finding it to be less insightful than PC6.

DIS cluster manual tours manipulating each of the principal components can be viewed from the links: PC1, PC2, PC3, PC4, PC5, and PC6.

0.6 Source code and usage

Use the below code as a guide for installation and finding the vignette. The vignette offers a less technical discussion opting to focus on code usage and goes through a couple more use cases. If you prefer to follow along with the example in the algorithm then simplified code is also listed below.

```
# devtools::install_github("nspyrison/spinifex") # Development version
install.packages("spinifex")

# Also see vignette:
vignette("spinifex") # vignette 'spinifex' not found

## manual tour of std flea from holes-index:
library(spinifex)
f_dat <- tourr::rescale(flea[,1:6])
f_cat <- factor(flea$species)
f_path <- save_history(f_dat, guided_tour(holes()))
f_bas <- matrix(f_path[, , max(dim(f_path)[3])], ncol=2)
f_mvar <- 5
f_lab <- colnames(f_dat)

# View the basis
view_basis(f_bas, data = f_dat, labels = f_lab)
# View the manip space
view_manip_space(basis = f_bas, manip_var = f_mvar, labels = f_lab)
# Play animation as HTML5 from plotly
play_manual_tour(data = f_dat, basis = f_bas, manip_var = f_mvar,
                 col = f_cat, angle = f_angle)
```

0.6.1 Acknowledgments

This article was created in R (R Core Team 2018), using **bookdown** (Xie 2016) and **rmarkdown** (Xie, Allaire, and Golemund 2018), with code generating the examples inline. The source files for this article be found at github.com/nspyrison/confirmation/. The source code for the **spinifex** package can be found at github.com/nspyrison/spinifex/.

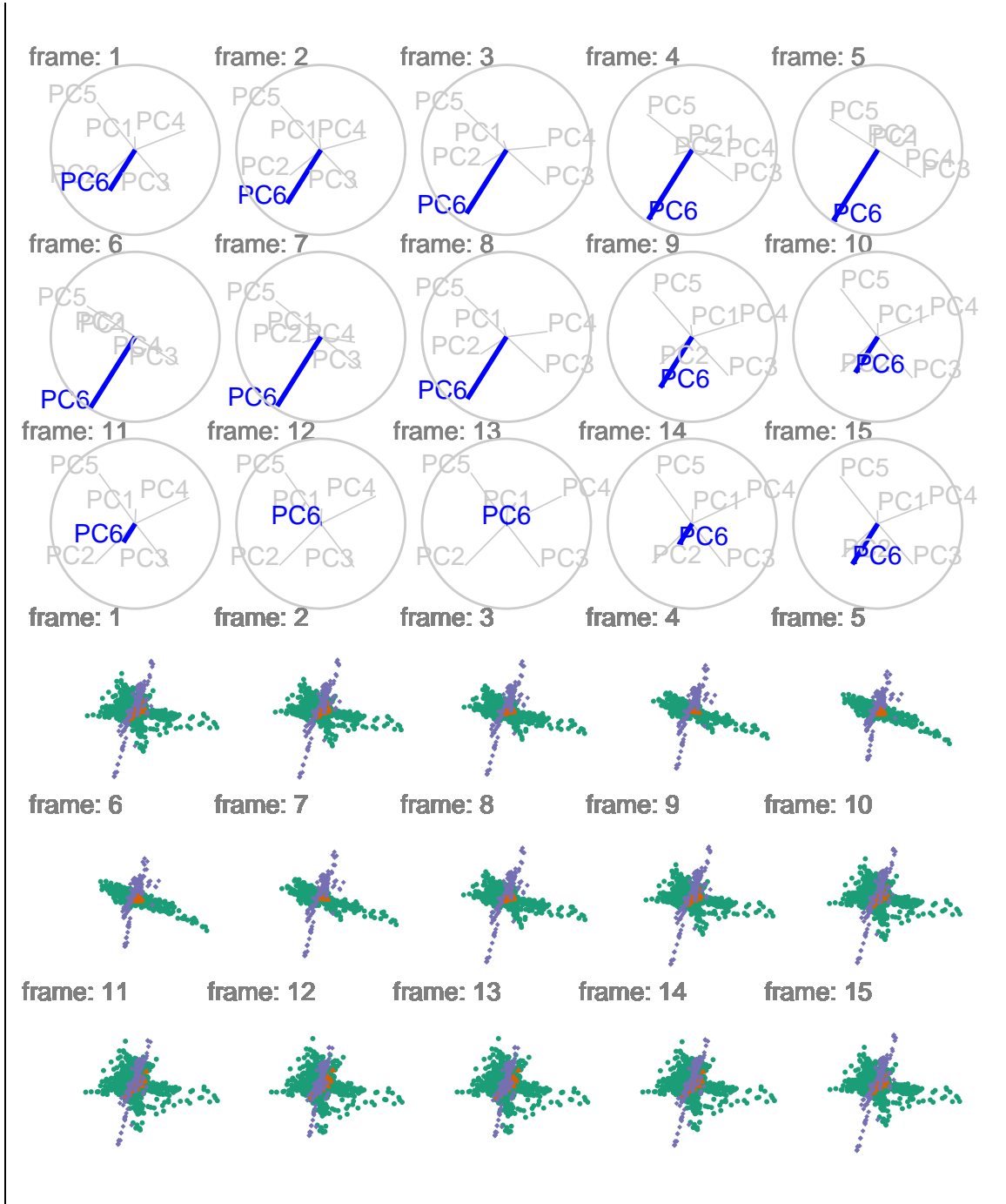


Figure 6: DIS cluster, a radial manual tour of PC6. colored by experiment type: DIS HERA1+2 in green, dimuon SIDIS in purple, and charm SIDIS in orange. When the contribution PC 6 is large we see that dimuon SIDIS (purple) data are nearly orthogonal to DIS HERA (green) data. As the projection is rotated, we can also see that DIS HERA (green) practically lies on a plane in this 6D subspace. When the contribution of PC6 is near zero, dimuonSIDIS (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/.

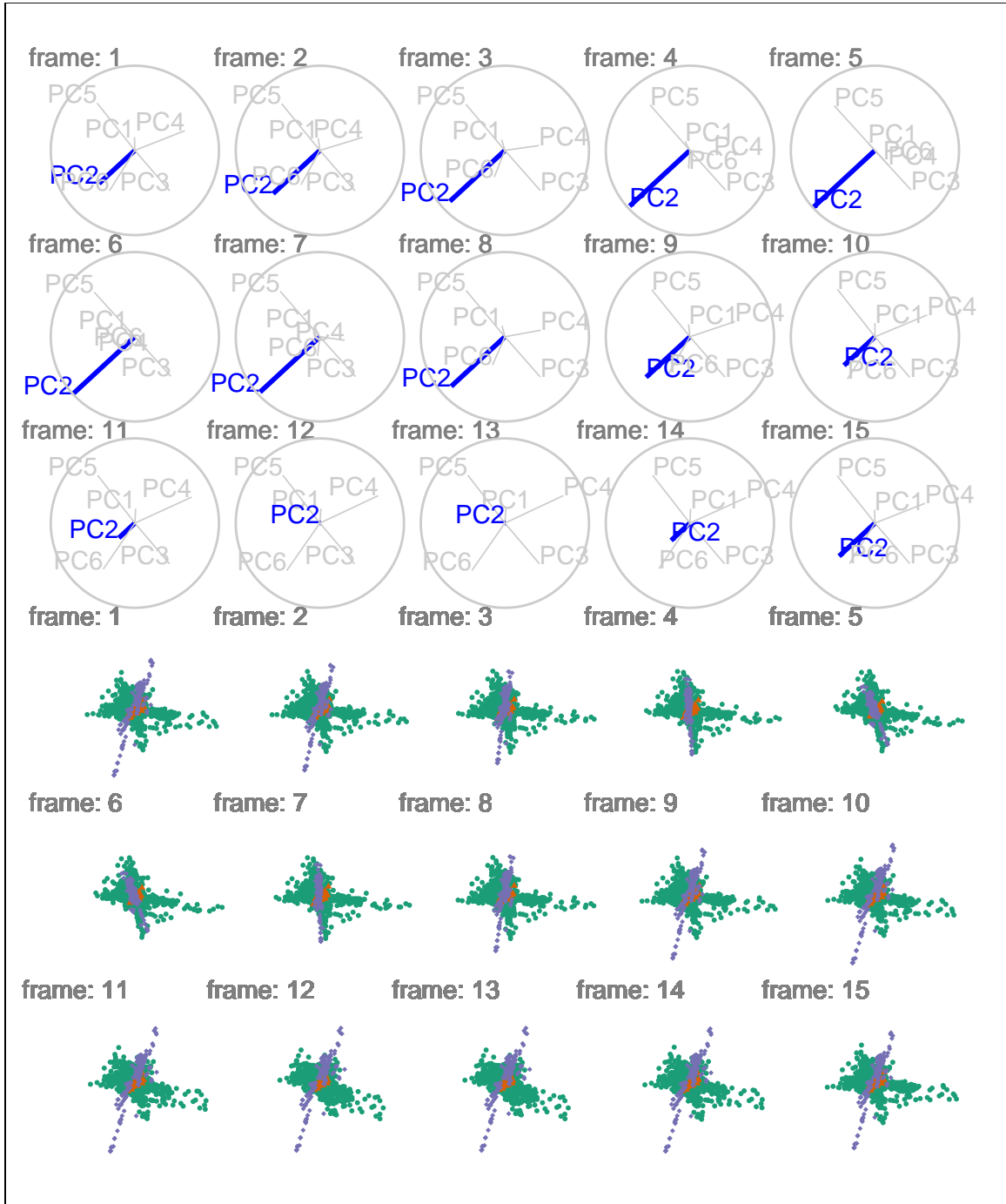


Figure 7: DIS cluster, a radial manual tour of PC2. Colored by experiment type: DIS HERA1+2 in green, dimuon SIDIS in purple, and charm SIDIS in orange. The structure of previously described plane of DIS HERA (green) and nearly orthogonal dimuon SIDIS (purple) is present, however, the manipulating PC2 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/.

0.7 Discussion

Tours, the dynamic linear projection of multivariate data, is an important aspect of data visualization extending the display of data-space as data dimensionality increases. This research has modified the algorithm producing manual tours, applied this functionality in R and offers extends the graphics offerings that can be used to display tours. The paragraphs below explore how this work might be extended.

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 graphs while **spinifex** utilizes **ggplot2** graphics.

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 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.

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