Robust Outlier Detection

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

Derek Beaton

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

August 01, 2018

The other authors

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Acknowledgements

ONTARIO BRAIN INSTITUTE INSTITUT ONTARIEN DU CERVEAU

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Acknowledgements

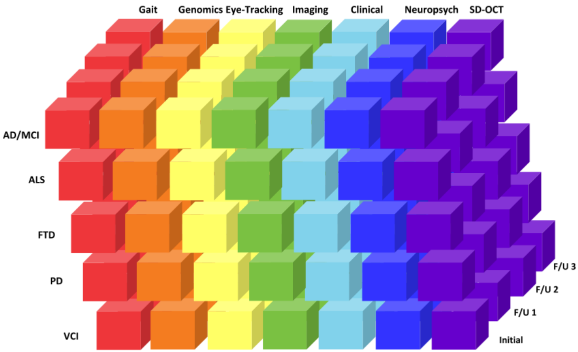
ONTARIO
NEURODEGENERATIVE
DISEASE RESEARCH
INITIATIVE

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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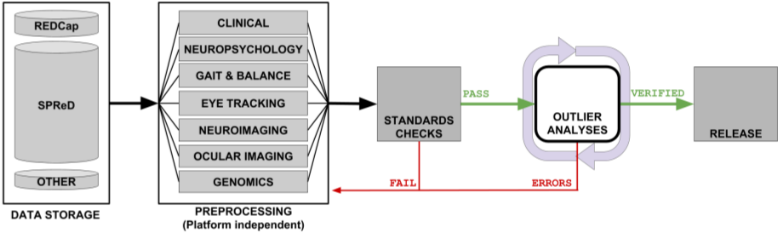
- Almost everything multivariate with varying complexities
- How to ensure data are of highest quality?

Outlier detection



The ONDRI preprocessing to release pipeline

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  - 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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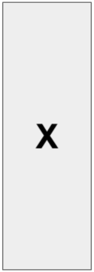
  - We'll bring these up later

PCA



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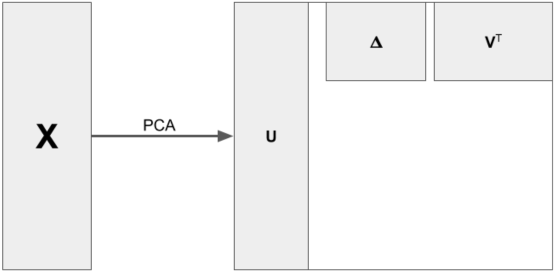

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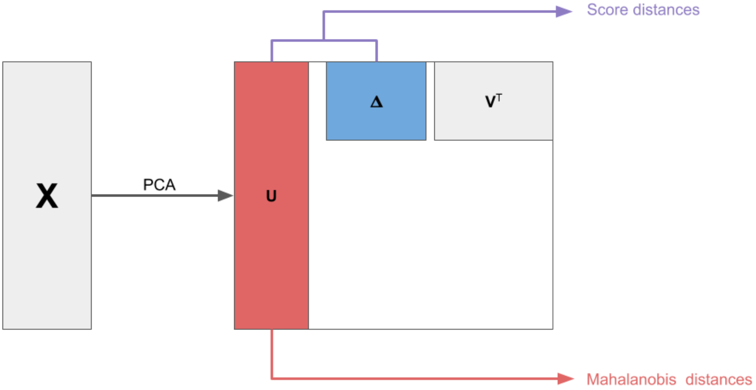
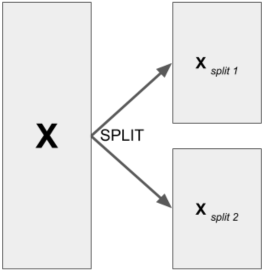


PCA


X
PCA
MAGIC EIGEN BOX
Score distances
Mahalanobis distances

Single split PCA



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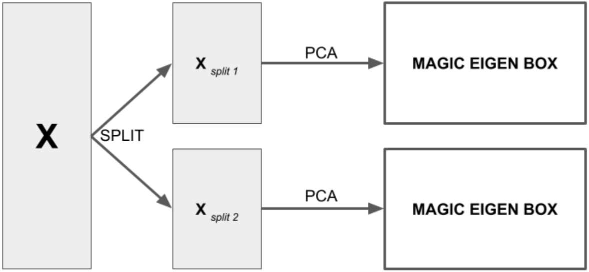

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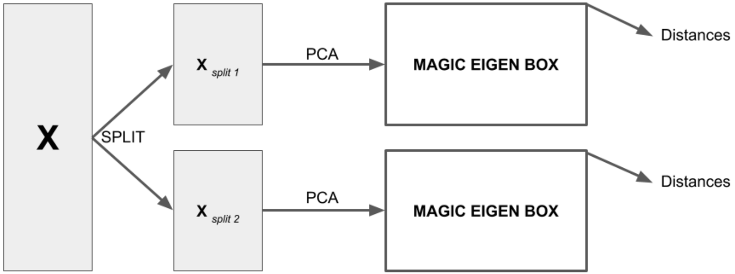
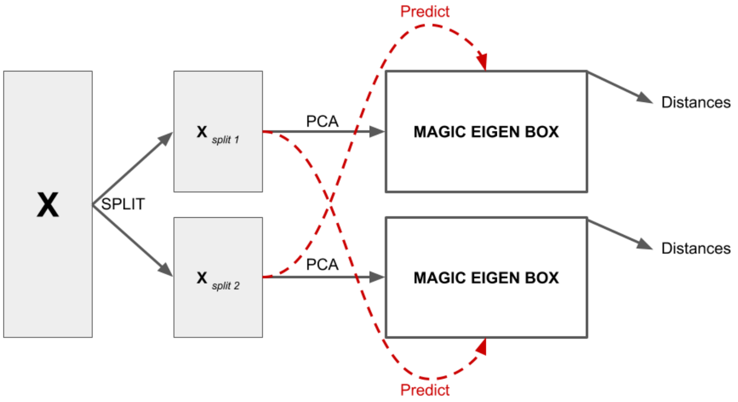


Prediction from split PCAs



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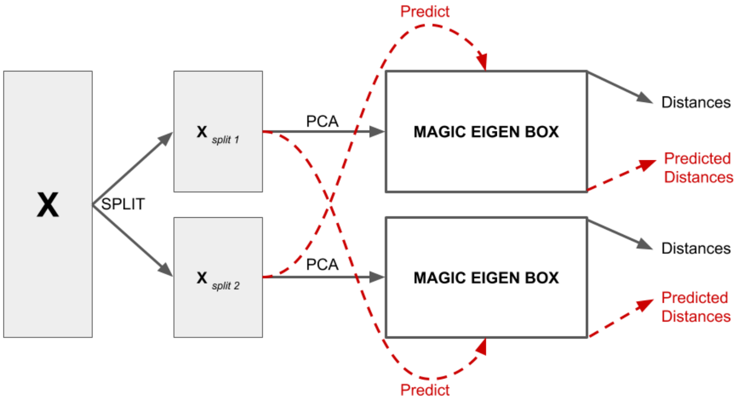

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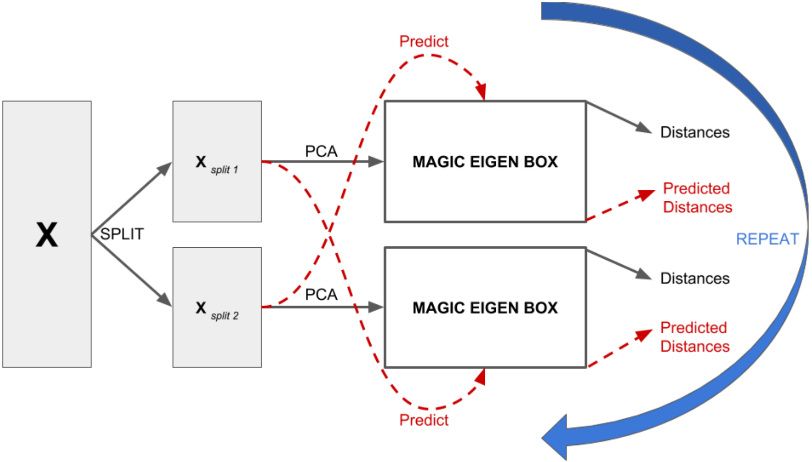
    - Some techniques (e.g., MCD [4], ROBPCA [5]) no longer work
    - **Predicted** distances can always be computed
- But: just one pass at split PCA is not enough

Resampling


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

PCA+SHR

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

3

PCA+SHR walkthrough

Data

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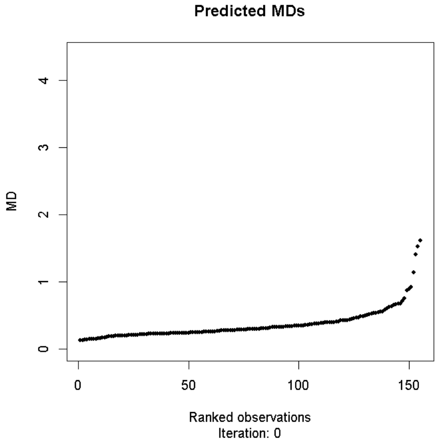
- $N = 1000$ iterations

Predicted MD distributions



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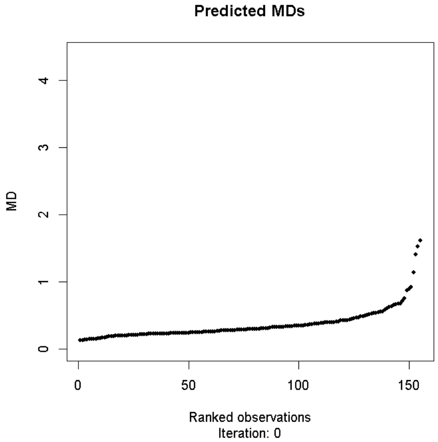
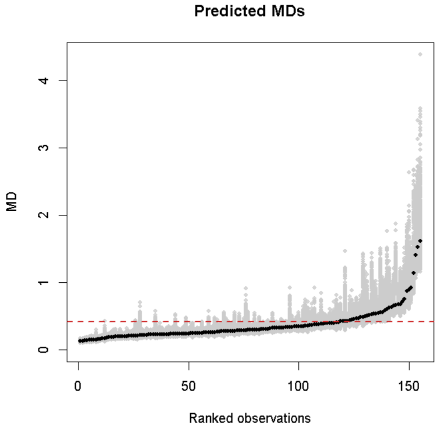
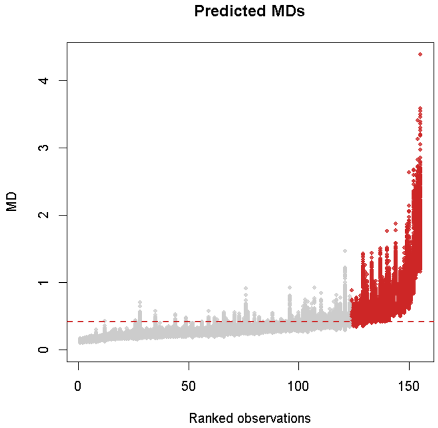


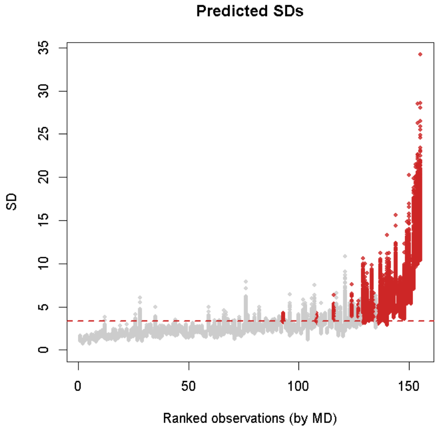
MD distribution threshold



Mahalanobis distribution outliers



Score distribution outliers



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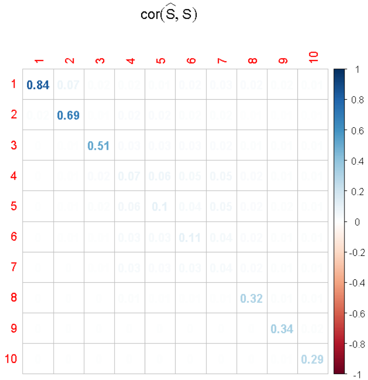
Reproducibility



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

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- We can use those to rebuild a robust version of $\mathbf{X}$:
  - $\mathbf{X}$ - original data
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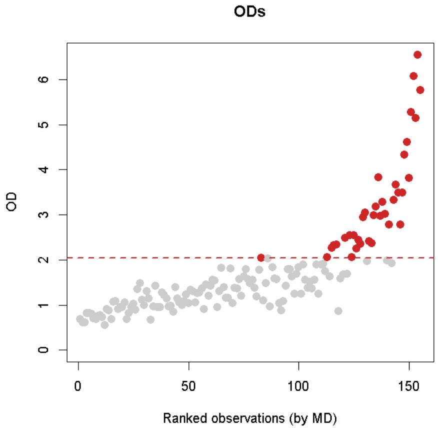
- How much do observations change between $\mathbf{X}$ and robust $\mathbf{X}'$?

Orthogonal distance (OD)

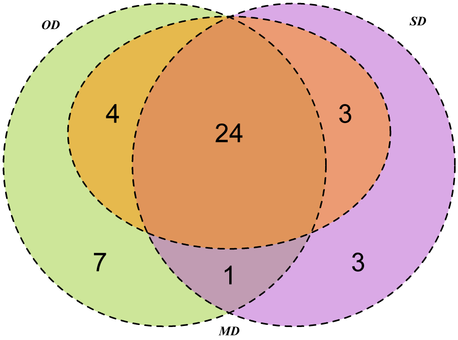
- Distance between observation and itself for $\mathbf{X}$ and robust $\mathbf{X}'$

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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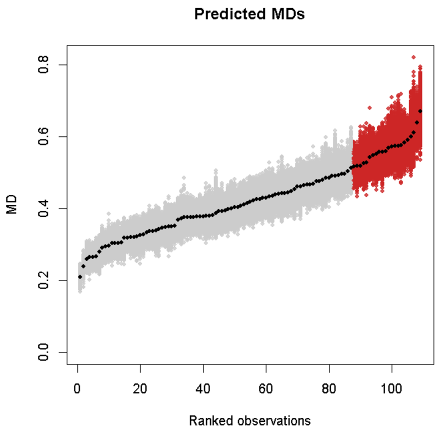
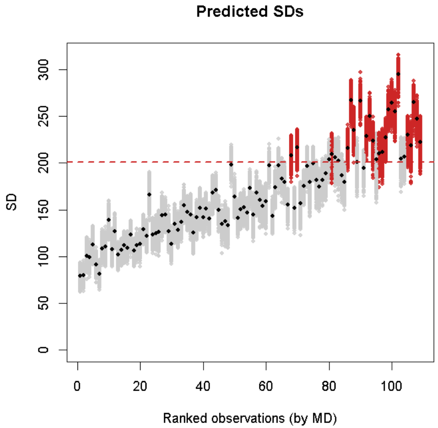
  - OPPNI pipeline (Churchill et al., 2015)

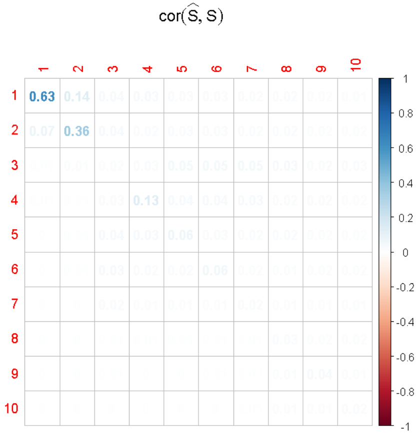
Outliers


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

Outliers

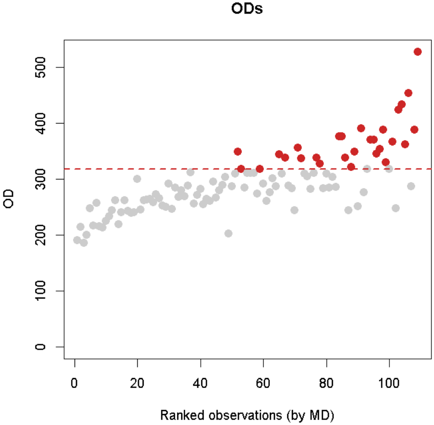

Predicted SDs
SD
0
50
100
150
200
250
300
0
20
40
60
80
100
Ranked observations (by MD)

Subspace



Only the first 10 of 108 Components shown

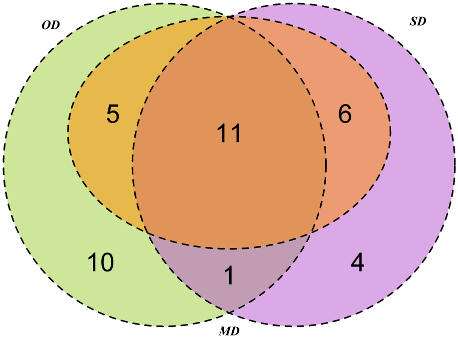
Outliers



OD computed from two components

Outliers

Outliers



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

4 Discussion

Conclusions

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

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  - Multiple distances, distributions to help make decisions

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- Can be slow

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

References

[1] Beaton, D., Sunderland, K. M., Levine, B., Mandzia, J., Masellis, M., Swartz, R. H., ... & Strother, S. C. (2018). Generalization of the minimum covariance determinant algorithm for categorical and mixed data types. bioRxiv, 333005.

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

5 Bonus material

PCA

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

PCA

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

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- $\mathbf{U}$ and $\mathbf{V}$ are orthonormal: $\mathbf{U^T U} = \mathbf{I} = \mathbf{V^T V}$

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Single split PCA

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

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

Predicted distances

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Predicted SD:

$$
\begin{aligned}
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- 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:

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