

Outliers App 0.10.2.9001 - Reference Guide

On behalf of the Neuroinformatics and Biostatistics (NIBS) Platform

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This reference guide helps you install and use the ONDRI Outliers App, with instructions on how to run the app, and some of the common errors while using the app.

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1 Overview

The purpose of this app is to help identify anomalous observations that may require additional checks or verification by data curators. We use a combination of techniques: (1) ordination, which is principal components analysis (PCA) and correspondence analysis (CA), (2) minimum covariance determinant (MCD) and a generalized MCD, (3) the Garthwaite-Koch partition, a.k.a. “CorrMax” transformation and a generalized CorrMax, as well as (4) resampling (bootstrap) to help assess and identify anomalies. For more details see Beaton et al. (2019) and Sunderland et al. (2019).

2 Installation and Deployment

1. Install R first and then RStudio. Please choose the correct installer carefully as it will depend on your computer’s operating system.

2. Install the `GSVD` and `ours` packages (which are not available through CRAN) with the following lines of code:

```
if (!require("devtools")){
  install.packages("devtools")
}

if (!require("GSVD")){
  Sys.setenv(R_REMOTES_NO_ERRORS_FROM_WARNINGS = TRUE)
  devtools::install_github("derekbeaton/GSVD")
}
if (!require("ours")){
  Sys.setenv(R_REMOTES_NO_ERRORS_FROM_WARNINGS = TRUE)
  devtools::install_github("derekbeaton/OuRS", subdir = "/OuRS")
}
```

3. Download and install the shiny app directly with the following lines of code:

```
if (!require("devtools")){
  install.packages("devtools")
}
devtools::install_github(repo = "ondri-nibs/outliers_app")
```

4. Type `ONDRIOutliersApp::installPackages()` to install any missing packages and/or dependencies. If you get the following message in your RStudio console, please type 3.
5. When installation is complete, type `ONDRIOutliersApp::runApp()` to open the app.

```
These packages have more recent versions available.  
It is recommended to update all of them.  
Which would you like to update?
```

```
1: All  
2: CRAN packages only  
3: None
```

Figure 1: This message may appear multiple times during the installation process.

3 How to Use

To start, load your data into your RStudio environment as a numeric matrix making sure there are no non-numeric values or NA within your data.

```
# Read our data into a data.frame  
ONDRI_synthetic_dataset <- read.csv("baycrest/datapacks/synth_data/JUL26/  
                                     OND01_ALL_01_NIBS_SYNTHDATA_2020JUL26_DATA.csv")  
  
# Make sure there are no NAs in your data. This should be integer(0).  
which(sapply(ONDRI_synthetic_dataset, is.na))  
  
# Make sure all these values are TRUE for variables you are including  
lapply(ONDRI_synthetic_dataset, is.numeric)  
  
# ...  
  
# Convert data frame into matrix  
ONDRI_synth_num_matrix <- as.matrix(ONDRI_synthetic_dataset_prepped)
```

Once again, your data must be a numeric *matrix* and not a data frame after you make sure there are no NA or non-numeric values.

3.1 Step 1: Data and Document Parameters

Select your data in the Step 1 sidebar, then select *Strictly continuous* if all of your columns are continuous, otherwise select *Non-continuous*. **NOTE:** data must be prepared in advance to make sure that they are appropriately transformed and ready for analyses in either pipeline. Please make sure to see the **DataPrep** app, as well as many of the utilities in the **OuRS** package.

If you are generating a report, set the title, subtitle, and author of your report and select the folder which the report files will be saved to. You may also choose a random seed for the bootstrapping procedure. Then, click the next button.

After choosing your data, you can view a scaled visualization of your data matrix in the *Heatmap* tab. You can zoom in by clicking and drawing a rectangle with the mouse to see subjects that may be omitted at a large scale. You can also double-click to zoom back out.

3.2 Step 2 & 3: Ordination & MCD

In this stage, we choose the parameters for the bootstrapping and MCD.

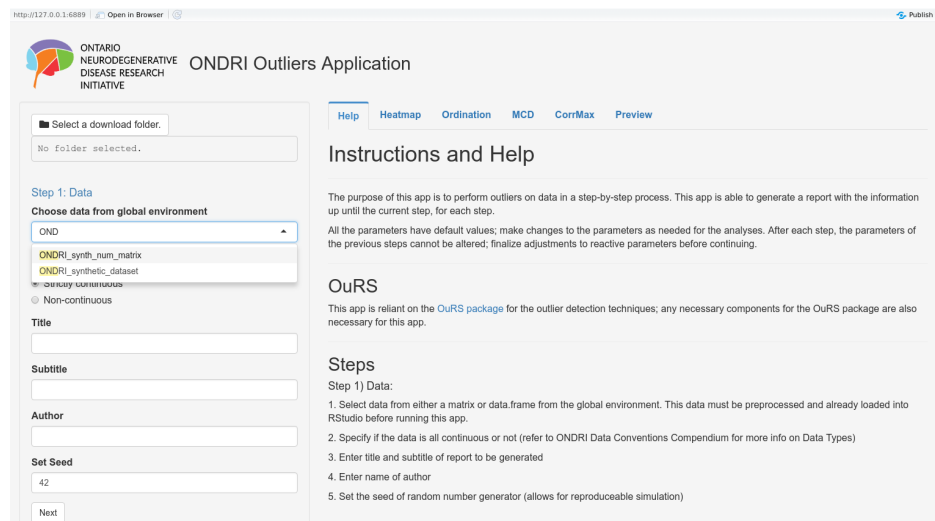


Figure 2: All output from the app will be added to the download folder selected.

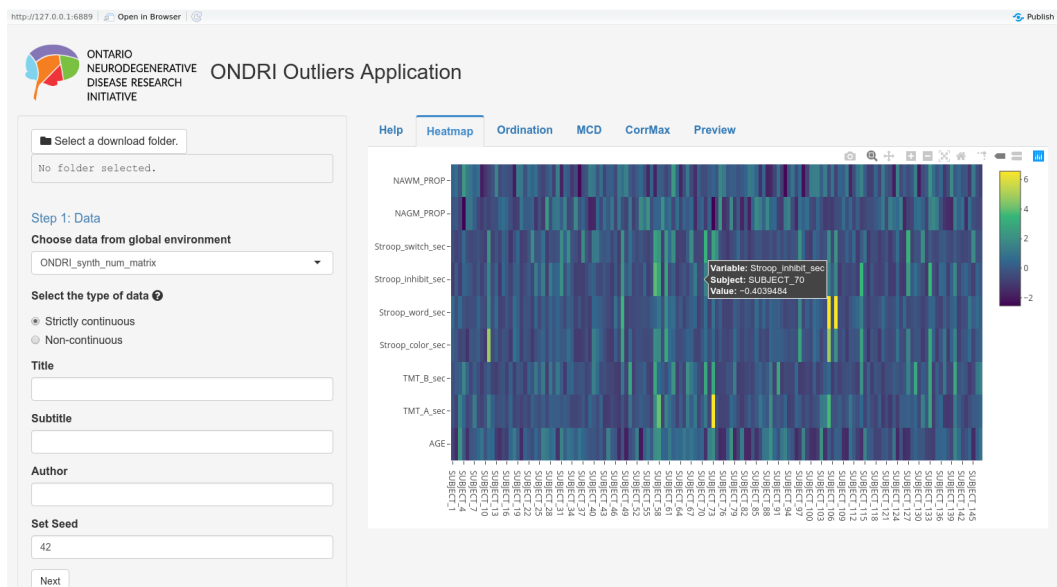


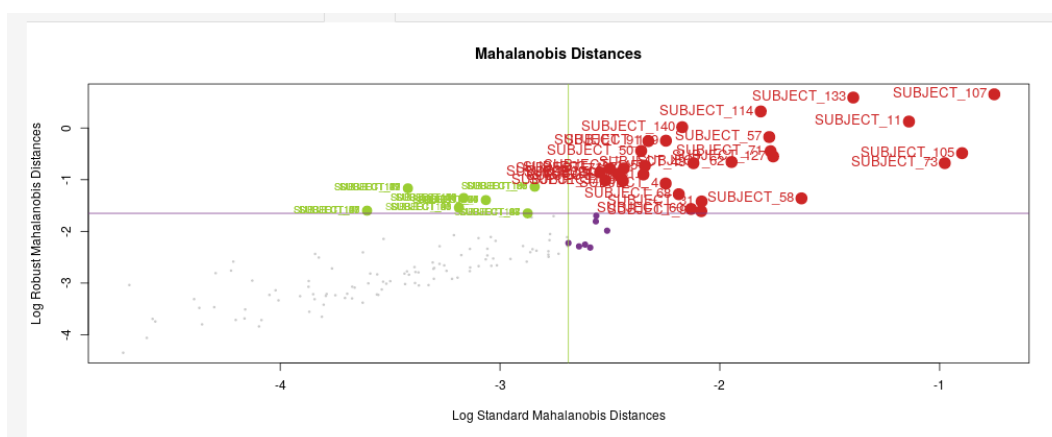
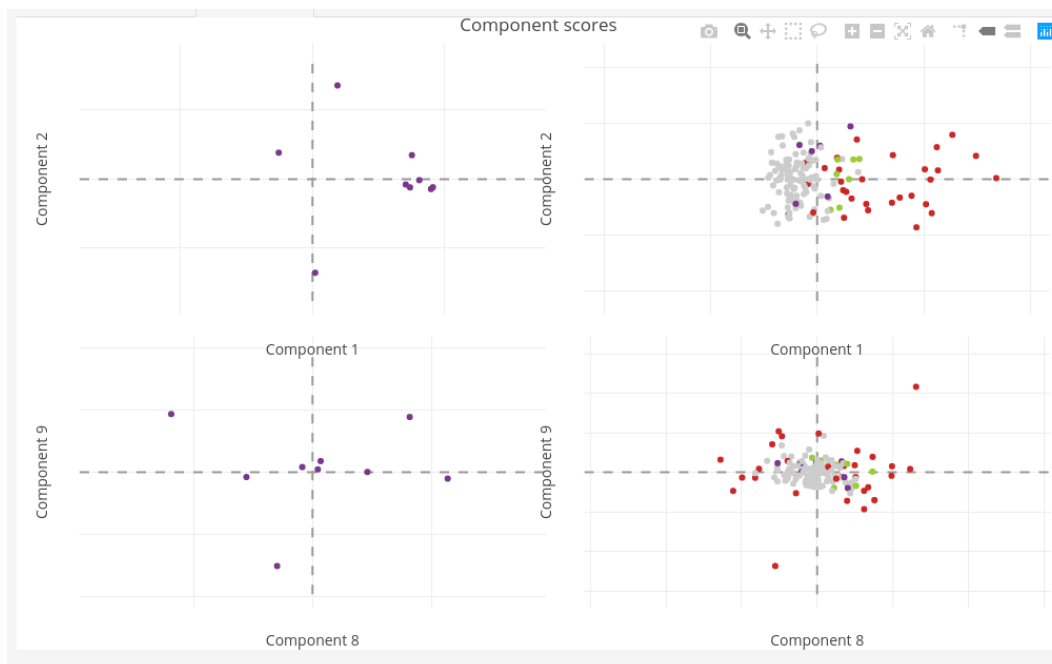
Figure 3: Heatmap tab.

The screenshot shows the ONDRI Outliers Application interface. At the top, there is a logo for the Ontario Neurodegenerative Disease Research Initiative and the title "ONDRI Outliers Application". Below the logo, there is a section for selecting a download folder, which currently shows "No folder selected.". To the right of this section, there are tabs for "Help", "Heatmap", "Ordination", "MCD", "CorrMax", and "Preview". The "Ordination" tab is currently selected. Below the tabs, there is a message: "Finish Step #2 to display ordination results.". The main area of the interface is titled "Steps 2 & 3: Ordination & MCD". It contains several sliders and input fields for parameter selection: "Standard Bootstrap Cutoff" (ranging from 0.5 to 0.99, with a value of 0.75 selected), "Robust Bootstrap Cutoff" (ranging from 0.5 to 0.99, with a value of 0.75 selected), "Alpha Level" (ranging from 0.5 to 0.9, with a value of 0.75 selected), "Bootstrap Iterations" (input field with the value 500), and "Outlier Iterations" (input field with the value 500). A "Next" button is located at the bottom of the parameter selection area.

Figure 4: Selection of parameters prior to ordination.

- *Alpha Level*: Alpha value used to compute sample size for MCD.
- *Outlier Iterations*: Number of subsets for MCD.
- *Bootstrap Iterations*: Number of samples in bootstrapping.
- *Standard Bootstrap Cutoff*: Cutoff for Mahalanobis distances in MCD plot which determines which subjects are flagged as outliers.
- *Robust Bootstrap Cutoff*: Cutoff for Robust Mahalanobis distances in MCD plot which determines which subjects are flagged as outliers.

After accepting these fields, two plots should render in the *Ordination* and *MCD* tab respectively. The left side of the Ordination plot contains the component scores of the variables and the right side contains the scores of the the subjects. The top two plots are plotted on the top two components (i.e. the ones explaining the most amount of the variance) and the bottom two plots are plotted with the last two components (i.e. the ones explaining the least amount of the variance). The MCD plot shows the standard and robust Mahalanobis distances of each subject and the bootstrap cutoffs on a log scale. After the MCD plot is rendered, the subjects on the Ordination plot will be coloured with the results of the MCD plot.



3.3 Step 4: CorrMax

After Step 4 input is accepted, the *CorrMax* tab will show a heatmap of percentage contributions of the points flagged corresponding to the MCD plot. Like in the Heatmap tab, you can hover the cursor over the heatmap to see these values. You can also adjust the CorrMax threshold which will adjust the percentage at which a subject-variable pair will be displayed as non-zero in the CorrMax plot.

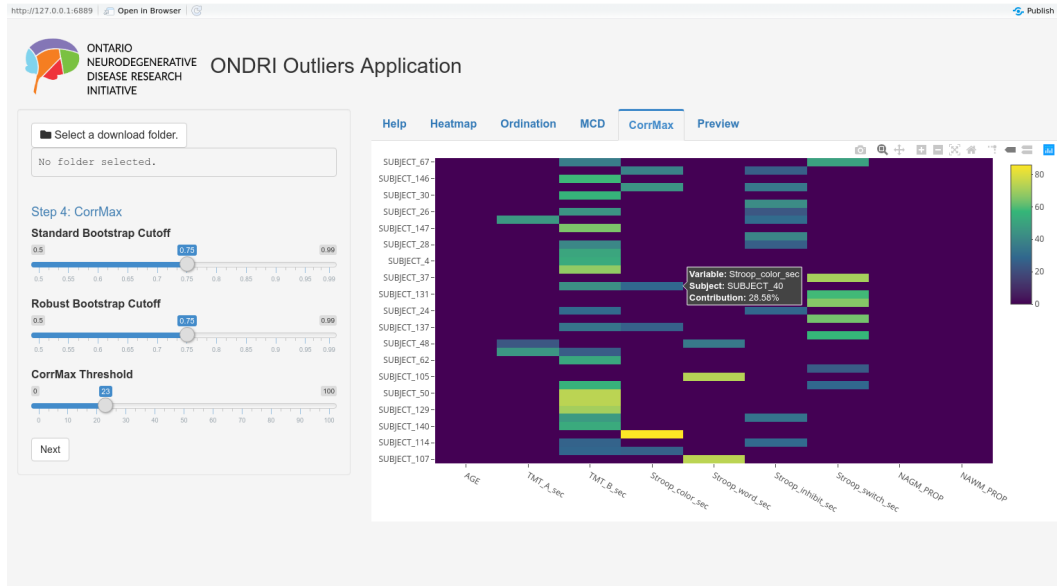


Figure 7: CorrMax tab.

3.4 Generate Report

After the four steps are completed you can click the Generate Report button to create a PDF of the results, including the plots shown in Ordination, MCD, and CorrMax. You can preview the report at any time by visiting the *Preview* tab, but note that if a step has not yet been completed, the plots will not show in the preview.

Note if you have not yet viewed the MCD tab, the program will first take you to it when you hit the ‘Generate Report’ button. Then you will have to press the button again to generate the report. This is because in order to fully run the lazy-evaluated shiny processes in the MCD stage, it is required that the MCD plot be rendered by the user.

4 Common Errors

4.1 Including non-numeric values in your data or NAs

You might receive the “‘x’ must be numeric” error or the ‘non-numeric argument to a mathematical function’ error.

Often, values that look like numbers in a data frame can be character vectors. To check that your entries are numeric, you can use

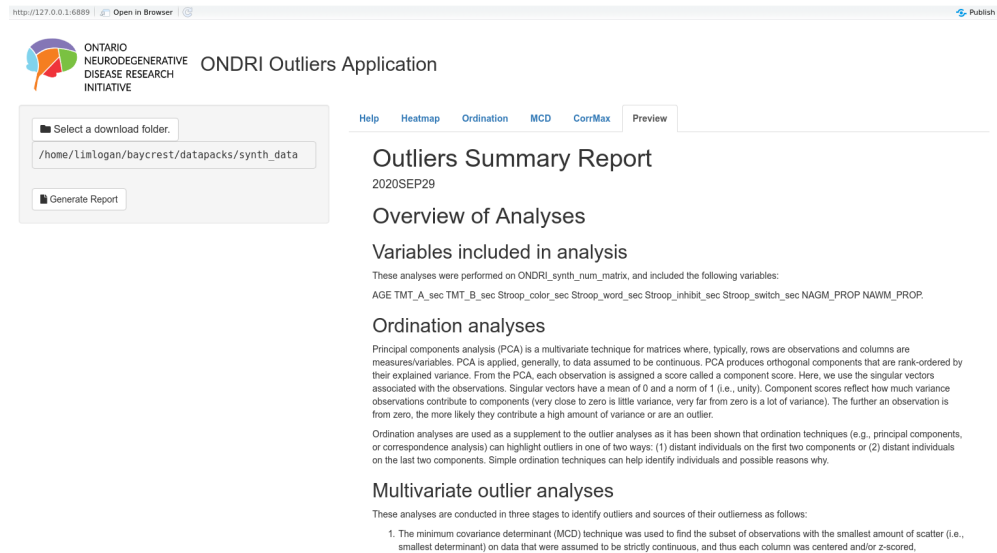


Figure 8: Report preview.

```
which(!sapply(mydata, is.numeric))
```

to see all non-numeric entries in your matrix. To find NA's, you can use

```
which(sapply(mydata, is.na))
```

4.2 Using a data.frame object instead of a matrix as data

This can cause a few problems with the internal mathematical functions that take matrices. Using a data.frame object as your data is not recommended or supported at this time.

To check if your object is a matrix or data.frame, use:

```
class(mydata)
```

To convert a data.frame to a matrix, you can use:

```
my_matrix <- as.matrix(mydata)
```

You can also view the object in RStudio to make sure your new object has the correct rows, columns and values:

```
View(my_matrix)
```

4.3 Using data that is too wide

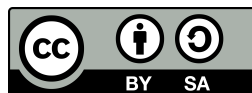
If your data does not satisfy


```
nrow(data()) < ceiling(ncol(data())*.9)
```

then you will not be able to continue with the outlier detection process and may instead be given the 'Data is too wide' message.

5 References

- Beaton, D., Sunderland, K. M., Levine, B., Mandzia, J., Masellis, M., Swartz, R. H., Troyer, A. K., Binns, M. A., Abdi, H., & Strother, S. C. (2019). Generalization of the minimum covariance determinant algorithm for categorical and mixed data types. *bioRxiv*. <https://doi.org/10.1101/333005>
- Garthwaite, P. H., & Koch, I. (2016). Evaluating the contributions of individual variables to a quadratic form. *Australian & New Zealand Journal of Statistics*, 58(1), 99–119.
- Hubert, M., & Debruyne, M. (2010). Minimum covariance determinant. *Wiley Interdisciplinary Reviews: Computational Statistics*, 2(1), 36–43.
- Sunderland, K. M., Beaton, D., Fraser, J., Kwan, D., McLaughlin, P. M., Montero-Odasso, M., Peltsch, A. J., Pieruccini-Faria, F., Sahlas, D. J., Swartz, R. H., & others. (2019). The utility of multivariate outlier detection techniques for data quality evaluation in large studies: An application within the ONDRI project. *BMC Medical Research Methodology*, 19(1), 1–16.



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