Toward Tidy Principles for Matrix-Decomposed Data

New Developments in Graphing Multivariate Data
Section on Statistical Graphics
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Support

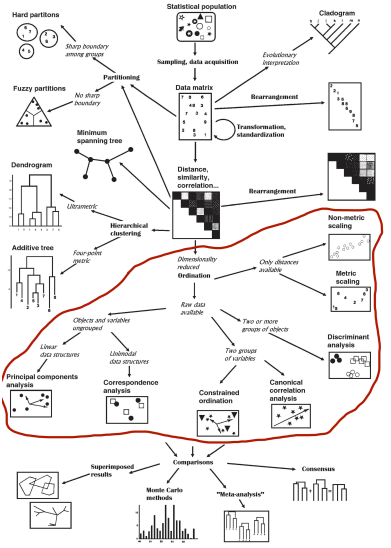
UCONN HEALTH

UF UNIVERSITY of FLORIDA

Ordination

"[A]ny technique that extracts artificial variables in order to reduce the dimensionality of the data is referred to as ***ordination****."*

		model: unsupervised	model: supervised
data	discrete	clustering	classification
data	continuous	dimension reduction	regression



Podani J • 2000 • *Introduction to the Exploration of Multivariate Biological Data* • https://web.archive.org/web/20200221000313/http://ramet.elte.hu/~podani/books.html

Principal components analysis

Derivation

- $X_{n\times p}$ data
- $\overline{x}_{n\times 1}$ data centroid
- $Y = X - 1\overline{x}^\top$ centered data
- $Y = U_{n\times q} D_{q\times q} V^\top_{q\times p}$ singular value decomposition

Interpretation

- D inertia
- U_r, V_r standard coordinates (orthonormal)
- $U_r D_r$, $V_r D_r$ principal coordinates
- V_r variable loadings
- $U_r D_r$ case scores

Application

- X' new data
- $(X' - 1\overline{x}^\top)V_r$ scores (supplementary)

Linear discriminant analysis

Derivation

- $G_{n\times k}$ groups
- $N = \text{diag}(n_1, \ldots, n_k)$ group counts
- $\overline{X}_{k\times p} = N^{-1}G^\top X$ group centroids
- $C = \frac{1}{n}X^\top X$ covariance matrix
- $\overline{Y} = \overline{X} - 1\overline{x}^\top$ centered group centroids
- $\overline{Y}C^{-1/2} = U_{k\times q}D_{q\times q}V^\top_{q\times p}$

Interpretation

- V_r variable loadings
- $U_rD_r = \overline{Y}C^{-1/2}V$ group centroid scores

Application

- $YC^{-1/2}V_r$ case scores (supplementary)
- X' new data
- $X'C^{-1/2}V_r$ scores (supplementary)

General Multidimensional Analysis

1. Preprocess data $X \rightsquigarrow Y$
   - centering
   - double-centering
2. Generalized SVD $Y = NDM^\top = (A^{-1/2}U)D(B^{-1/2}V)^\top$, where A, B are positive semi-definite and $N^\top AN = M^\top BM = I$ (orthonormalization)
   - weights
   - sphering

   Low-rank approximation $Y \approx N_r D M_r^\top$
3. Biplot of $F = U_r D^a$ and $G = V_r D^b$, with $a + b = 1$
   - row-principal
   - column-principal
   - symmetric

Greenacre M • 1984 • *Theory and applications of correspondence analysis* • http://www.carme-n.org/

Need

R is replete with ordination methods!

CRAN Task View: Multivariate Statistics

Maintainer: Paul Hewson
Contact: Paul.Hewson at plymouth.ac.uk
Version: 2014-09-19

CRAN Task View: Analysis of Ecological and Environmental Data

Maintainer: Gavin Simpson
Contact: ucfagls at gmail.com
Version: 2014-05-31

… but they are

- **specialized**: unweildy & uninformative inspection methods
- **heterogeneous**: diverse, dissimilar, domain-specific conventions
- **standalone**: not easily interoperable with other tools or integrable into external workflows

Design

Typical implementations:

General implementation:

Tidy management:

Inspiration

*[T]he **tidyverse** is a collection of R packages that share a high-level design philosophy and low-level grammar and data structures, so that learning one package makes it easier to learn the next.*

The tidyverse strives to be

- **human-centered**: supports data analysis conducted by humans
- **consistent**: ensures learning transfers between packages
- **composable**: enables modular thinking and doing
- **inclusive**: developed and informed by a broad community

Wickham &al • 2019 • *The Journal of Open Source Software* • doi:10.21105/joss.01686
Tidyverse team • *Tidyverse design guide* • https://design.tidyverse.org/

Inspiration

lazy, surly, & pithy data frames

relational algebra for data sets

convenient summarization
of statistical models

grammatical production
of statistical graphics

Implementation

Engine

Recovery methods for (your!) S3 model classes:

- left & right matrix factors (singular vectors)
  $U_{n\times k}$, $V_{p\times k}$
- transformations of coordinate spaces
  $A_{n\times n}$, $B_{p\times p}$
- inertia and its distribution unto the factors
  $D = \text{diag}(d_1, \ldots, d_k)$, (a, b)
- active & supplementary elements
  $U_r D_r = XV_r$, $X'V_r$

Dashboard

Class 'tbl_ord':

- wrapper for ordination models
- clear & consistent formatting

Functions:

- augment with model metadata
- redistribution of inertia
- tidily inspect & summarize
- annotate rows and columns
- build biplots grammatically
- add ordination plot layers

Example workflow

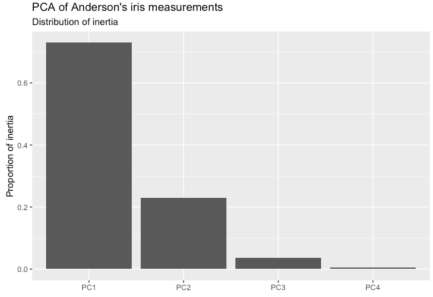
```
head(iris)
#>   Sepal.Length Sepal.Width Petal.Length Petal.Width Species
#> 1          5.1         3.5          1.4         0.2  setosa
#> 2          4.9         3.0          1.4         0.2  setosa
#> 3          4.7         3.2          1.3         0.2  setosa
#> 4          4.6         3.1          1.5         0.2  setosa
#> 5          5.0         3.6          1.4         0.2  setosa
#> 6          5.4         3.9          1.7         0.4  setosa
summary(iris)
#>   Sepal.Length    Sepal.Width     Petal.Length    Petal.Width
#>  Min.   :4.300   Min.   :2.000   Min.   :1.000   Min.   :0.100
#>  1st Qu.:5.100   1st Qu.:2.800   1st Qu.:1.600   1st Qu.:0.300
#>  Median :5.800   Median :3.000   Median :4.350   Median :1.300
#>  Mean   :5.843   Mean   :3.057   Mean   :3.758   Mean   :1.199
#>  3rd Qu.:6.400   3rd Qu.:3.300   3rd Qu.:5.100   3rd Qu.:1.800
#>  Max.   :7.900   Max.   :4.400   Max.   :6.900   Max.   :2.500
#>        Species
#>  setosa    :50
#>  versicolor:50
#>  virginica :50
#>
#>
#>
```

```
(iris_pca <- ordinate(iris, cols = 1:4, model = ~ prcomp(., scale. = TRUE)))
#> # A tbl_ord of class 'prcomp': (150 x 4) x (4 x 4)'
#> # 4 coordinates: PC1, PC2, ..., PC4
#> #
#> # Rows (principal): [ 150 x 4 | 1 ]
#>     PC1    PC2     PC3 ... |   Species
#>                            |   <fct>
#> 1 -2.26 -0.478  0.127      | 1 setosa
#> 2 -2.07  0.672  0.234  ... | 2 setosa
#> 3 -2.36  0.341 -0.0441     | 3 setosa
#> 4 -2.29  0.595 -0.0910     | 4 setosa
#> 5 -2.38 -0.645 -0.0157     | 5 setosa
#> # … with 145 more rows
#> # ℹ Use `print(n = ...)` to see more rows
#> #
#> # Columns (standard): [ 4 x 4 | 3 ]
#>      PC1     PC2     PC3 ... |   .name        .center .scale
#>                              |   <chr>         <dbl>  <dbl>
#> 1  0.521 -0.377   0.720     | 1 Sepal.Length   5.84  0.828
#> 2 -0.269 -0.923  -0.244 ... | 2 Sepal.Width    3.06  0.436
#> 3  0.580 -0.0245 -0.142     | 3 Petal.Length   3.76  1.77
#> 4  0.565 -0.0669 -0.634     | 4 Petal.Width    1.20  0.762
```

Example workflow

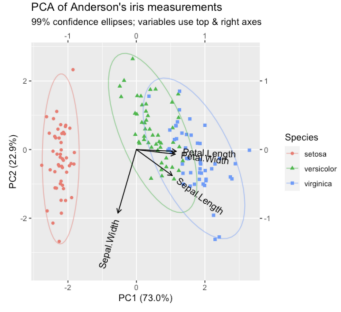
```
iris_meta <- data.frame(
  Species = c("setosa", "versicolor", "virginica"),
  Colony = c(1L, 1L, 2L),
  Cytotype = c("diploid", "hexaploid", "tetraploid"),
  Ploidy = c(2L, 6L, 4L)
)
(iris_pca <- left_join_rows(iris_pca, iris_meta, by = "Species"))
#> # A tbl_ord of class 'prcomp': (150 x 4) x (4 x 4)'
#> # 4 coordinates: PC1, PC2, ..., PC4
#> #
#> # Rows (principal): [ 150 x 4 | 4 ]
#>      PC1    PC2     PC3 ... |   Species Colony Cytotype Ploidy
#>                             |   <chr>    <int> <chr>     <int>
#> 1 -2.26 -0.478  0.127      | 1 setosa       1 diploid       2
#> 2 -2.07  0.672  0.234  ... | 2 setosa       1 diploid       2
#> 3 -2.36  0.341 -0.0441     | 3 setosa       1 diploid       2
#> 4 -2.29  0.595 -0.0910     | 4 setosa       1 diploid       2
#> 5 -2.38 -0.645 -0.0157     | 5 setosa       1 diploid       2
#> # … with 145 more rows
#> # ℹ Use `print(n = ...)` to see more rows
#> #
#> # Columns (standard): [ 4 x 4 | 3 ]
#>      PC1     PC2     PC3 ... |   .name        .center .scale
#>                              |   <chr>          <dbl>  <dbl>
#> 1  0.521 -0.377   0.720     | 1 Sepal.Length    5.84  0.828
#> 2 -0.269 -0.923  -0.244 ... | 2 Sepal.Width     3.06  0.436
#> 3  0.580 -0.0245 -0.142     | 3 Petal.Length    3.76  1.77
#> 4  0.565 -0.0669 -0.634     | 4 Petal.Width     1.20  0.762
```

```
tidy(iris_pca) %T>% print() %>%
  ggplot(aes(x = .name, y = .prop_var)) +
  geom_col() +
  labs(x = "", y = "Proportion of inertia") +
  ggtitle("PCA of Anderson's iris measurements",
          "Distribution of inertia")
#> # A tibble: 4 × 4
#>   .name .sdev .inertia .prop_var
#>   <fct> <dbl>    <dbl>     <dbl>
#> 1 PC1   1.71     435.      0.730
#> 2 PC2   0.956    136.      0.229
#> 3 PC3   0.383     21.9     0.0367
#> 4 PC4   0.144      3.09    0.00518
```

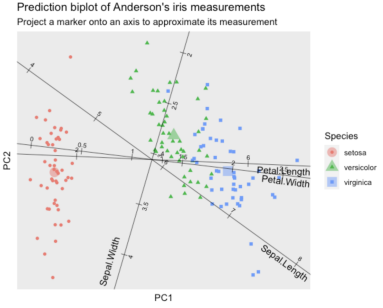


Example workflow

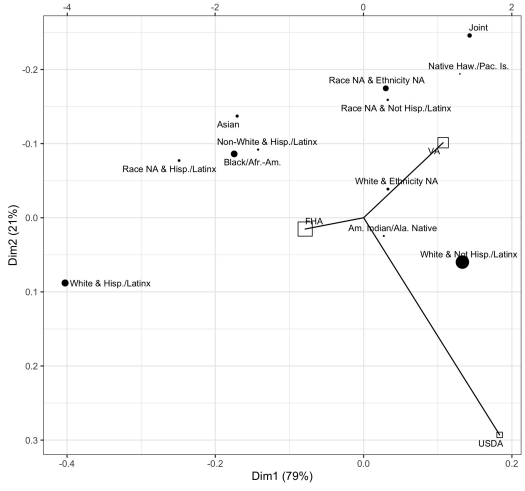
```
ggbiplot(iris_pca, sec.axes = "cols", scale.factor = 2) +
  geom_rows_point(aes(color = Species, shape = Species)) +
  stat_rows_ellipse(aes(color = Species), alpha = .5, level = .99) +
  geom_cols_vector() +
  geom_cols_text_radiate(aes(label = .name)) +
  expand_limits(y = c(-3.5, NA)) +
  ggtitle("PCA of Anderson's iris measurements",
          "99% confidence ellipses; variables use top & right axes")
```



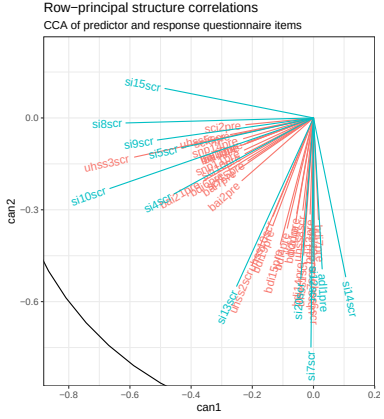

```
ggbiplot(iris_pca, axis.type = "predictive", axis.percents = FALSE) +
  theme_biplot() +
  geom_rows_point(aes(color = Species, shape = Species)) +
  stat_rows_center(
    aes(color = Species, shape = Species),
    size = 5, alpha = .5, fun.data = mean_se
  ) +
  geom_cols_axis(aes(label = .name, center = .center, scale = .scale)) +
  ggtitle("Prediction biplot of Anderson's iris measurements",
          "Project a marker onto an axis to approximate its measurement")
```

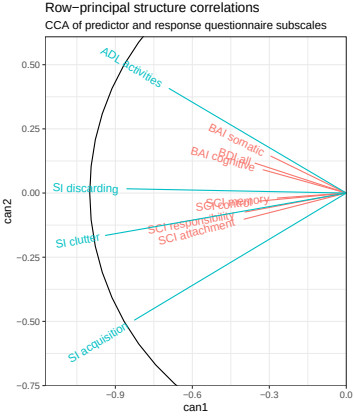


Origination of home loans by program and racial-ethnic group



Associations between hoarding and other mental health disorders





Use case 3

Limitations & needs

S3 class methods
- quality measures
- interpolation
- prediction
- predictive biplot elements

Biplot functionality
- predictive biplots
- joint row-and-column layers
  - interpolative vector sum
  - predictive projection

Involvement
- accessibility
- issues
- contributions

Fin

This is the end
Beautiful friend