

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

A thesis submitted for the degree of

Doctor of Philosophy

by

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Acknowledgements

I would like to thank ...

Declaration

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

Nicholas S Spyrison

Preface

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

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

Abstract

This thesis is about ...

Chapter 1

Introduction

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

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

Chapter 2

Literature review

2.1 Touring

2.1.1 Overview

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

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

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

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

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

Terminology

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

2.1.2 History

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

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

TALK ABOUT maths Here::

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

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

2.1.3 Tour path

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

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

- *cmass* (Cook, Buja, and Cabrera, 1993) - find the projection with the most density or mass in the center.
 - *lda* (Lee et al., 2005) - linear discriminant analysis, seeks a projection where 2 or more classes are most separated.
 - *pda* - principal component analysis finding where the data is most spread (1d only).
 - other user-defined objective function (Wickham et al., 2011).
- *planned tour*, Precomputed choice, In which the path has already been generated or defined.
 - *little tour* (McDonald, 1982), where every permutation of variables is stepped through in order, analogous to a brute-force or exhaustive search.
 - a saved path of any other tour
 - *manual tour* - Manual control, a constrained rotation on selected manipulation variable and magnitude (Cook and Buja, 1997). Typically used to explore the local area after identifying an interesting feature from another tour.
 - *dependance tour*, combination of n independent 1d tours. A vector describes the axis each variable will be displayed on. ie $c(1, 1, 2, 2)$ is a 4 to 2d tour with the first 2 variables on on the first axis, and the remaining on the second.
 - *correlation tour* (Buja, Hurley, and McDonald, 1987), a special case of the dependence tour, analogous to canonical correlation analysis

2.1.4 Geometrics and display dimension

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

- 1d geoms

- 1-d densities: such as histogram, average shifted histograms([scott85](#)), and kernel density([scott95](#)).
- image: ([Wegman](#))
- time series: where multivariate values are independently lagged to view peak and trough alignment. Currently no package implementation, but use case is discussed in (Cook and Buja, [1997](#)).
- 2d geoms
 - 2-d density ([NS](#))
 - scatterplot
 -
- 2.5d, 3d geoms {ADD FOOTNOTE ABOUT 2.5d vs 3d}
 - Anaglyphs, sometimes called stereo, where (typically) red images are positioned for the left channel and cyan for the right, when viewed with corresponding filter glasses give the depth perception of the image.
 - Depth, which use some subset of depth cues, most commonly size and/or color of data points.
- d -dim geoms
 - Andrews curves ([Andrews, 1972](#)), smoothed variant of parallel coordinate plots, discussed below.
 - Chernoff faces ([Chernoff, 1973](#)), variables linked to size of facial features for rapid cursory like-ness comparison of observations.
 - Parallel coordinate plots ([Ocagne, 1885](#)), where any number of variables are plotted in parallel with observations linked to their corresponding variable value by polylines.
 - Scatterplot matrix ([Becker and Cleveland, 1987](#)), showing a triangle matrix of bivariate scatterplots with 1-d density on the diagonal.
 - Radial glyphs, radial variants of parallel coordinates including radar, spider, and star glyphs ([Siegel et al., 1972](#)).

2.1.5 Application

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

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

2.2 Virtual reality

Chapter 3

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

3.1 Abstract

Touring techniques offer a great opportunity for data-space visualizations of $(\mathbf{X} \in \mathbb{R}^p, p > 3)$ multivariate data sets. This paper discusses the R package *spinifex*, which adds support for the manual tour, which is particularly usefully for exploring the local structure after identifying a feature of interest, perhaps via guided tour. Additionally, *spinifex* extends graphic outputs to *plotly* and *gganimation*. This work extends the functionality of and is compatible with *tourr*.

Keywords: grand tour, projection pursuit, manual tour, *tourr*, touring, high dimensional visualization, high dim vis, dimensionality reduction, visualization, statistical graphics, data-space.

3.2 Introduction

The manual tour was described in Cook and Buja (1997), and allows a user to rotate a variable into and out of a 2D projection of high-dimensional space. The primary purpose is to determine the sensitivity of structure visible in a projection to 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 (Hurley and Buja, 1990). In guided tours an index of interest defined on the space of all projections, and the function is optimised. It derives from projection pursuit (Friedman and Tukey, 1974), and the guided tour provides a visual interface to the optimisation. The manual tour can be used to help refine structure in the optimal projection, sharpening it by exploring the contributions of different variables, and simplifying by zeroing the coefficients of variables that don't contribute to the structure.

3.3 Manual tour algorithm

The algorithm contains several steps:

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

3.3.1 Notation

Given:

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

$\mathbf{B}_{[p, d]}$ An orthonormal¹ basis describing the current orientation projecting p down to d dimension.

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

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

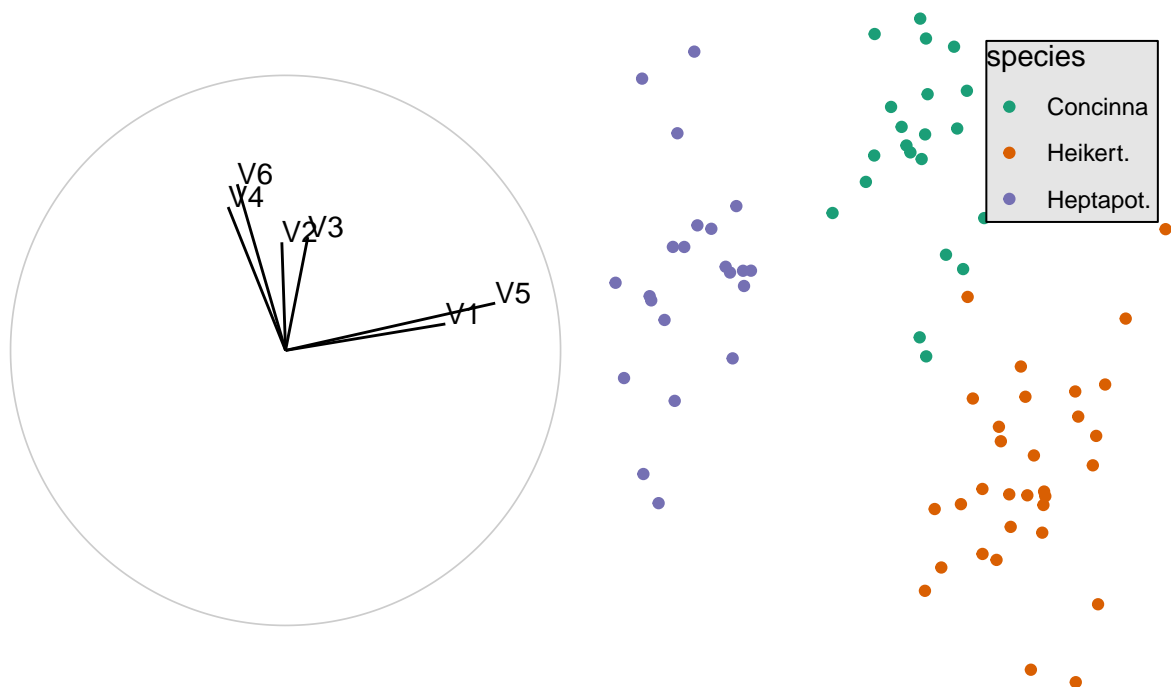
$$\mathbf{B}_{[p, d]} = \begin{bmatrix} B_{1, 1} & \dots & B_{1, d} \\ B_{2, 1} & \dots & B_{2, d} \\ \vdots & \ddots & \vdots \\ B_{p, 1} & \dots & B_{p, d} \end{bmatrix}$$

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

3.3.2 Flea data set

We'll illustrate with the flea data set from the R package *tourr* (Wickham et al., 2011), which contains different tours on the same data. The data comes from Lubischew (1962). The flea data contains 74 observations across 6 variables, physical measurements of each flea beetle. Each individual belonged to one of three species being observed.

We'll perform a guided tour on the flea data optimizing for the index holes (Cook, Swayne, and Buja, 2007). Where the basis is projected and the local area is explored for a projection that move the data further from the center. In figure ??, below, the left frame depicted the final basis of the holes tour; a unit circle with lines showing the x and y contributions of each variable in the projection space. The right frame projects the data through that basis and colors the points according to the observed species.



Call the `view_basis()` function to produce the left frame. In touring typically we want dynamic display that looks through many such views, however, 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 reproduce the right frame.

```
view_basis <- function(basis,
                        labels = paste0("V", 1:nrow(basis))
) {
  # Initialize
  p <- nrow(basis)
  if (!is.data.frame(basis)) basis <- as.data.frame(basis)
  ## circle
  angle <- seq(0, 2 * pi, length = 360)
  circ <- data.frame(x = cos(angle), y = sin(angle))

  # graphics (reference frame)
  ## circle and set options
  gg1 <- ggplot2::ggplot() + ggplot2::geom_path(
    data = circ, color = "grey80", size = .3, inherit.aes = F,
```



```
mapping = ggplot2::aes(x = circ$x, y = circ$y)
) +
ggplot2::scale_color_brewer(palette = "Dark2") +
ggplot2::theme_void() +
ggplot2::theme(legend.position = "none") +
ggplot2::coord_fixed() # Do not use with plotly!
## Axes line segments
gg2 <- gg1 +
  ggplot2::geom_segment(
    data = basis,
    mapping = ggplot2::aes(x = basis[,1], y = basis[,2], xend = 0, yend = 0)
  )
## Text labels
gg3 <- gg2 + ggplot2::geom_text(
  data = basis, size = 4, hjust = 0, vjust = 0, colour = "black",
  mapping = ggplot2::aes(x = basis[, 1], y = basis[, 1], label = labels)
)

gg3
}
```

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.

NOTE: Explanation has math, diagram and code

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

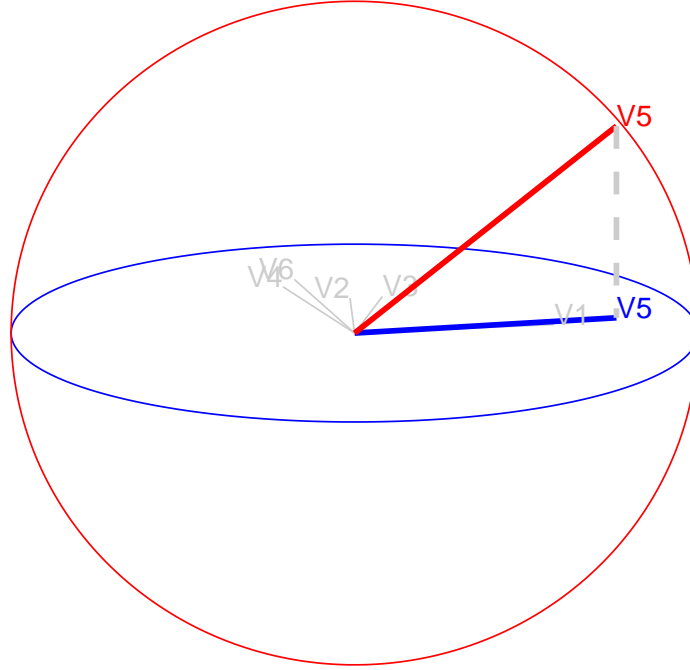
In figure ??, above, notice the the variables 1 and 5 are almost orthogonal to the other 4 variables and that V5 has a larger contribution than V1. As such, let's select the 5-th variable as our manipulation variable.

3.3.4 Step 2 Create the manip space

NOTE: Explanation has math, diagram and code

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

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



3.3.5 Step 3 Generate rotation

NOTE: Explanation has math, diagram and code

Select a vector ϕ_i , the angle of out-of plane rotation, orthogonal to the projection plane (relative to ϕ_1 , the transformation $\phi_i - \phi_1$ proved to be helpful to discuss ϕ relative to the Z axis).

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.

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

$$= \begin{bmatrix} M_{1,1} & M_{1,2} & M_{1,3} \\ M_{2,1} & M_{2,2} & M_{2,3} \\ \vdots & \vdots & \vdots \\ M_{p,1} & M_{p,2} & M_{p,3} \end{bmatrix}_{[p, d+1]}$$

For the $d = 2$ case:

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

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

To get back to data-space post multiply each projection basis by the data, for the data projection.

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

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

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

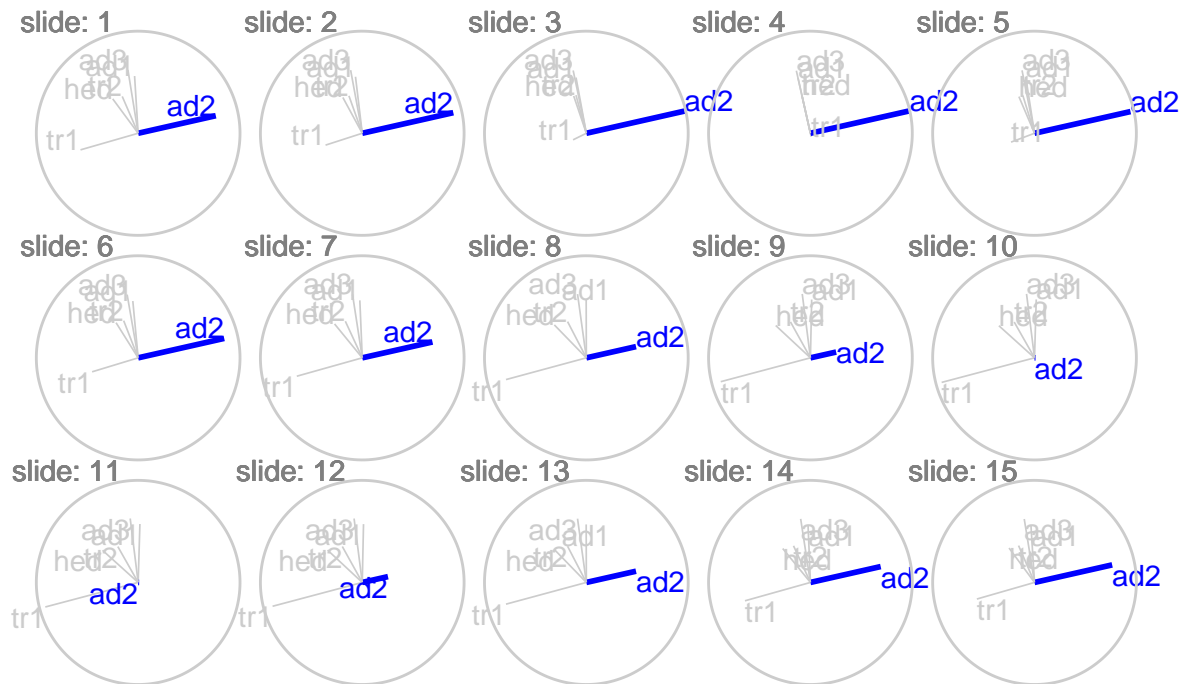


Figure 3.1: *manual tour, holes guided tour of flea data*

3.4 Display projection sequence

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.

3.5 Installation

spinifex is open source and hosted on [GitHub](https://github.com/nspyrison/spinifex). The development version is available for download by running `devtools::install_github("nspyrison/spinifex")` on your R console.

3.6 Application

apply manual tours to Ursula fig 1 here: NOTE: Examples from <https://arxiv.org/abs/1806.09742>

First stab at reproducing Fig8 from the PDFSense paper, is hosted here: nspyrison.netlify.com

3.7 Source

The code used to generate this chapter can be found at this [GitHub page](#).

3.8 Discussion

Future work:

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

Chapter 4

Display dimensionality

- XGobbi vs the C2

Chapter 5

Human-computer interaction of 3d projections

- Tour in 3D
- ImAxes / IATK

Appendix A

Additional stuff

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

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

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