

Robust Outlier Detection

for Low and High-Dimensional Neuroimaging Data with
Principal Components Analysis and Split-Half Resampling

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Twitter: @derek__beaton (that's two underscores!)
Github for today: <http://github.com/derekbeaton/ours>

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The other authors

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Acknowledgements



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Acknowledgements



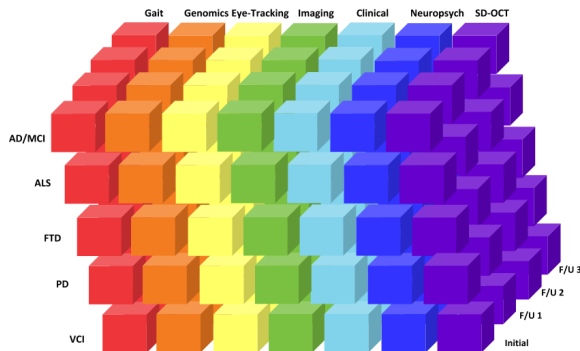
ONTARIO
NEURODEGENERATIVE
DISEASE RESEARCH
INITIATIVE

Ontario neurodegenerative disease research initiative (ONDRI)

1

Introduction

ONDRI



The ONDRI “cube” (Farhan et al., 2017). Ontario-wide, multi-site, longitudinal, multi-cohort, “deep-phenotyping”. Today’s focus: Alzheimer’s (AD/MCI) and Vascular Cognitive Impairment (VCI)

ONDRI

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 - Today's focus: structural and functional neuroimaging

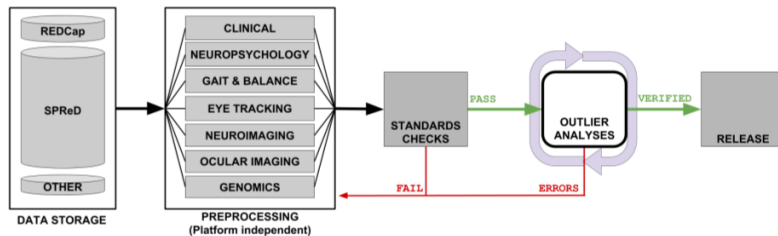
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- Most platforms have many modalities.
 - Today's focus: structural and functional neuroimaging
- Almost everything multivariate with varying complexities
- How to ensure data are of highest quality?

Outlier detection



The ONDRI preprocessing to release pipeline

Outlier detection

- ONDRI's Neuroinformatics & Biostatistics team performs multivariate outlier detection on all data sets (see Sunderland et al., in prep).

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- Why a new approach?

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- Identify anomalous data points; can be
 - observations that deviate from sample
 - interesting patterns (e.g., co- or multi-morbid)
 - errors
- Why a new approach?
 - There are substantial limitations of existing methods

2

PCA+SHR background

New framework

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New framework

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 - Principal components analysis (PCA) plus
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- The BIG goal
 - Provide flexible & robust multivariate outlier detection

Distances

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- Orthogonal distances

Distances

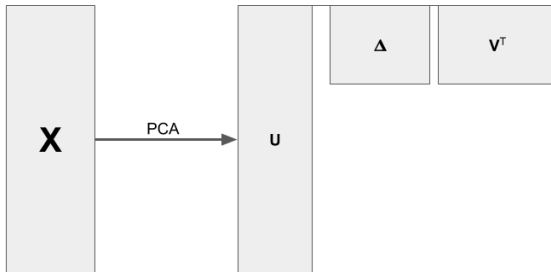
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 - MD scaled by explained variance per component
- Orthogonal distances
 - We'll bring these up later

PCA

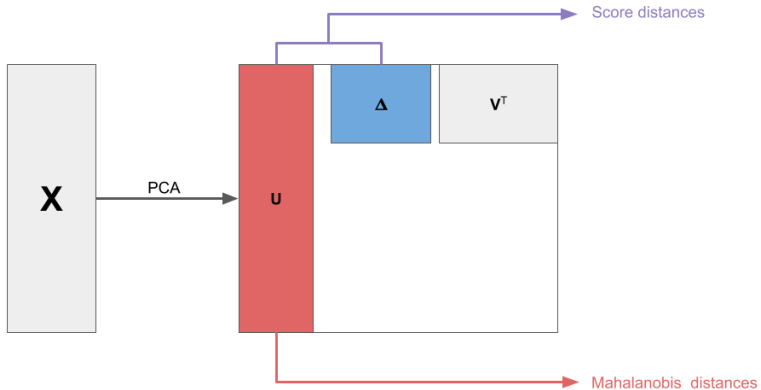


X

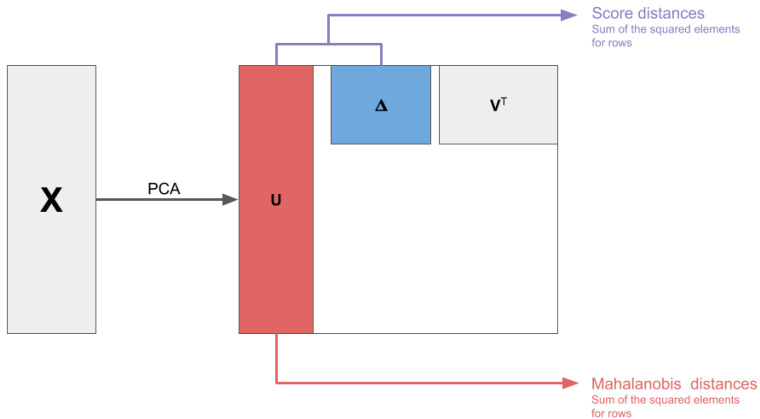
PCA



PCA



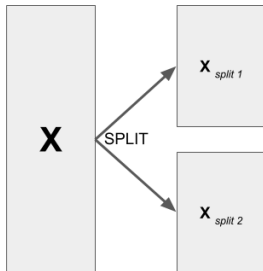
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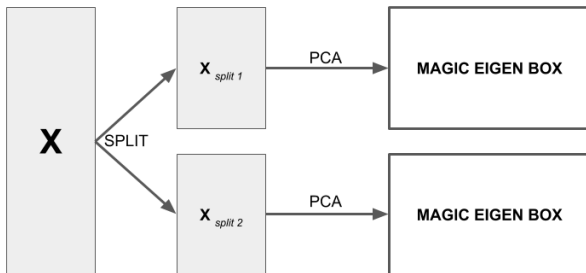
PCA



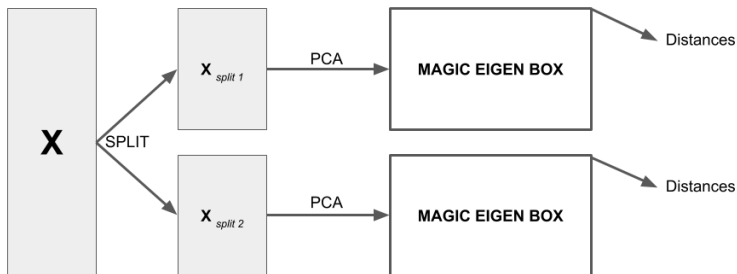
Single split PCA



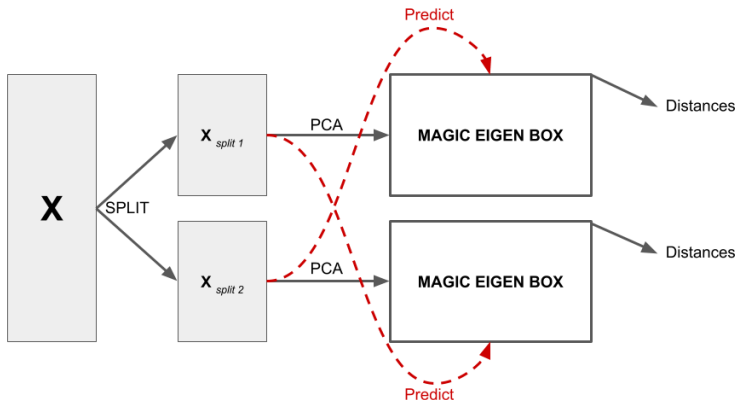
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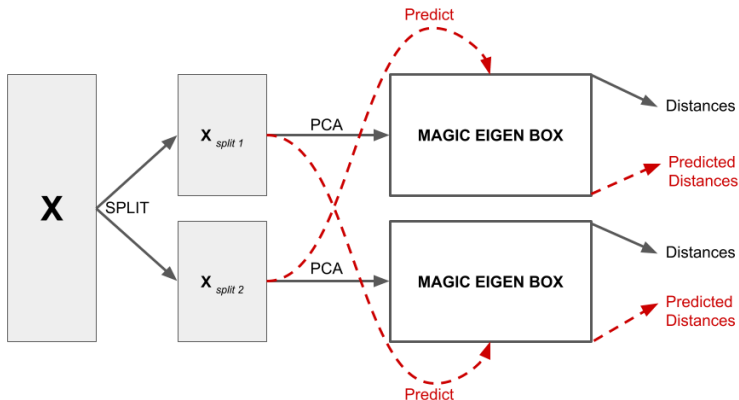
Single split PCA



Prediction from split PCAs



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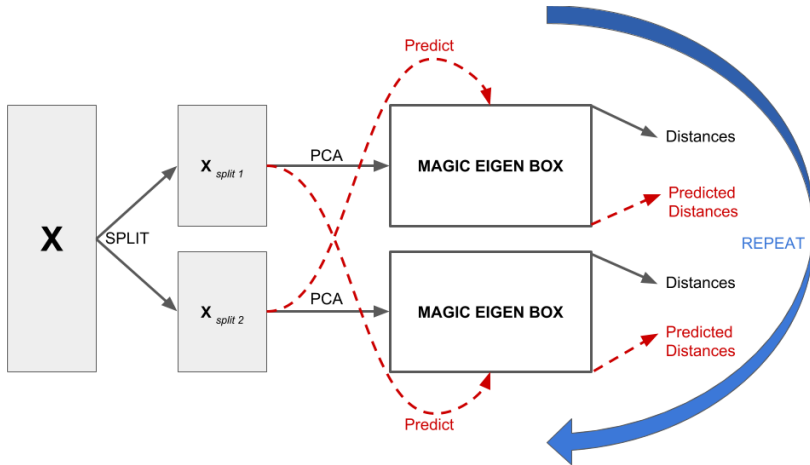
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- When data are singular, collinear, or rank deficient (e.g., $I < J$):
 - Standard MD cannot be computed
 - Some techniques (e.g., MCD [4], ROBPCA [5]) no longer work
 - **Predicted** distances can always be computed (see Bonus Material)
- But: just one pass at split PCA is not enough

Resampling



Introduction

PCA+SHR background

PCA+SHR walkthrough

Discussion

Bonus material

Distances

PCA

Resampling

PCA+SHR

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- Resampling provides distributions to estimate stability/spread and cutoffs.
- Estimates of reproducibility
 - Will come up later with orthogonal distances (OD).

3

PCA+SHR walkthrough

Data

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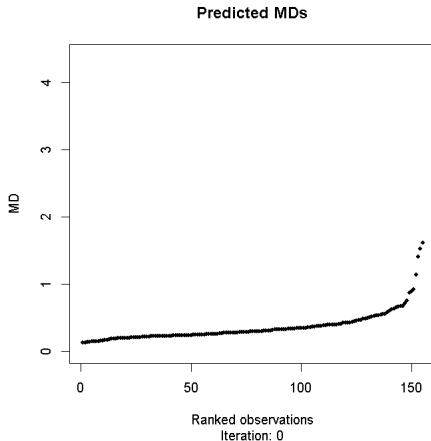
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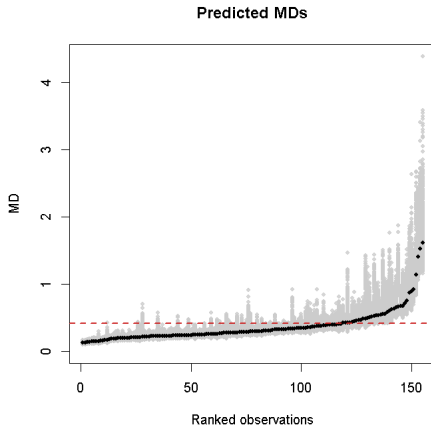
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- $N = 1000$ iterations

Predicted MD distributions

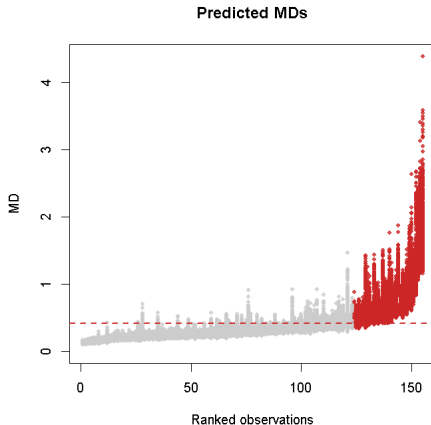


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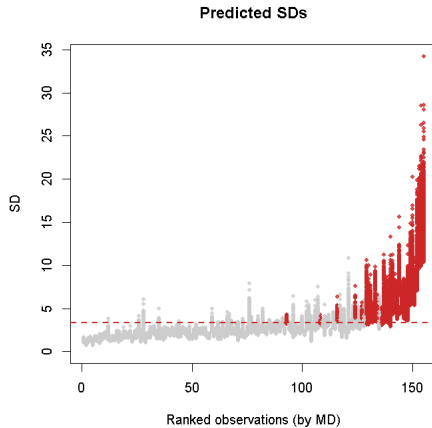
MD distribution threshold



Mahalanobis distribution outliers



Score distribution outliers



Reproducibility

- What else do we get?

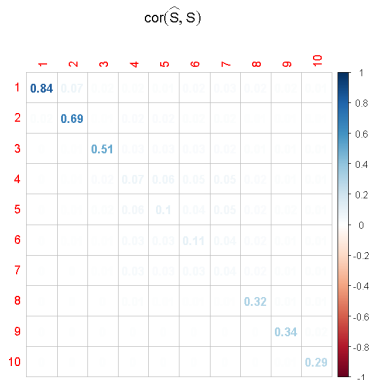
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Reproducibility

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 - Squared correlations between singular vectors and predicted singular vectors
 - Find reproducible & robust subspace (components)

Reproducibility



Median R^2 between split vectors and predicted vectors over 1000 iterations

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- We can use those to rebuild a robust version of \mathbf{X} :

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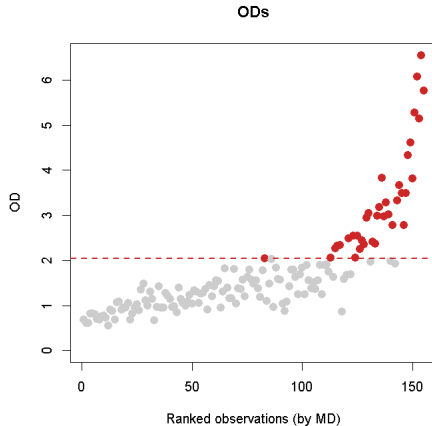
Resampling

- We can use those to rebuild a robust version of \mathbf{X} :
 - \mathbf{X}' - reconstructed from just first three components
- How much do observations change between \mathbf{X} and robust \mathbf{X}' ?

Orthogonal distance (OD)

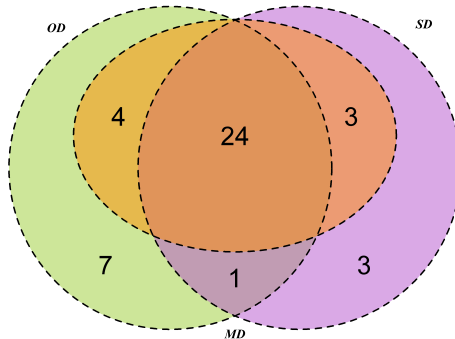
- Distance between observation and itself for \mathbf{X} and robust \mathbf{X}'

Orthogonal distance outliers



Outliers

Outliers



$I = 161$, Outliers = 42.

Summary of PCA+SHR

- Build (predictive) distributions

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- Find a reproducible subspace

Summary of PCA+SHR

- Build (predictive) distributions
- Find a reproducible subspace
- Three types of distances & outliers

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What about large data?

- High dimensional, low sample size
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 - Difficult to find robust subspaces
- PCA+SHR works the same regardless of size

Data

- $I = 109$ observations from the AD/MCI cohort

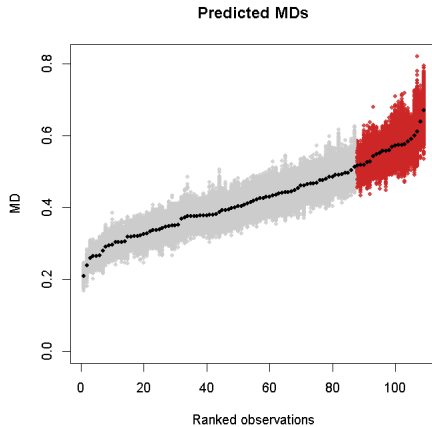
Data

- $I = 109$ observations from the AD/MCI cohort
- $J = 32,768$ voxels per person

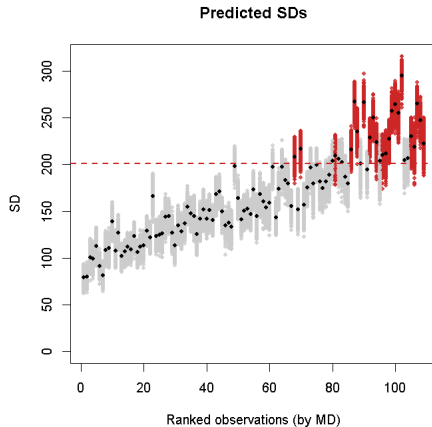
Data

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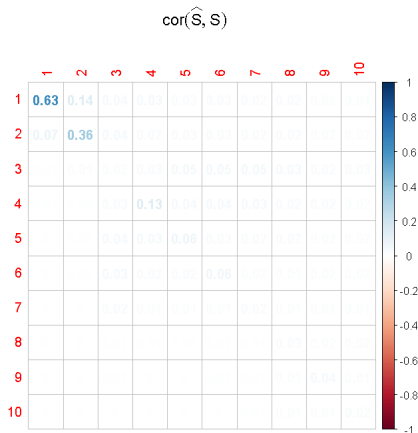
Outliers



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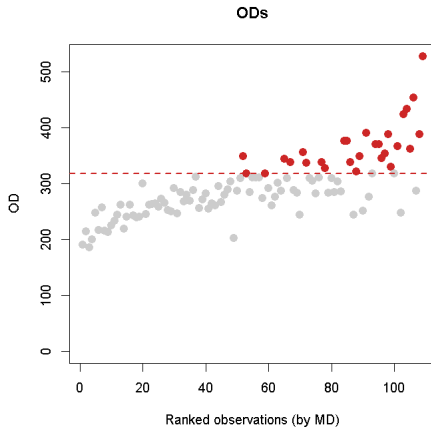


Subspace



Only the first 10 of 108 Components shown

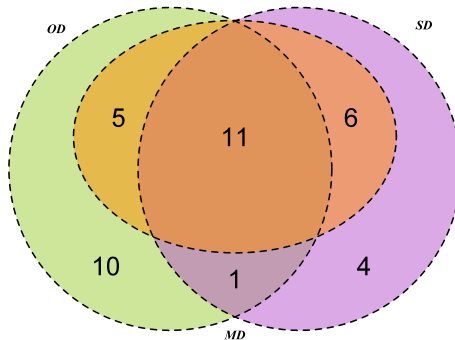
Outliers



OD computed from two components

Outliers

Outliers



$I = 109$, Outliers = 37.

4

Discussion

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 - Low: Find most outlying & unique outliers to each type

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- A lot of information available
 - Multiple distances, distributions to help make decisions

Limitations

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- Lots of options
 - How to decide outlier identification?
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 - But we provide defaults in the software that work well
- Can be slow

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 - Beaton et al., (2018) - extended MCD [1] to any data type

References

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 - Higher level overview of ONDRI curation-through-release pipeline

5

Bonus material

Notation

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- a - scalar

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- \mathbf{a} - vector

Notation

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Notation

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- \mathbf{A} - matrix
- \mathbf{A}^T - transpose
- \mathbf{AB} - matrix multiplication

PCA

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- \mathbf{V} is $J \times L$ (right singular vectors; columns of \mathbf{X})
- \mathbf{U} and \mathbf{V} are orthonormal: $\mathbf{U}^T\mathbf{U} = \mathbf{I} = \mathbf{V}^T\mathbf{V}$

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Given $\mathbf{X} = \mathbf{U}\mathbf{\Delta}\mathbf{V}^T$

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Score distances

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Score distances

Given $\mathbf{X} = \mathbf{U}\mathbf{\Delta}\mathbf{V}^T$

- Sum of squared component (factor) scores
- Can be computed regardless of rank
- Score distances (SD) are defined as:

$$\mathbf{S} = \text{diag}\{(\mathbf{U}\mathbf{\Delta})(\mathbf{U}\mathbf{\Delta})^T\} = \text{diag}\{(\mathbf{X}\mathbf{V})(\mathbf{X}\mathbf{V})^T\} \quad (2)$$

Mahalanobis

Given $\mathbf{X} = \mathbf{U}\mathbf{\Delta}\mathbf{V}^T$

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- Sum of squared singular vectors

$$\begin{aligned}\mathbf{M} = \text{diag}\{\mathbf{U}\mathbf{U}^T\} &= \text{diag}\{(\mathbf{X}\mathbf{V}\mathbf{\Delta}^{-1})(\mathbf{X}\mathbf{V}\mathbf{\Delta}^{-1})^T\} \\ &= \text{diag}\{(\mathbf{S}\mathbf{\Delta}^{-1})(\mathbf{S}\mathbf{\Delta}^{-1})^T\}\end{aligned}\tag{3}$$

Mahalanobis

Given $\mathbf{X} = \mathbf{U}\mathbf{\Delta}\mathbf{V}^T$

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- Can only be computed when not rank deficient

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 - if $I \gg L$; when $I \leq L$, $\mathbf{M} = \mathbf{I}_c$ where $c = L \times I^{-1}$
- Mahalanobis distances (MD) are defined as:

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Single split PCA

For some subset H and its complement \bar{H} we have two PCAs:

$$\begin{aligned}\mathbf{X}_H &= \mathbf{U}_H \mathbf{\Delta}_H \mathbf{V}_H^T \\ \mathbf{X}_{\bar{H}} &= \mathbf{U}_{\bar{H}} \mathbf{\Delta}_{\bar{H}} \mathbf{V}_{\bar{H}}^T\end{aligned}\tag{4}$$

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Size of H could be $\alpha = .5$ (split half) or e.g., $\alpha = .9$ (90-10)

Predicted distances

Predicted distances

Predicted SD:

$$\begin{aligned}\hat{\mathbf{S}}_H &= \text{diag}\{(\mathbf{X}_H \mathbf{V}_{\bar{H}})(\mathbf{X}_H \mathbf{V}_{\bar{H}})^T\} \\ \hat{\mathbf{S}}_{\bar{H}} &= \text{diag}\{(\mathbf{X}_{\bar{H}} \mathbf{V}_H)(\mathbf{X}_{\bar{H}} \mathbf{V}_H)^T\}\end{aligned}\tag{5}$$

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Predicted MD:

$$\begin{aligned}\hat{\mathbf{M}}_H &= \text{diag}\{(\hat{\mathbf{S}}_H \Delta_{\bar{H}}^{-1})(\hat{\mathbf{S}}_H \Delta_{\bar{H}}^{-1})^T\} \\ \hat{\mathbf{M}}_{\bar{H}} &= \text{diag}\{(\hat{\mathbf{S}}_{\bar{H}} \Delta_H^{-1})(\hat{\mathbf{S}}_{\bar{H}} \Delta_H^{-1})^T\}\end{aligned}\tag{6}$$

Predicted distances

Predicted SD:

$$\begin{aligned}\hat{\mathbf{S}}_H &= \text{diag}\{(\mathbf{X}_H \mathbf{V}_{\bar{H}})(\mathbf{X}_H \mathbf{V}_{\bar{H}})^T\} \\ \hat{\mathbf{S}}_{\bar{H}} &= \text{diag}\{(\mathbf{X}_{\bar{H}} \mathbf{V}_H)(\mathbf{X}_{\bar{H}} \mathbf{V}_H)^T\}\end{aligned}\tag{5}$$

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$$\begin{aligned}\hat{\mathbf{M}}_H &= \text{diag}\{(\hat{\mathbf{S}}_H \Delta_{\bar{H}}^{-1})(\hat{\mathbf{S}}_H \Delta_{\bar{H}}^{-1})^T\} \\ \hat{\mathbf{M}}_{\bar{H}} &= \text{diag}\{(\hat{\mathbf{S}}_{\bar{H}} \Delta_H^{-1})(\hat{\mathbf{S}}_{\bar{H}} \Delta_H^{-1})^T\}\end{aligned}\tag{6}$$

Orthogonal distance

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- We can use subspace to rebuild a robust version of \mathbf{X} :
 - $\mathbf{X}' = \mathbf{U}_{1:3} \mathbf{\Delta}_{1:3} \mathbf{V}_{1:3}^T$
- How much do observations change between \mathbf{X} and robust \mathbf{X}' ?

Orthogonal distance

Given two commensurate matrices, \mathbf{X} and \mathbf{X}' , orthogonal distances (OD) are defined as:

$$\mathbf{O} = \|\mathbf{X} - \mathbf{X}'\| \quad (7)$$