Robust Outlier Detection

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

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Rotman Research Institute, Baycrest Health Sciences

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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ONTARIO BRAIN INSTITUTE

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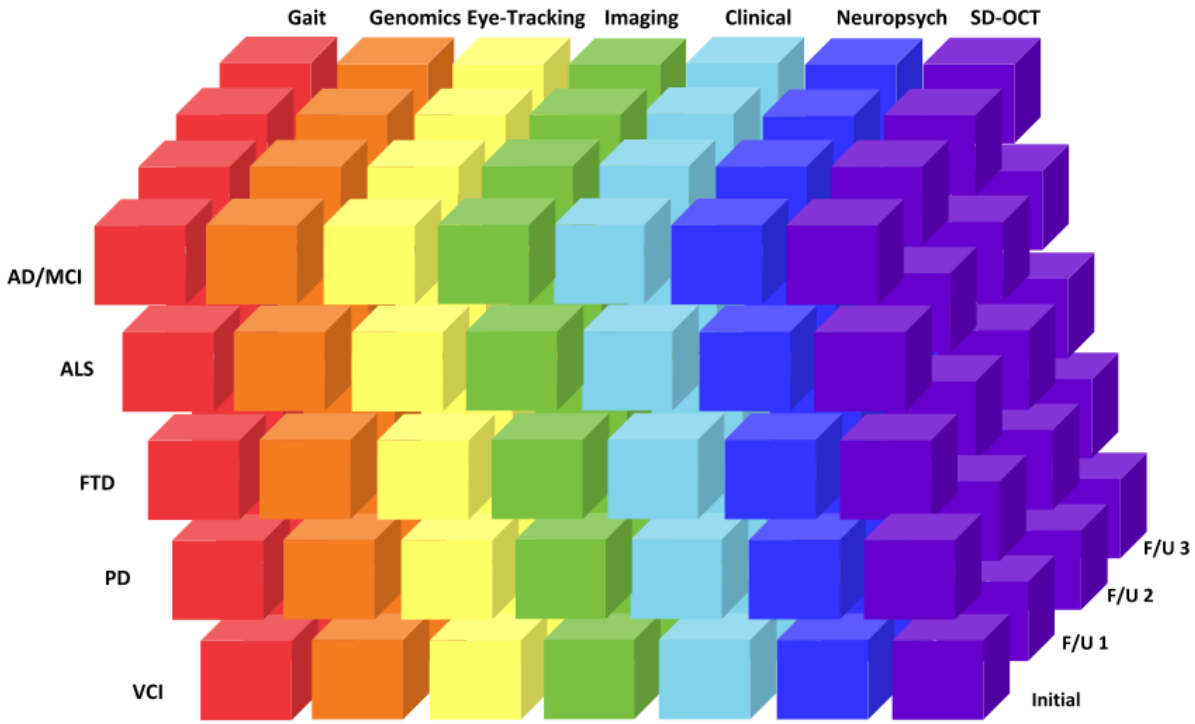
Introduction

ONDRI

ONTARIO
NEURODEGENERATIVE
DISEASE RESEARCH
INITIATIVE

Ontario neurodegenerative disease research initiative (ONDRI)

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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- Almost everything multivariate with varying complexities

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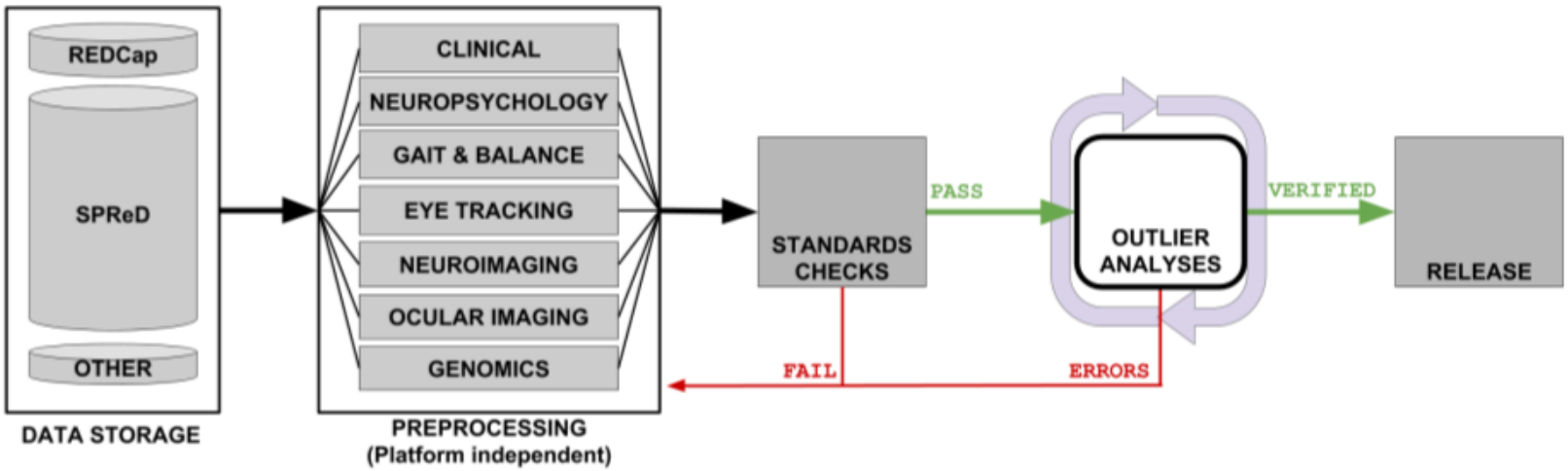
  - Today's focus: structural and functional neuroimaging
- Almost everything multivariate with varying complexities
- How to ensure data are of highest quality?

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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  - 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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- The BIG goal
  - Provide flexible & robust multivariate outlier detection

Distances

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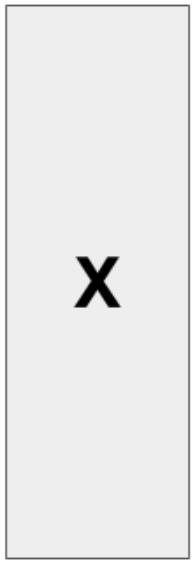
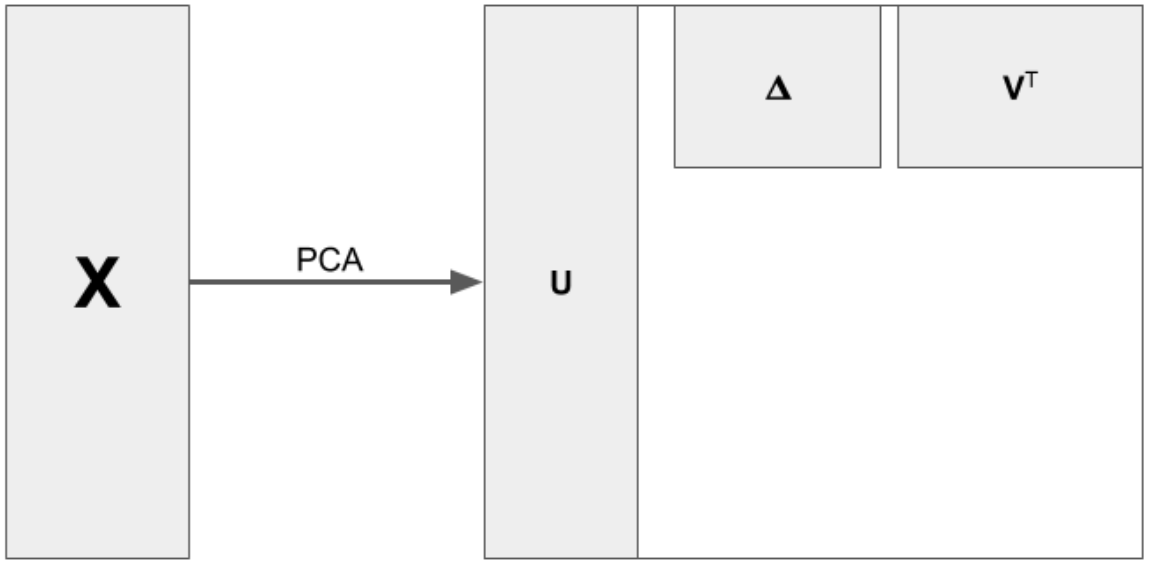
  - We'll bring these up later

PCA



PCA



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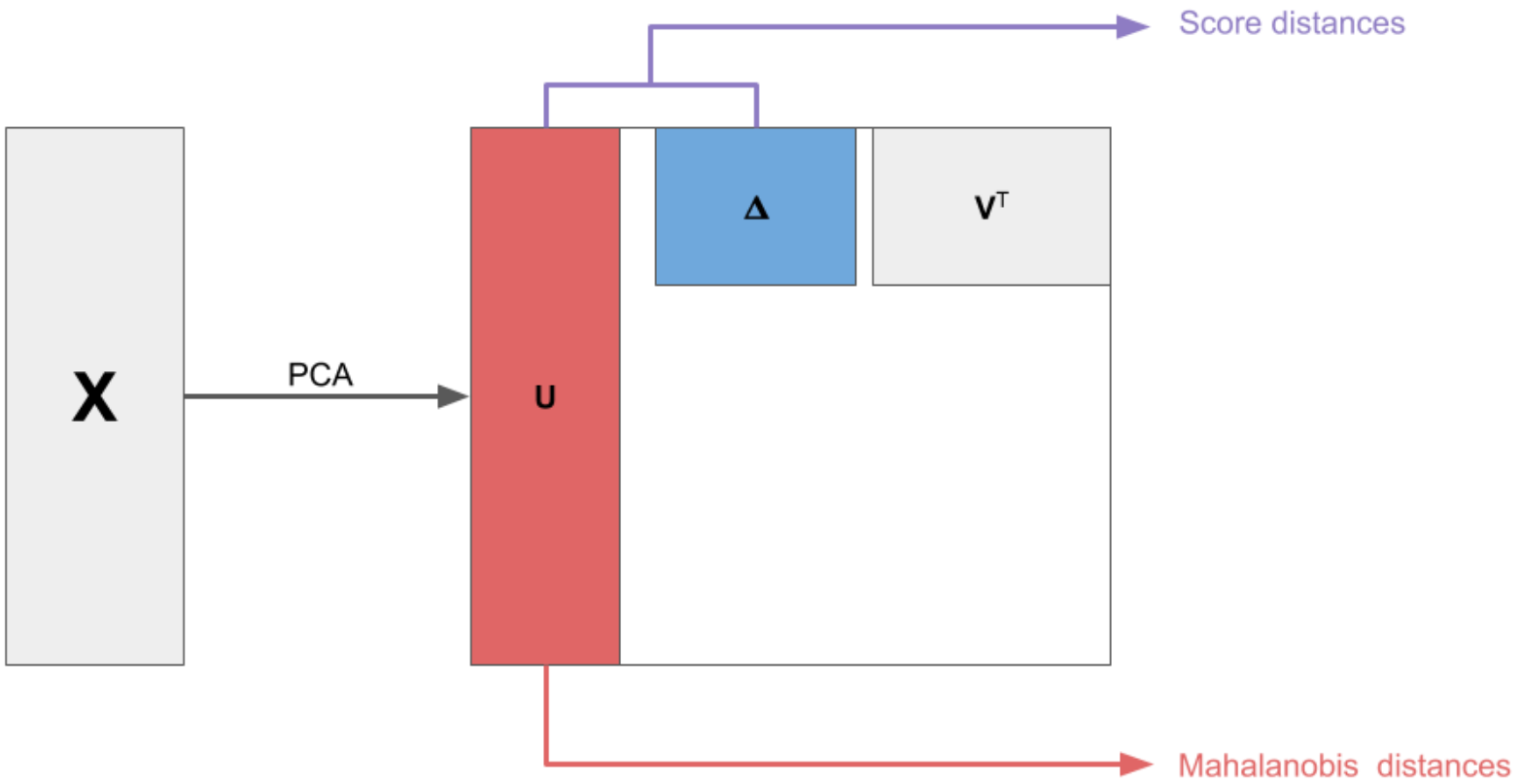

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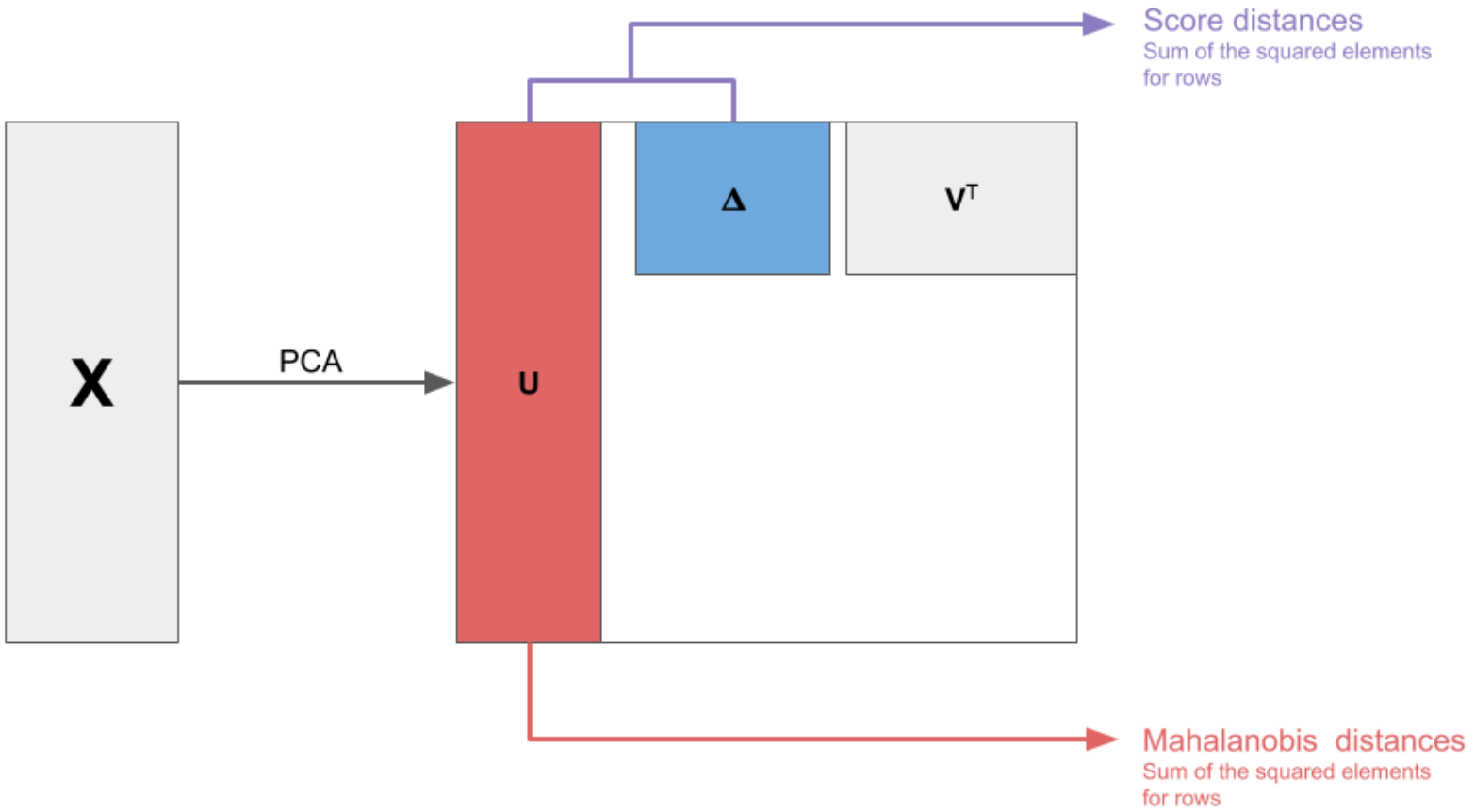
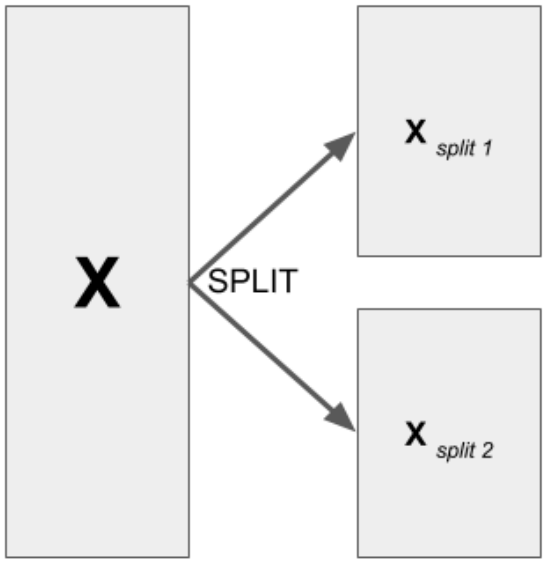

Score distances
Sum of the squared elements
for rows
X
PCA
U
Δ
V^T
Mahalanobis distances
Sum of the squared elements
for rows

PCA


X
PCA
MAGIC EIGEN BOX
Score distances
Mahalanobis distances

Single split PCA



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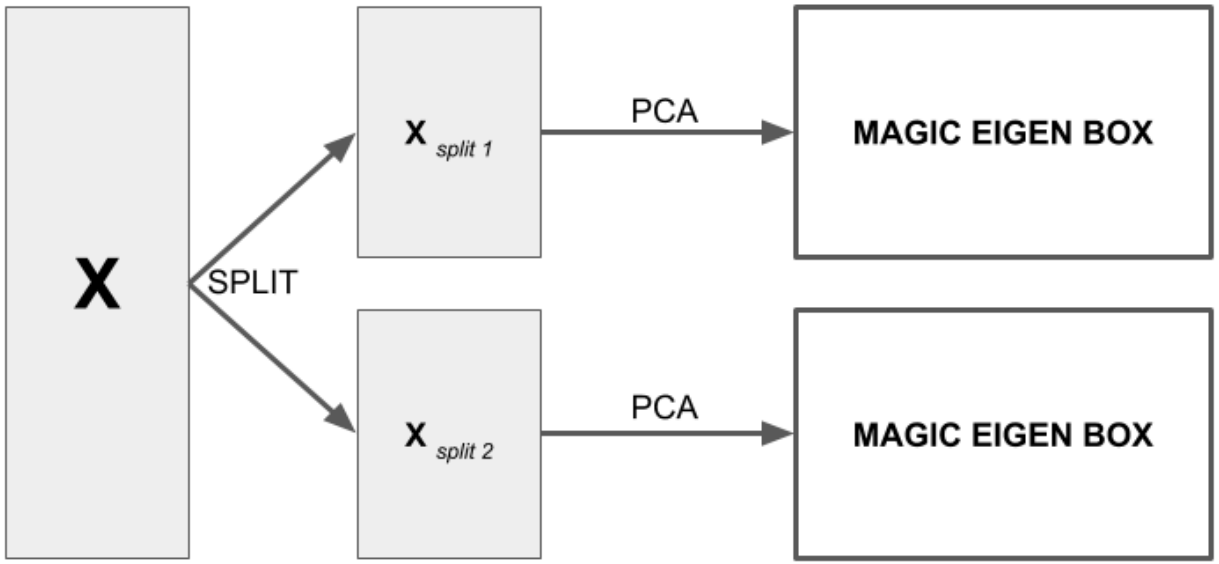
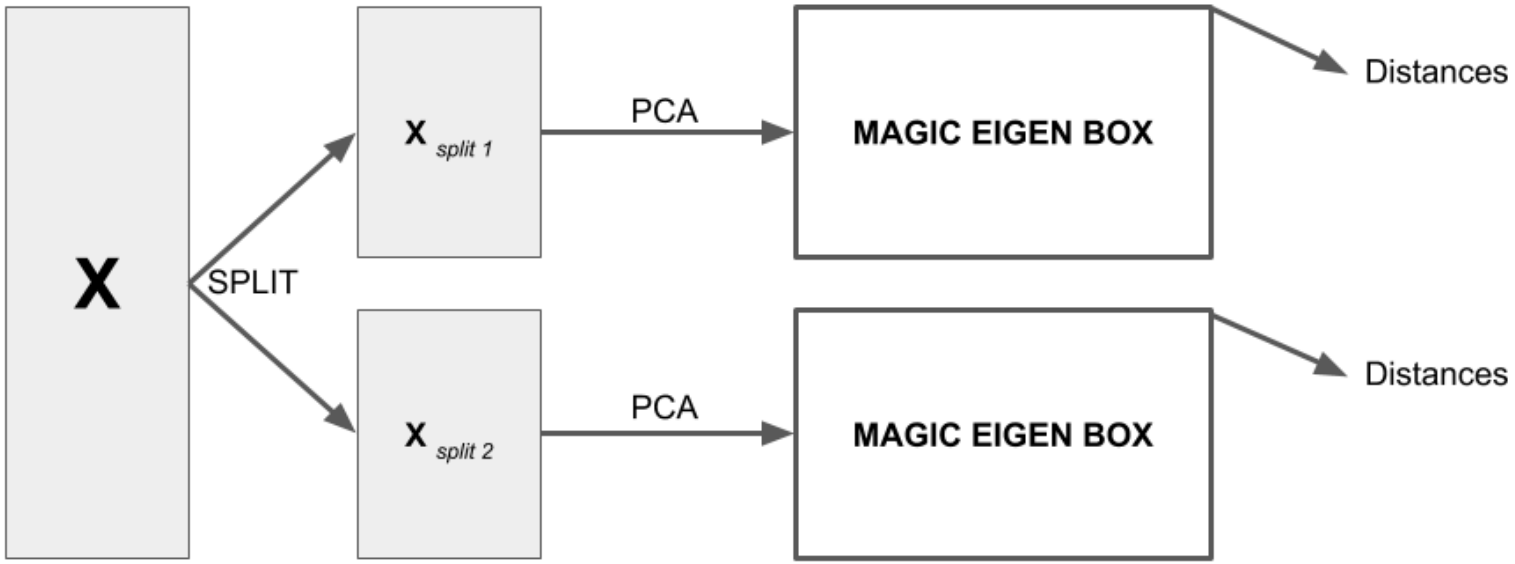
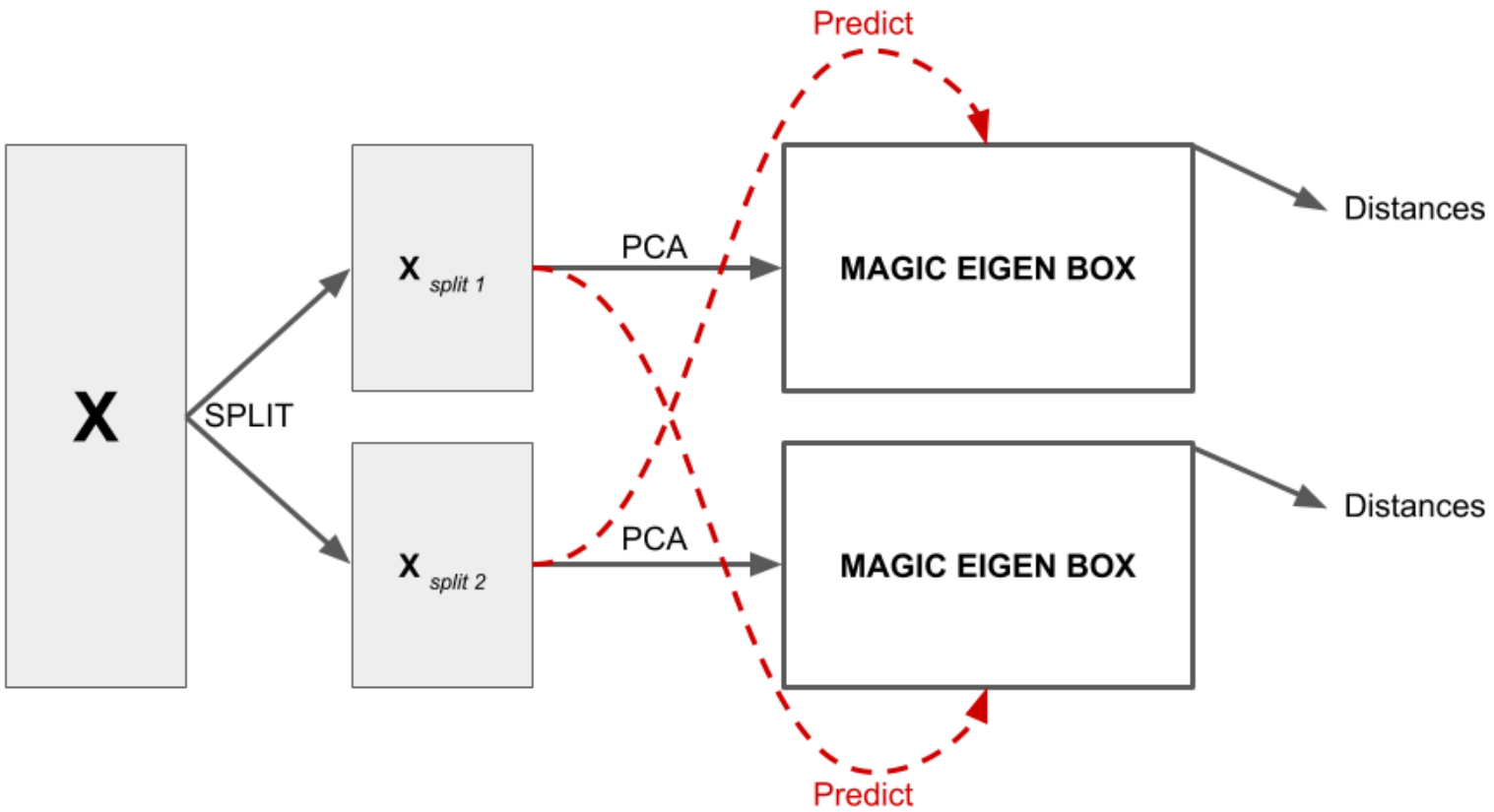


Single split PCA



Prediction from split PCAs



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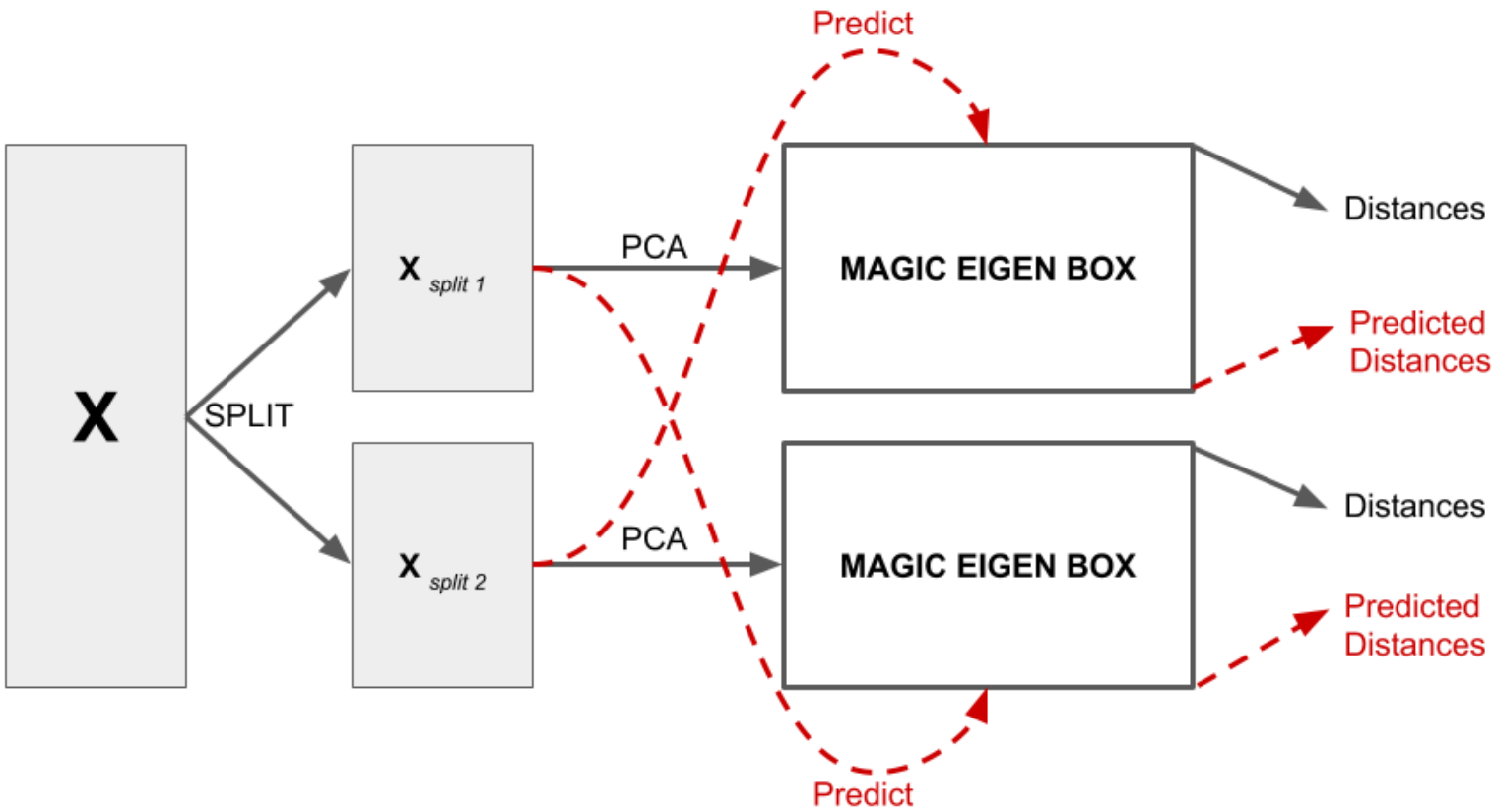

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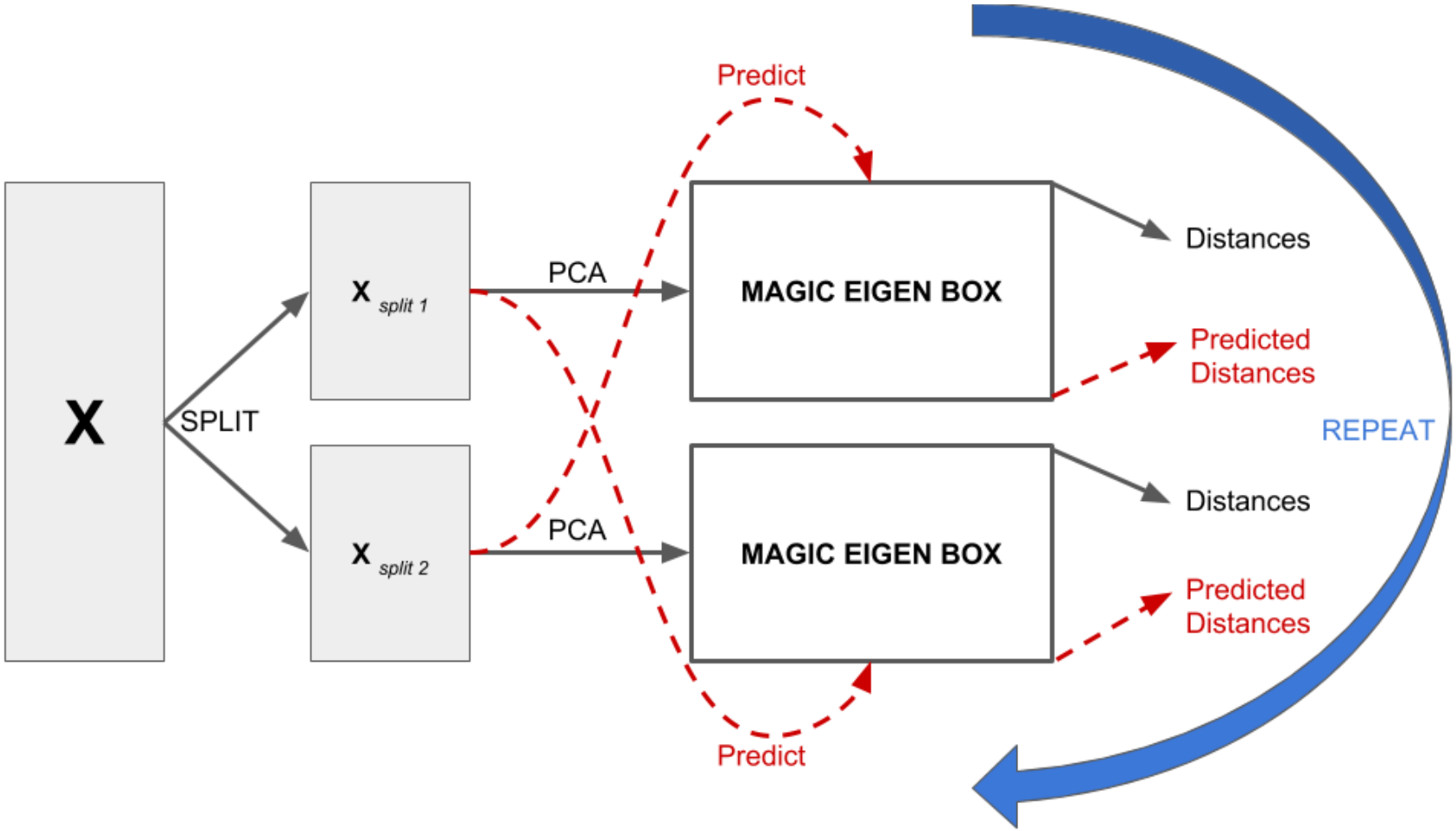
  - **Predicted** distances can always be computed (see Bonus Material)
- But: just one pass at split PCA is not enough

Resampling


X
SPLIT
X split 1
X split 2
PCA
PCA
MAGIC EIGEN BOX
MAGIC EIGEN BOX
Predict
Predict
Distances
Predicted Distances
Distances
Predicted Distances
REPEAT

PCA+SHR

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  - Will come up later with orthogonal distances (OD).

3

PCA+SHR walkthrough

Data

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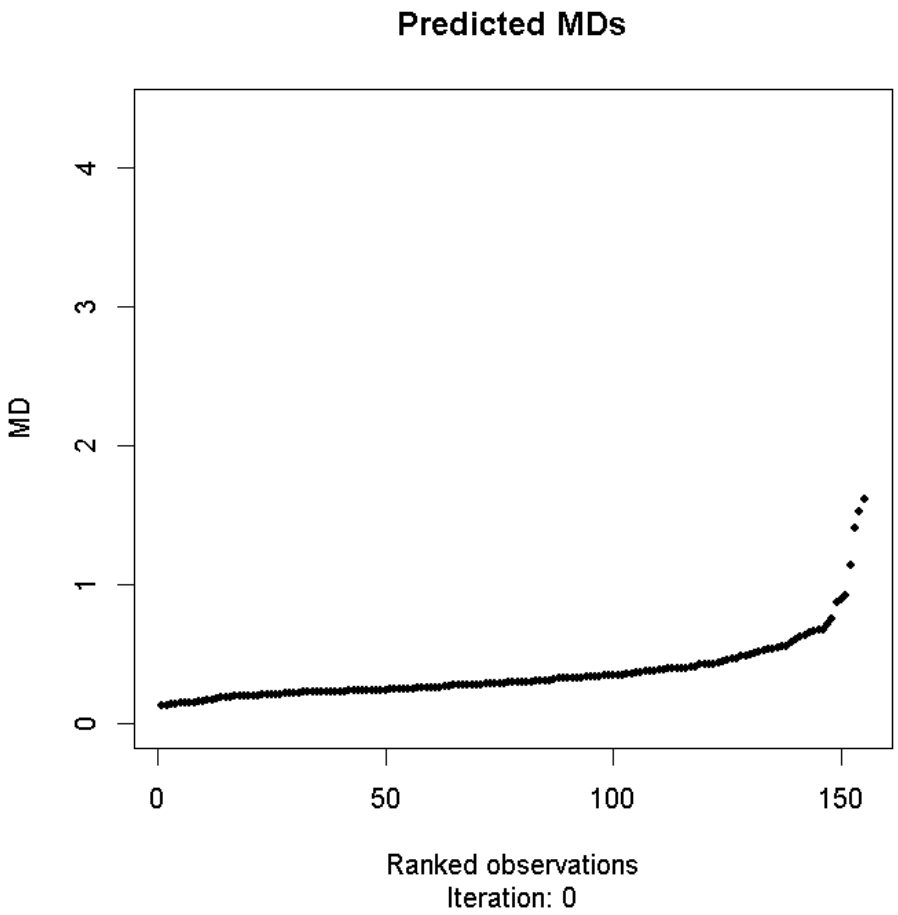
- $N = 1000$ iterations

Predicted MD distributions



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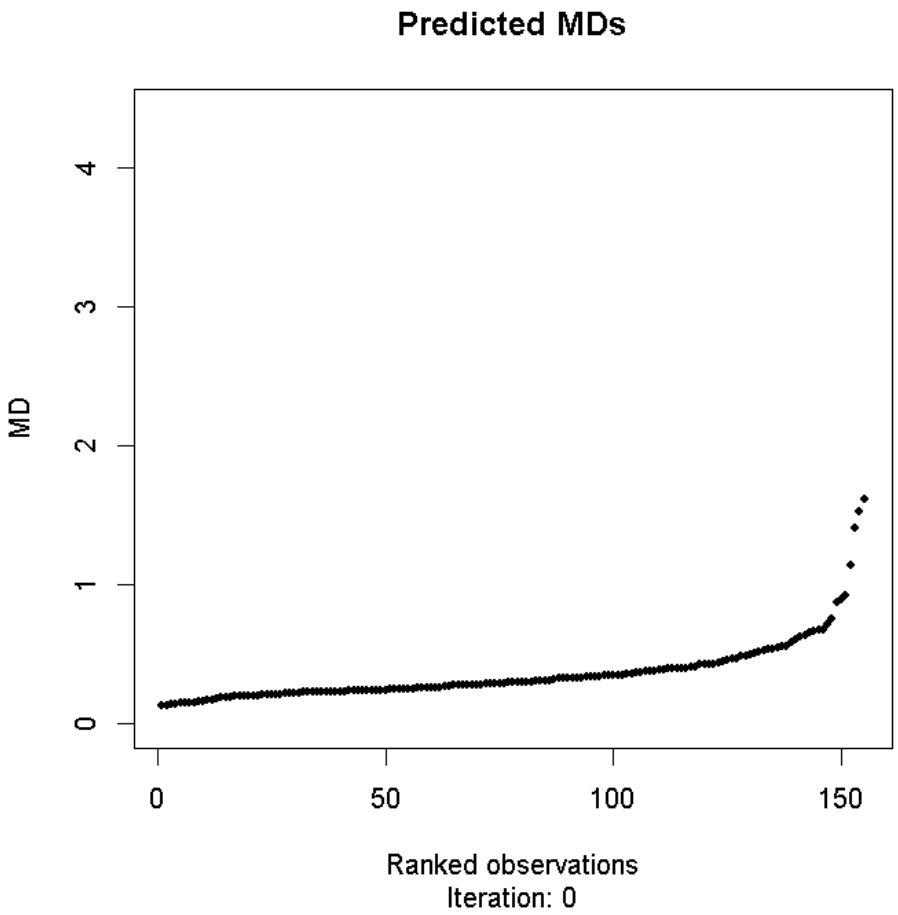
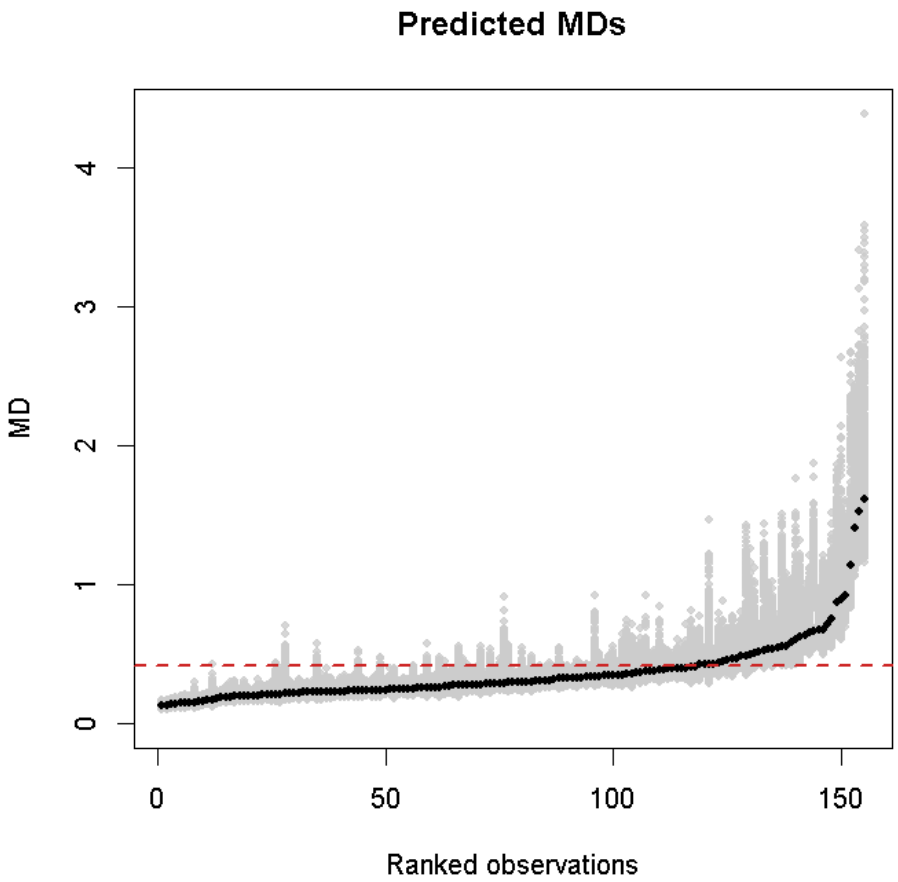
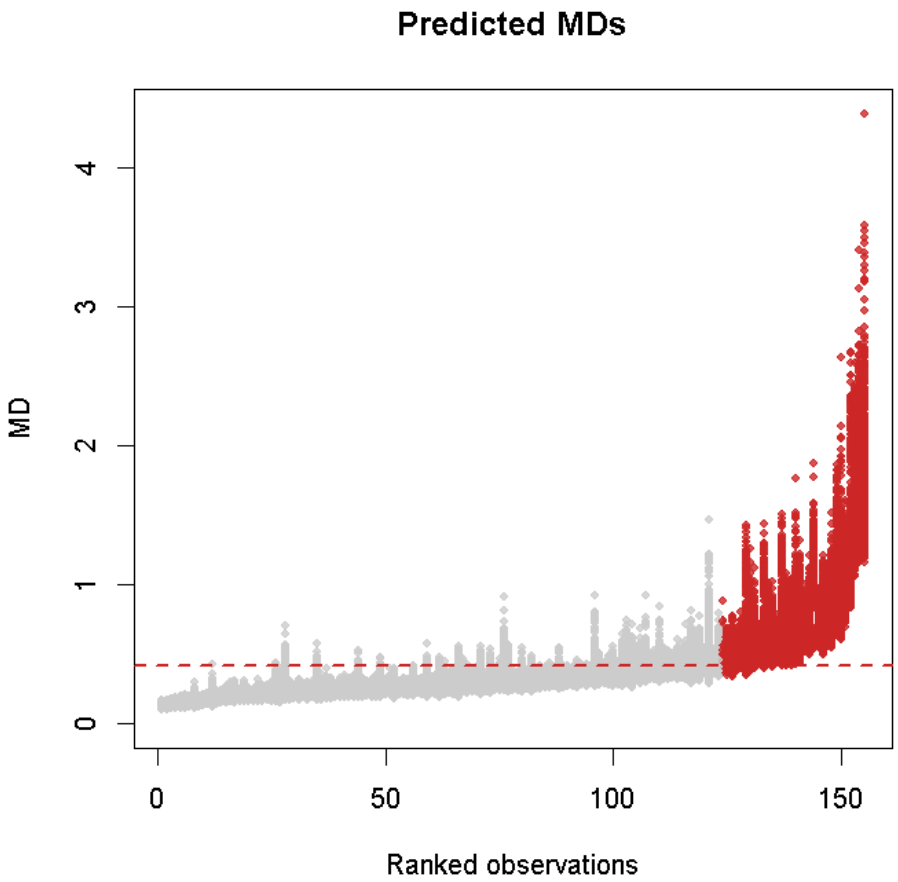


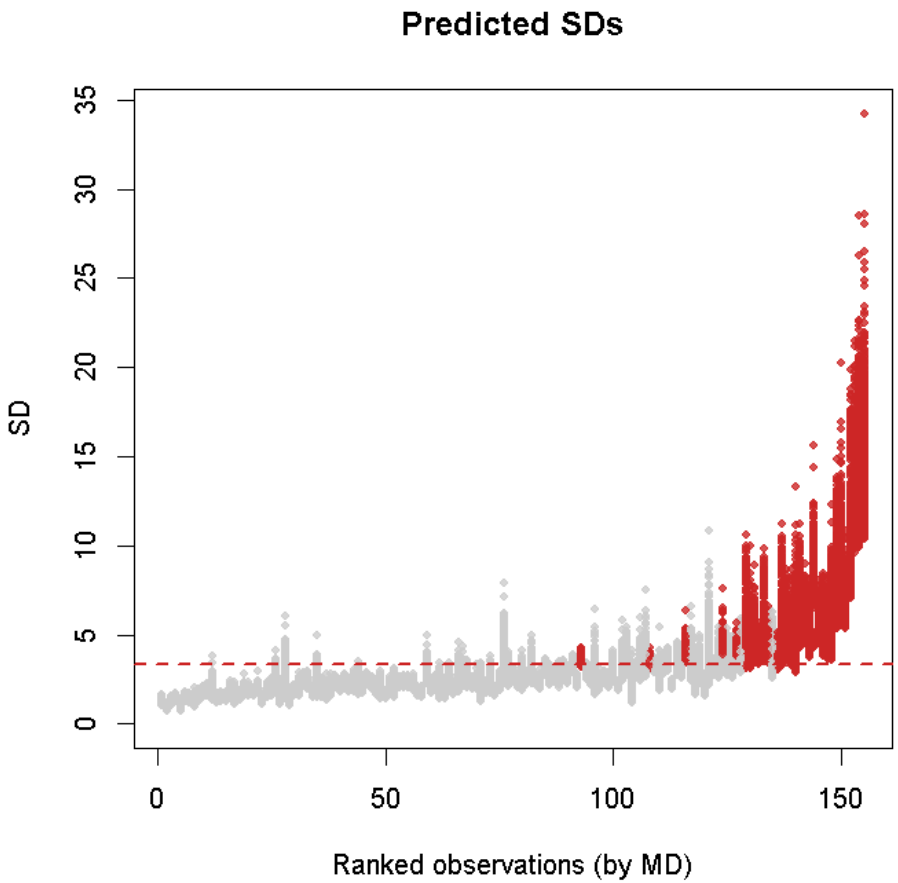
MD distribution threshold



Mahalanobis distribution outliers



Score distribution outliers



Reproducibility

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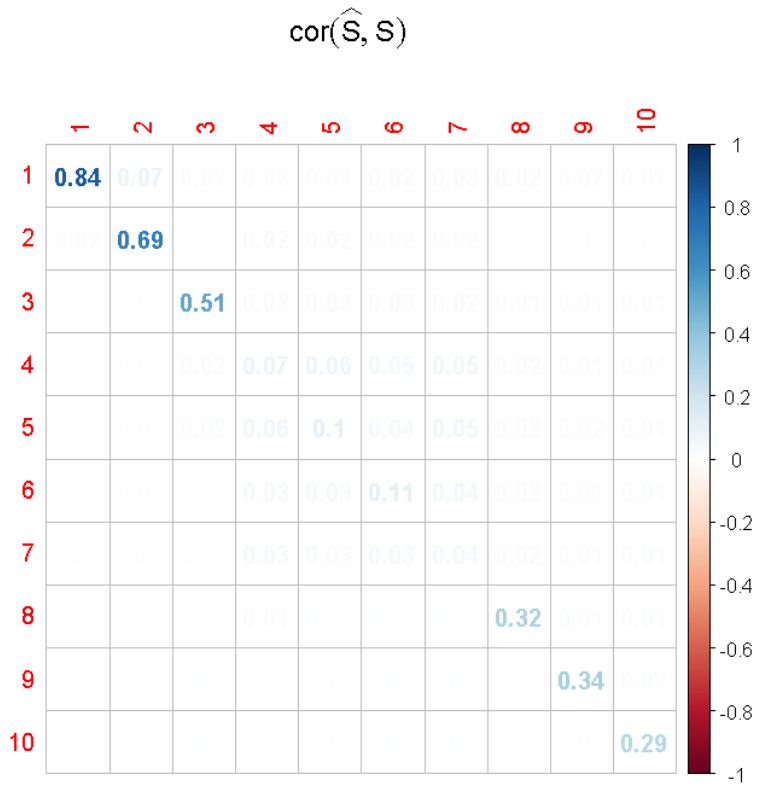

Median R^2 between split vectors and predicted vectors over 1000 iterations

Resampling

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

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  - $\mathbf{X}'$ - reconstructed from just first three components

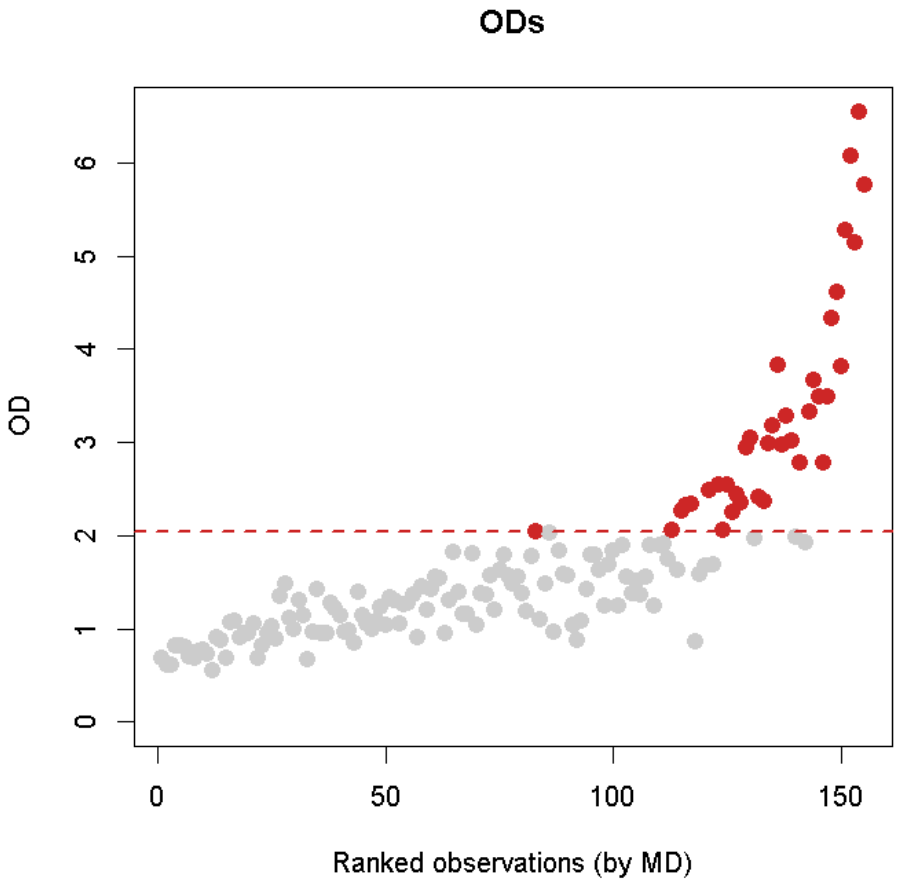
Resampling

- 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)

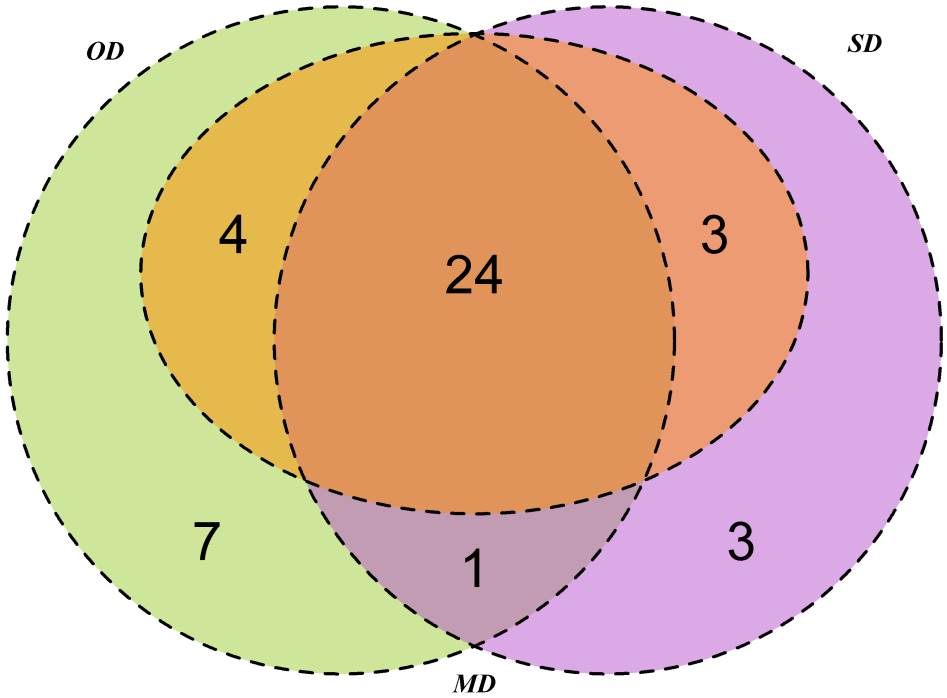
- Distance between observation and itself for $\mathbf{X}$ and robust $\mathbf{X}'$

Orthogonal distance outliers



Outliers

Outliers



$I = 161$, Outliers $= 42$.

Summary of PCA+SHR

- Build (predictive) distributions

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- Find a reproducible subspace

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

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  - Difficult to find robust subspaces
- PCA+SHR works the same regardless of size

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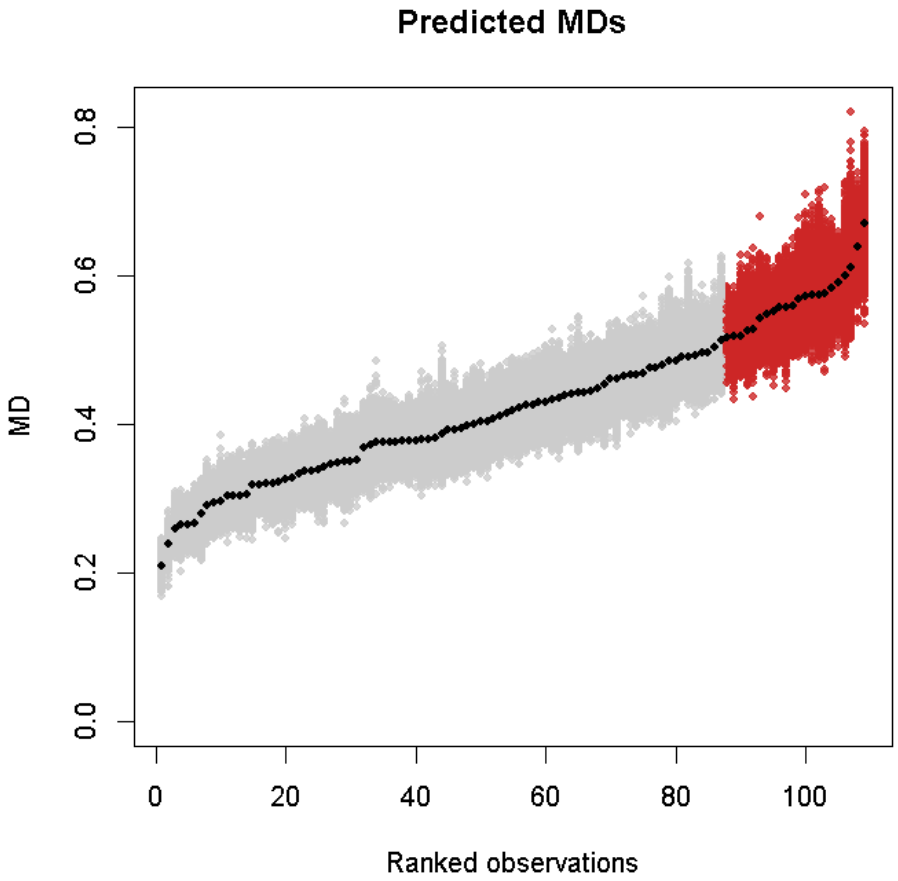
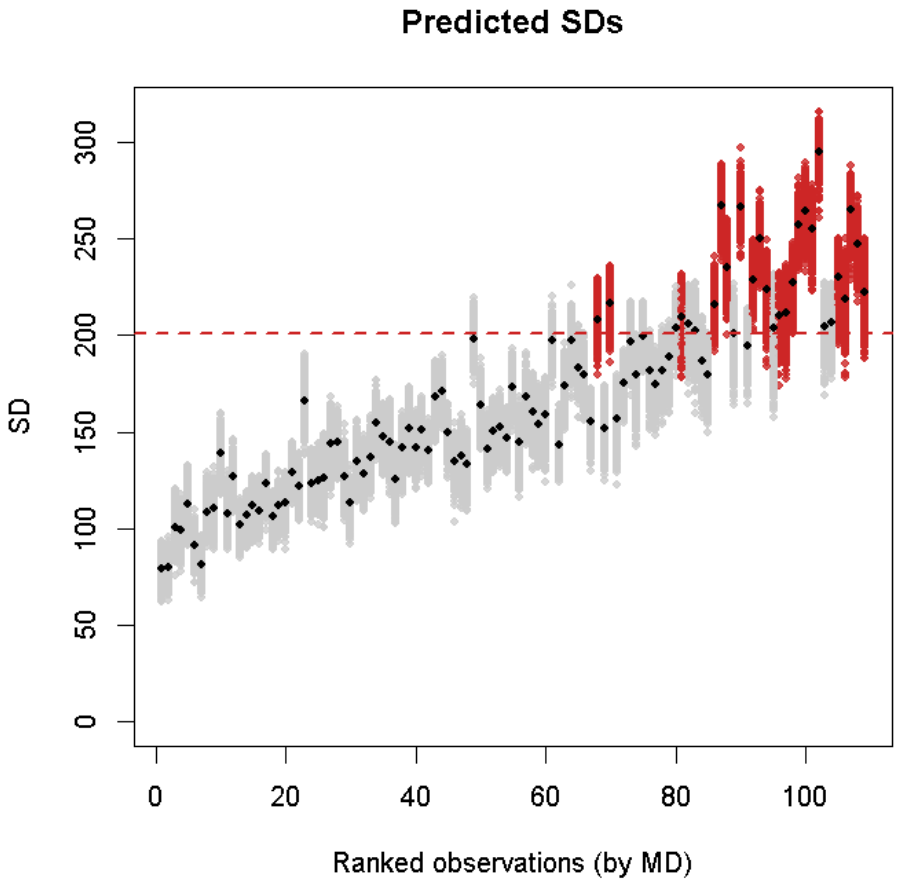
- $J = 32,768$ voxels per person
  - Resting state fMRI processed via OPPNI (Churchill et al., 2015)

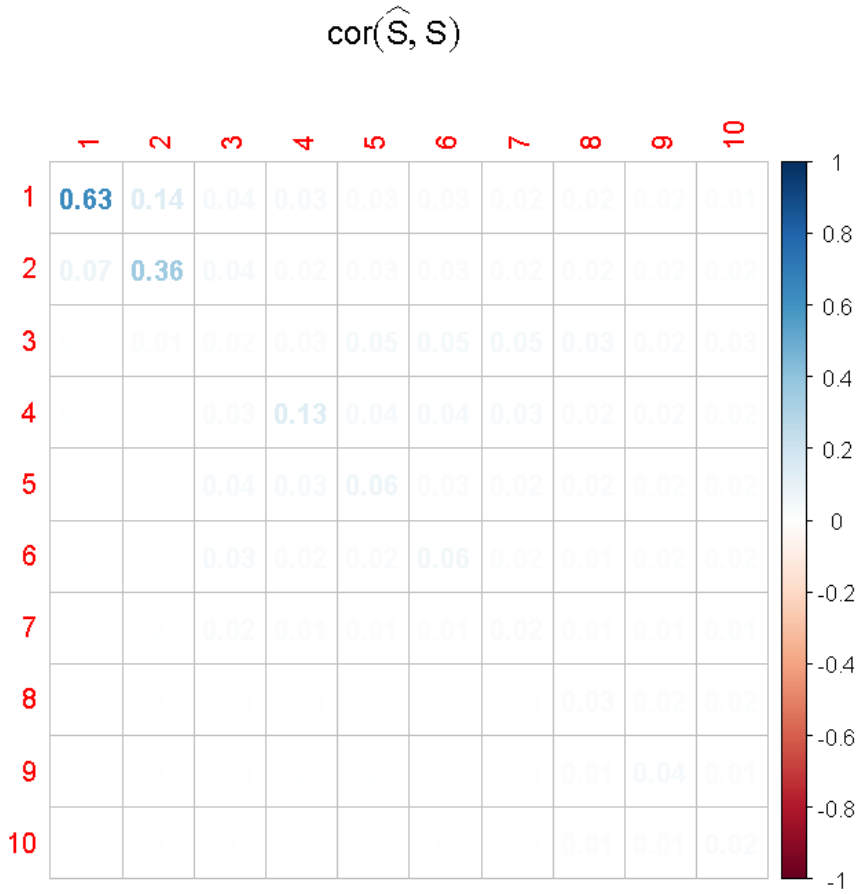
Outliers


Predicted MDs
MD
0.0
0.2
0.4
0.6
0.8
0
20
40
60
80
100
Ranked observations

Outliers

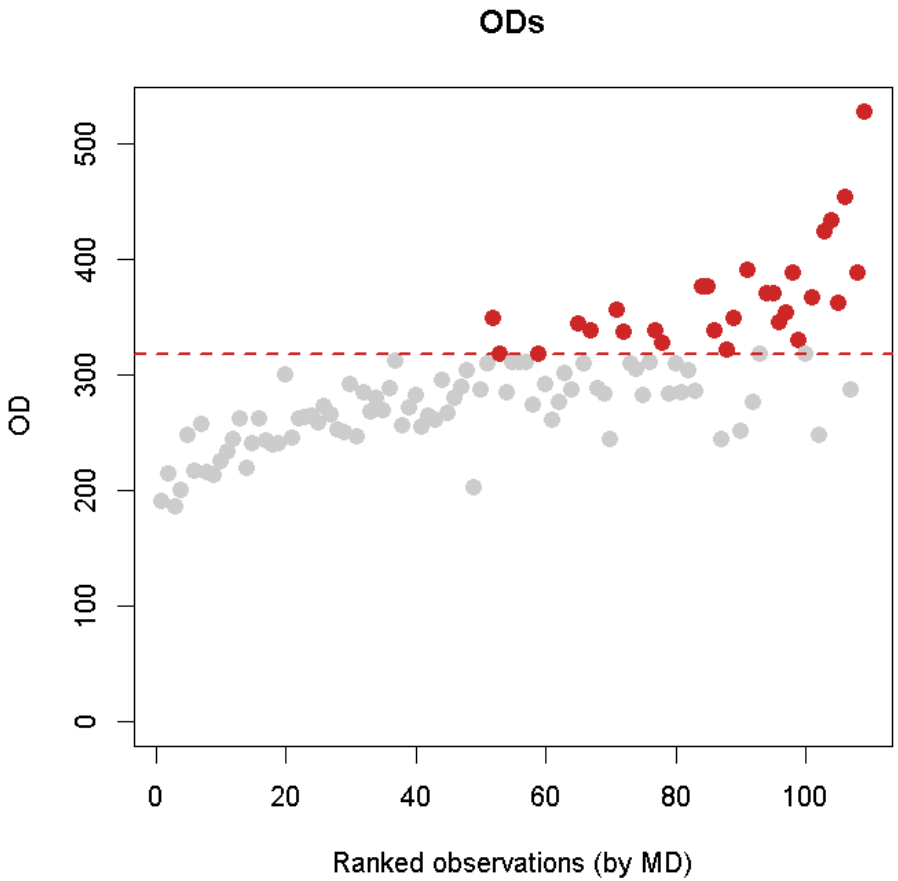

Predicted SDs
SD
0
50
100
150
200
250
300
0
20
40
60
80
100
Ranked observations (by MD)

Subspace



Only the first 10 of 108 Components shown

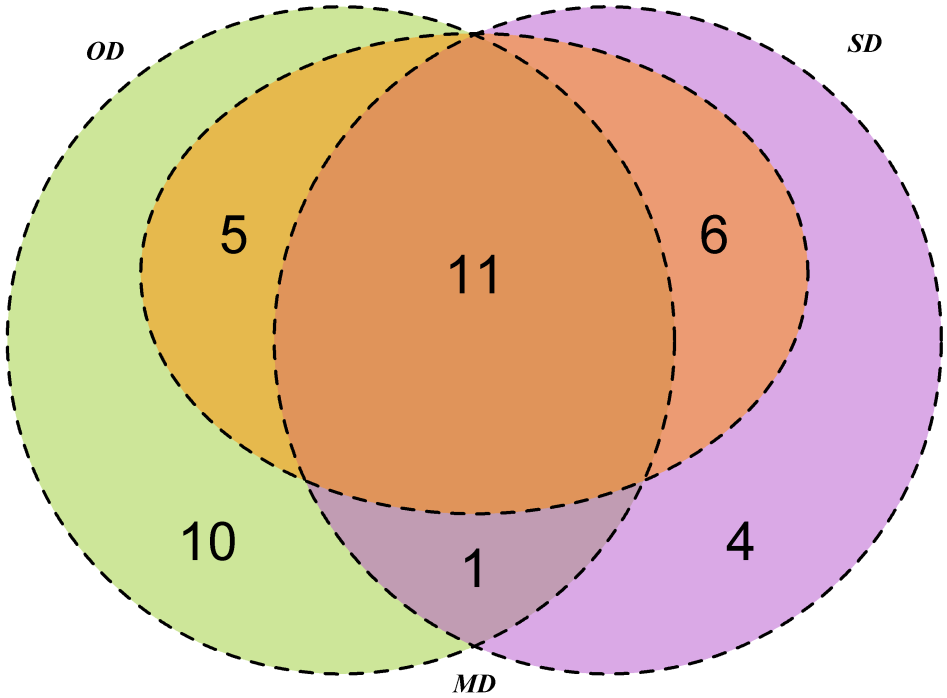
Outliers



OD computed from two components

Outliers

Outliers



$I = 109$, Outliers $= 37$.

4

Discussion

Conclusions

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  - High: Tends to intersect, find most outlying individuals
  - Low: Find most outlying & unique outliers to each type

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  - Most methods don't work for high dimensional/low sample size data
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  - Multiple distances, distributions to help make decisions

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  - Distributions, point, spread?
  - But we provide defaults in the software that work well
- Can be slow

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  - Continuous, categorical, ordinal, or mixed
  - Beaton et al., (2018) - extended MCD [1] to any data type

References

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- ONDRI Neuroinformatics & Biostatistics team will be in Montreal next week at **INCF: Neuroinformatics 2018**
  - More detailed explanation of outlier process (Sunderland et al., in prep)
  - Higher level overview of ONDRI curation-through-release pipeline

5

Bonus material

Notation

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- a - scalar

Notation

- a - scalar
- $\mathbf{a}$ - vector

Notation

- a - scalar
- $\mathbf{a}$ - vector
- $\mathbf{A}$ - matrix

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- a - scalar
- $\mathbf{a}$ - vector
- $\mathbf{A}$ - matrix
- $\mathbf{A}^T$ - transpose

Notation

- a - scalar
- $\mathbf{a}$ - vector
- $\mathbf{A}$ - matrix
- $\mathbf{A}^T$ - transpose
- $\mathbf{AB}$ - matrix multiplication

PCA

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The SVD of a matrix $\mathbf{X}$ of size $I \times J$ (at least column-wise centered, i.e., covariance)

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- Rank is L where $L \leq \min(I, J)$

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- $\mathbf{U}$ is $I \times L$ (left singular vectors; rows of $\mathbf{X}$)

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

Score distances

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

Score distances

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

- Sum of squared component (factor) scores

$$\mathbf{S} = \text{diag}\{(\mathbf{U\Delta})(\mathbf{U\Delta})^T\} = \text{diag}\{(\mathbf{XV})(\mathbf{XV})^T\} \qquad (2)$$

Score distances

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

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Score distances

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

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

$$\mathbf{S} = \mathrm{diag}\{(\mathbf{U\Delta})(\mathbf{U\Delta})^T\} = \mathrm{diag}\{(\mathbf{XV})(\mathbf{XV})^T\} \qquad (2)$$

Mahalanobis

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

Mahalanobis

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

- Sum of squared singular vectors

$$\begin{aligned}\mathbf{M} = \mathrm{diag}\{\mathbf{UU}^T\} = \mathrm{diag}\{(\mathbf{XV\Delta}^{-1})(\mathbf{XV\Delta}^{-1})^T\} \\ = \mathrm{diag}\{(\mathbf{S\Delta}^{-1})(\mathbf{S\Delta}^{-1})^T\}\end{aligned} \tag{3}$$

Mahalanobis

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

- Sum of squared singular vectors
- Can only be computed when not rank deficient

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Mahalanobis

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

- Sum of squared singular vectors
- Can only be computed when not rank deficient
  - if $I >> L$; when $I \leq L$, $\mathbf{M} = \mathbf{I}c$ where $c = L \times I^{-1}$

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- Can only be computed when not rank deficient
  - if $I >> L$; 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:

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

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Predicted MD:

$$\begin{aligned}\widehat{\mathbf{M}}_H &= \mathrm{diag}\{(\widehat{\mathbf{S}}_H\mathbf{\Delta}_{\bar{H}}^{-1})(\widehat{\mathbf{S}}_H\mathbf{\Delta}_{\bar{H}}^{-1})^T\} \\ \widehat{\mathbf{M}}_{\bar{H}} &= \mathrm{diag}\{(\widehat{\mathbf{S}}_{\bar{H}}\mathbf{\Delta}_H^{-1})(\widehat{\mathbf{S}}_{\bar{H}}\mathbf{\Delta}_H^{-1})^T\}\end{aligned} \tag{6}$$

Predicted distances

Predicted SD:

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

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Orthogonal distance

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

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  - $\mathbf{X}' = \mathbf{U}_{1:3}\mathbf{\Delta}_{1:3}\mathbf{V}_{1:3}^T$

Orthogonal distance

- 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:

$$\mathbf{O} = \| \mathbf{X} - \mathbf{X}' \| \tag{7}$$