Unveiling Patterns in High Dimensions:

AI/ML Innovations in Multivariate Analysis, Dimension Reduction, and Clustering

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AI/ML Applications in Astronomy and Astrophysics,
10th January 2025

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Introduction

Astronomical data, from any domain, is usually available in forms:

- High dimensions: An increase in dimension reduces the data visibility, increases sparsity and computational complexity.
- Presence of outlying observations and their proper detection.
- Presence of missing values
- Presence of '0' values

- All these issues increases manifold with increase in the data size, and without proper handling of which, it may cause serious problems in the modeling and inference.

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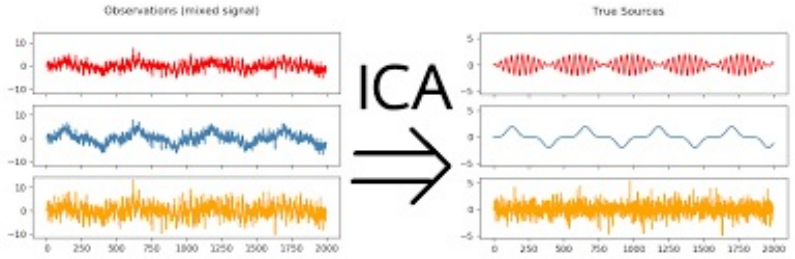
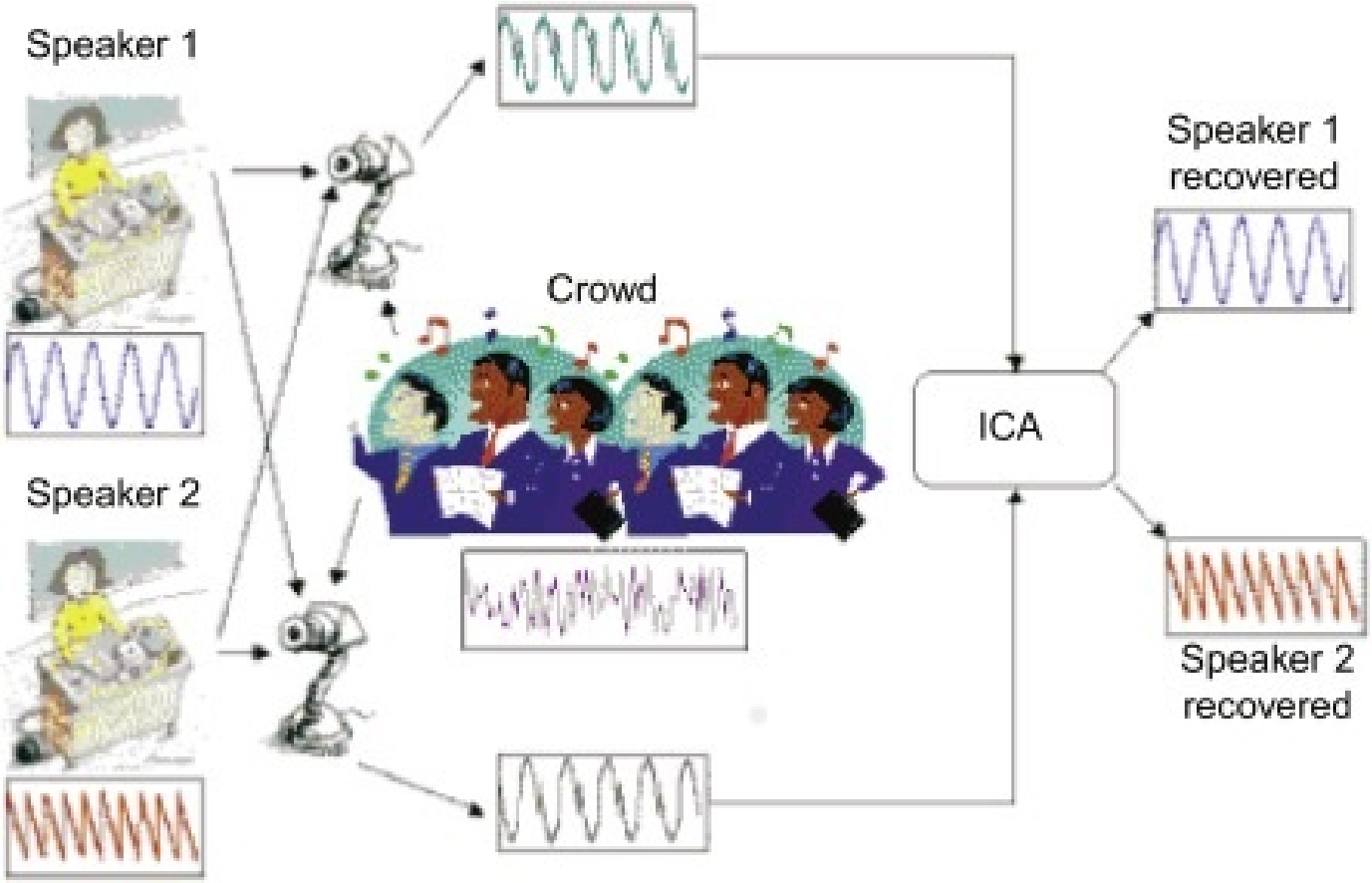
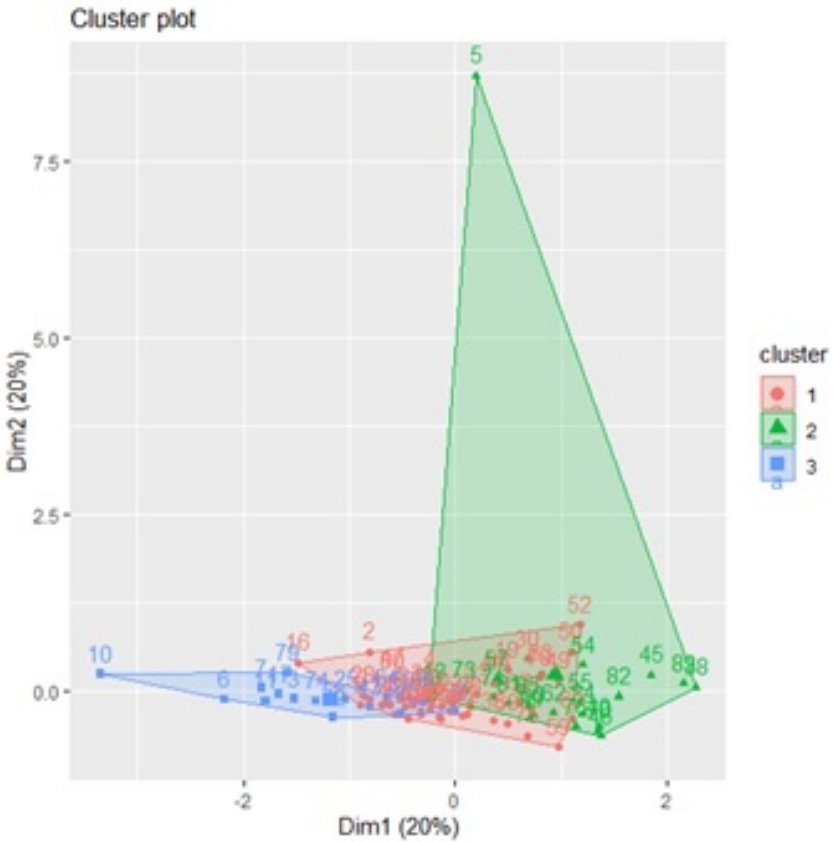
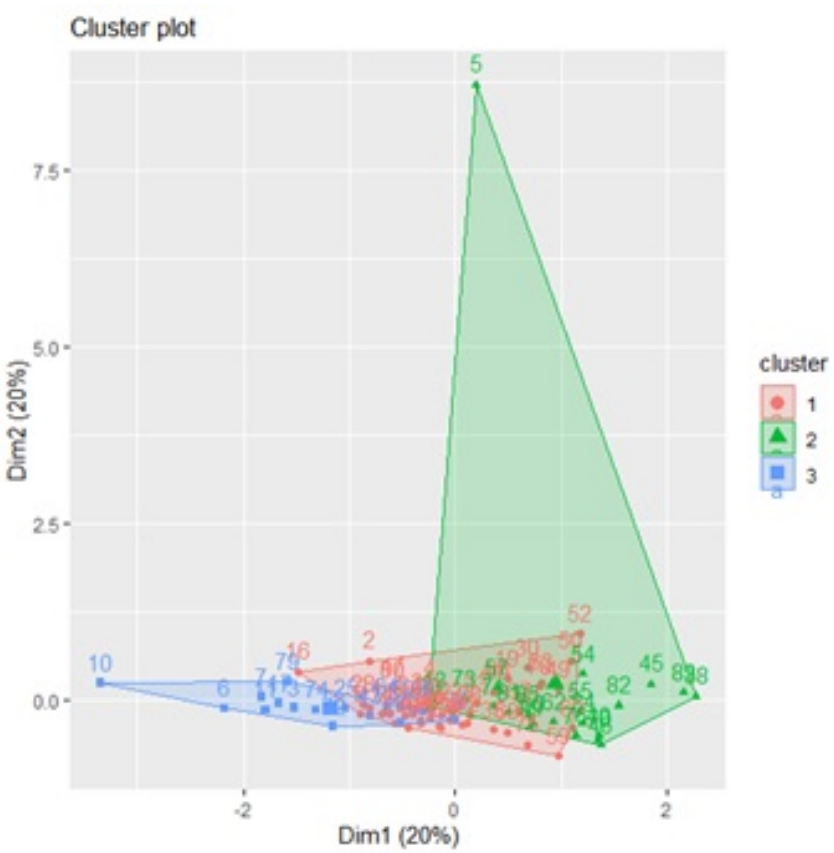
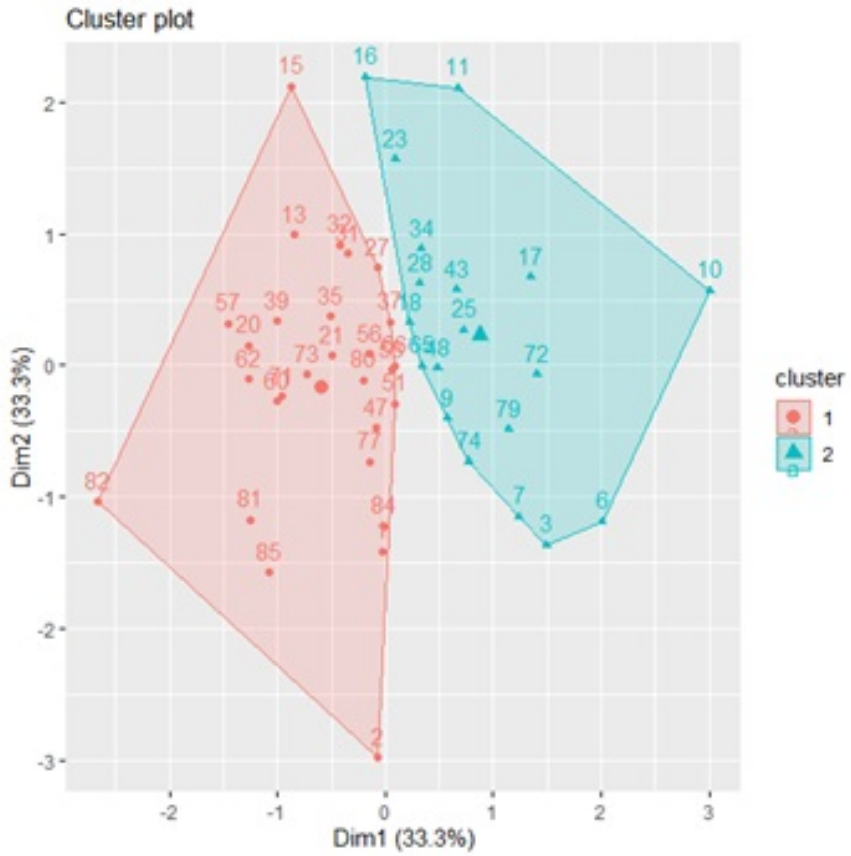


ICA


Speaker 1
Speaker 2
Crowd
ICA
Speaker 1
recovered
Speaker 2
recovered


Cluster plot
Dim2 (20%)
Dim1 (20%)
7.5
5.0
2.5
0.0
-2
0
2
cluster
1
2
3


Cluster plot
Dim2 (20%)
Dim1 (20%)
cluster
1
2
3


Cluster plot
Dim2 (33.3%)
Dim1 (33.3%)
cluster
1
2

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Outlier may be defined as those data point which differs *significantly* from other observations.
There are various tools available in Statistics/ ML for outlier detection.

Robust PCA

Without prior detection and even removal of outliers, the Robust PCA is a better option than the conventional PCA or ICA. If the data is represented in form of $n \times p$ matrix with n being the number of objects and p being the original number of variables, $p \geq n$, the ROBPCA method involves both the methods of projection pursuit and robust estimation.

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In the final step, the scatter matrix of the data points is estimated using the MCD estimator.

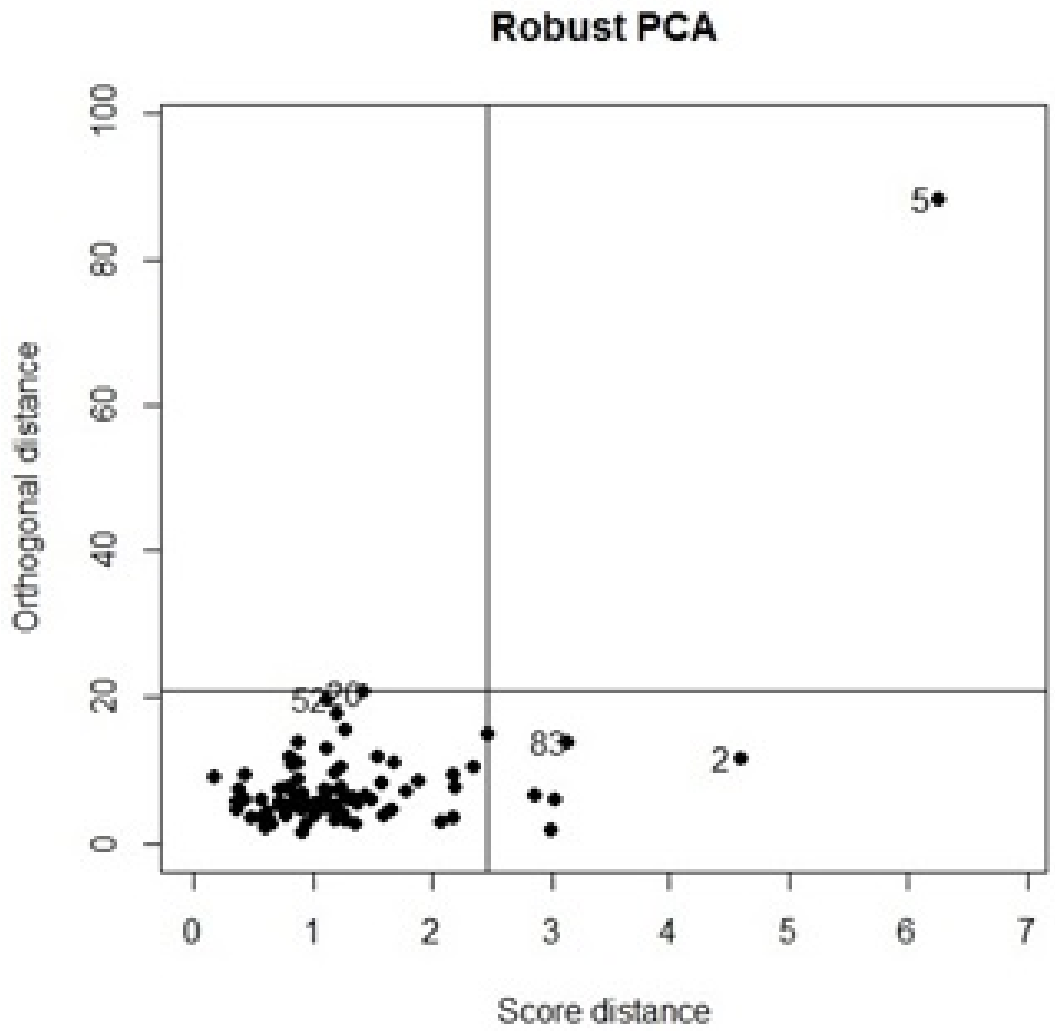
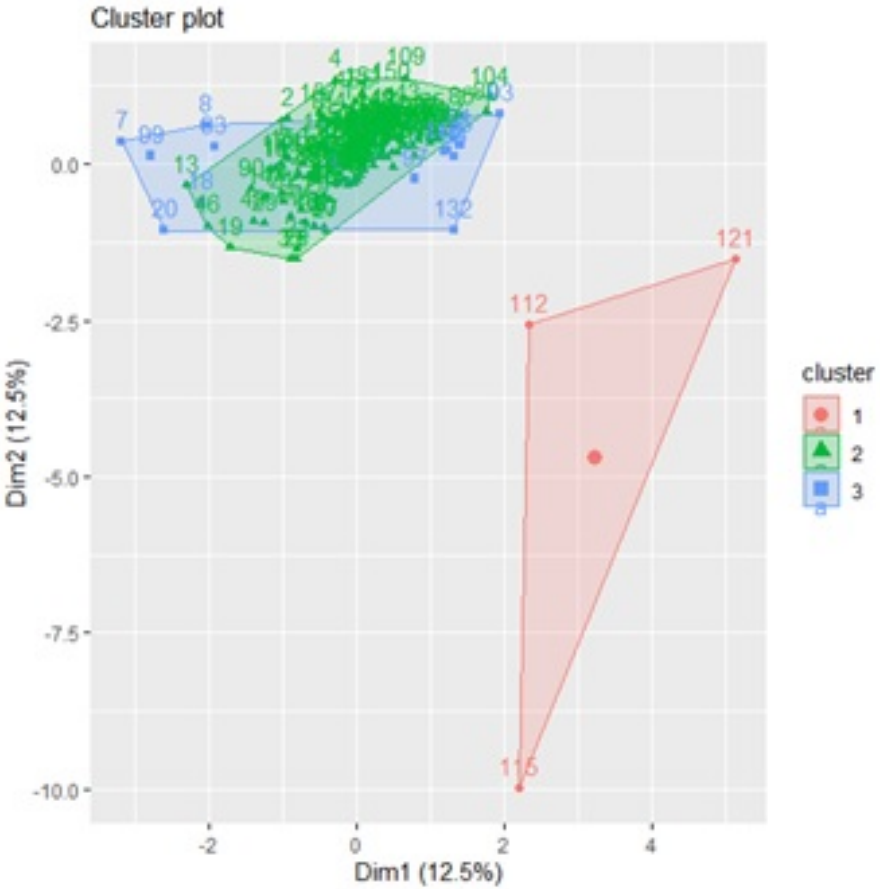
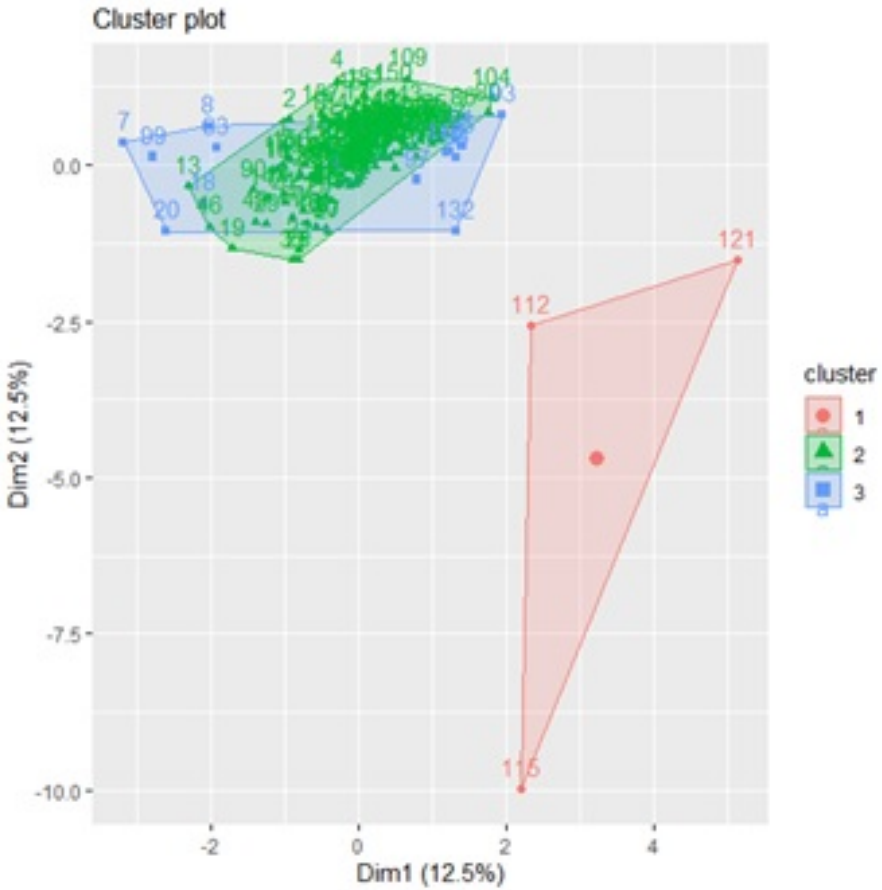


Figure: Diagonistic Plot of ROBPCA


Cluster plot
Dim2 (12.5%)
Dim1 (12.5%)
0.0
-2.5
-5.0
-7.5
-10.0
-2
0
2
4
121
112
115
132
cluster
1
2
3


Cluster plot
Dim2 (12.5%)
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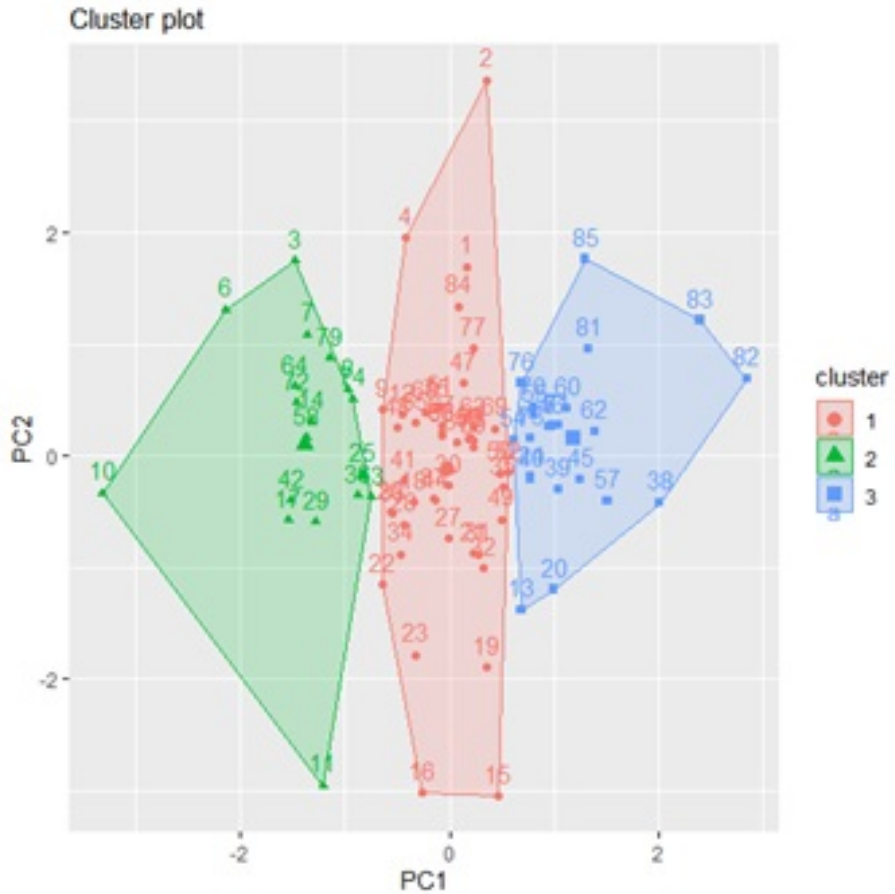
cluster
1
2
3


Cluster plot
PC2
PC1
cluster
1
2
3

VBSE

A more recent variation on principal component analysis is called sparse PCA. In particular, sparse weight vectors, or loading that is, weight vectors with a small number of "active" (nonzero) values—are what the SPCA looks for. Because the principal components of this approach are produced as a linear combination of only a few of the original variables, the model's interpret-ability is improved. In a high-dimensional data context, when the number of variables p exceeds the number of observations n, SPCA also prevents over fitting. Overfitting is a ML syndrome when a model is trained to fit a training set too closely loosing its ability to accurately predict a new one.

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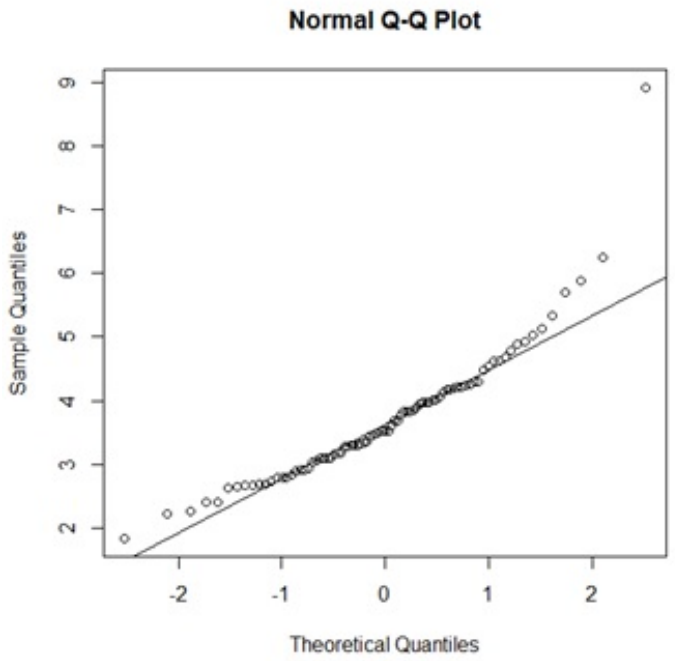

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Multivariate Outlier Detection Methods

- Mahalanobis Distance: based on Mahalanobis $D_i^2 = (X_i - \bar{X})' S_d^{-1} (X_i - \bar{X})$.

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- Hotelling T^2 Test: based on the assumption that the data follows multivariate Gaussian distribution.

Visualizing outliers

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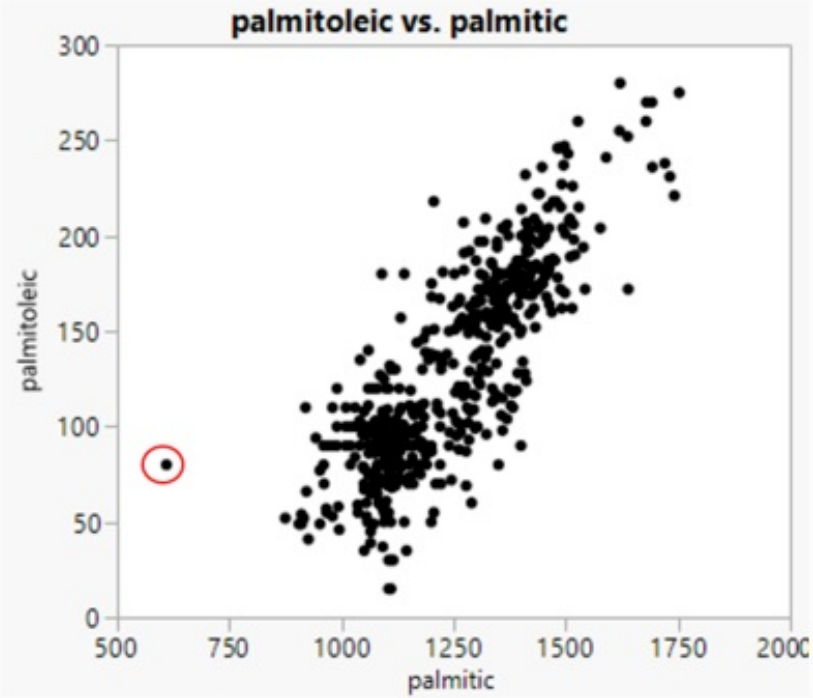
- χ^2 Plot: a plot of the ranked ordered values of the Generalized or Mahalanobis distance vs values of the χ^2 statistic. This procedure is based on the covariance matrix of the data. The resulting diagram would be interpreted much as a univariate probability plot where the presence of more than one straight-line segment is taken as evidence of multiple populations, and outliers as individuals or small groups are separated from the remaining data by gaps on the plot.

Scatter Plot and Density Plot



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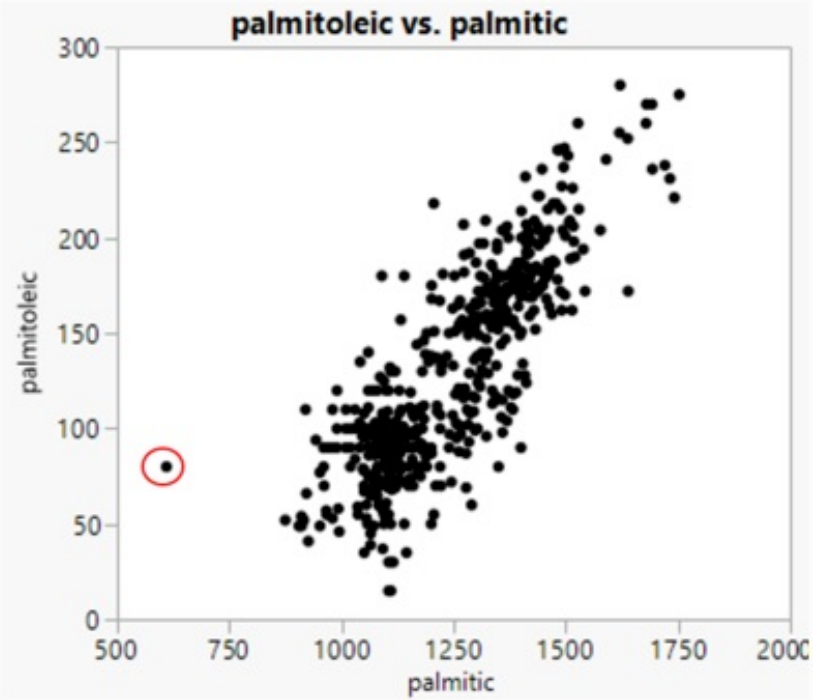
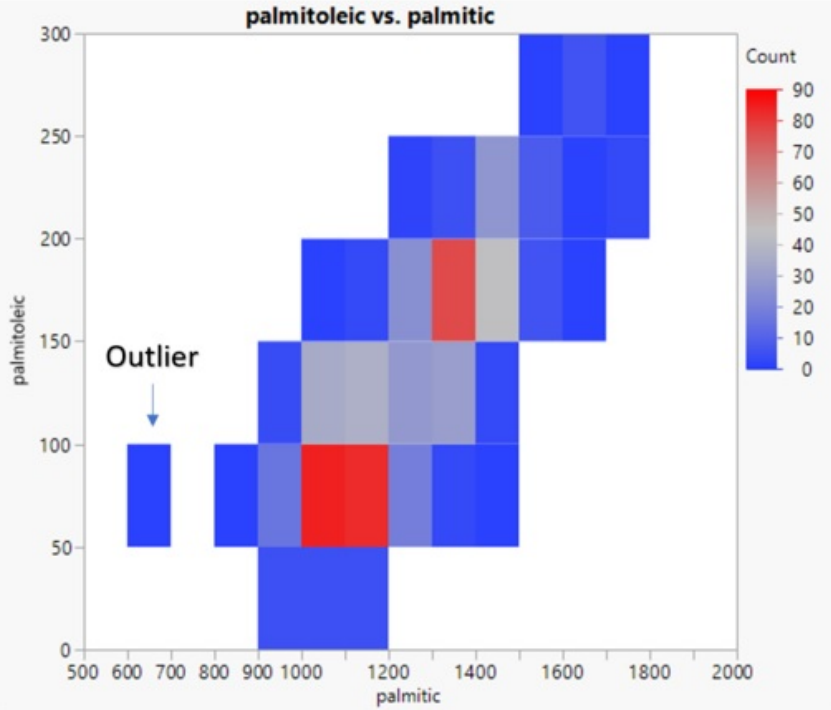
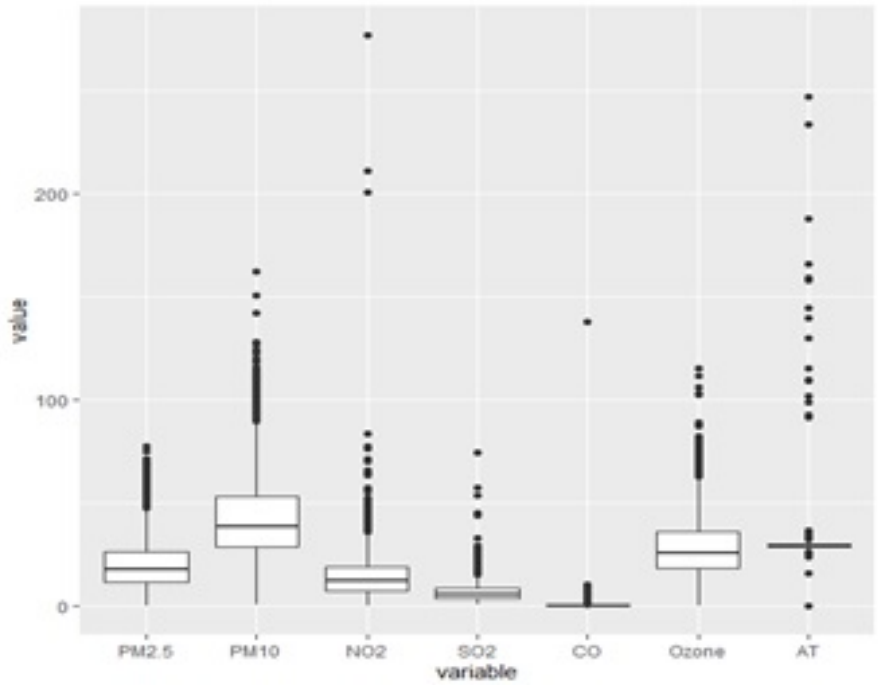
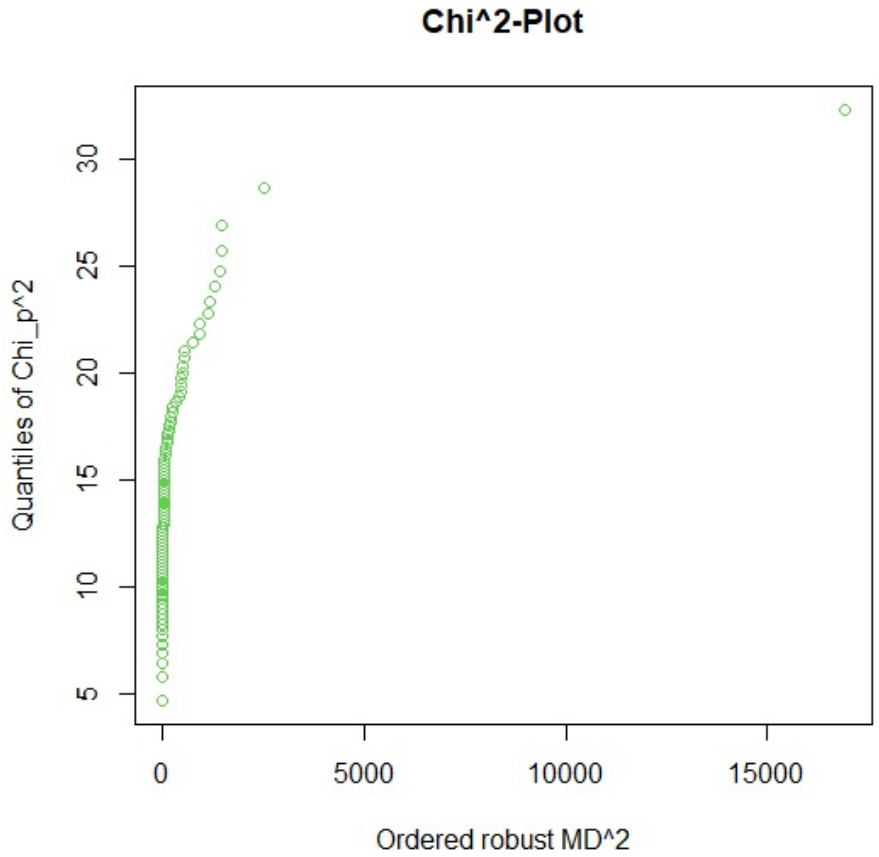




Box-plot and χ^2 Plot





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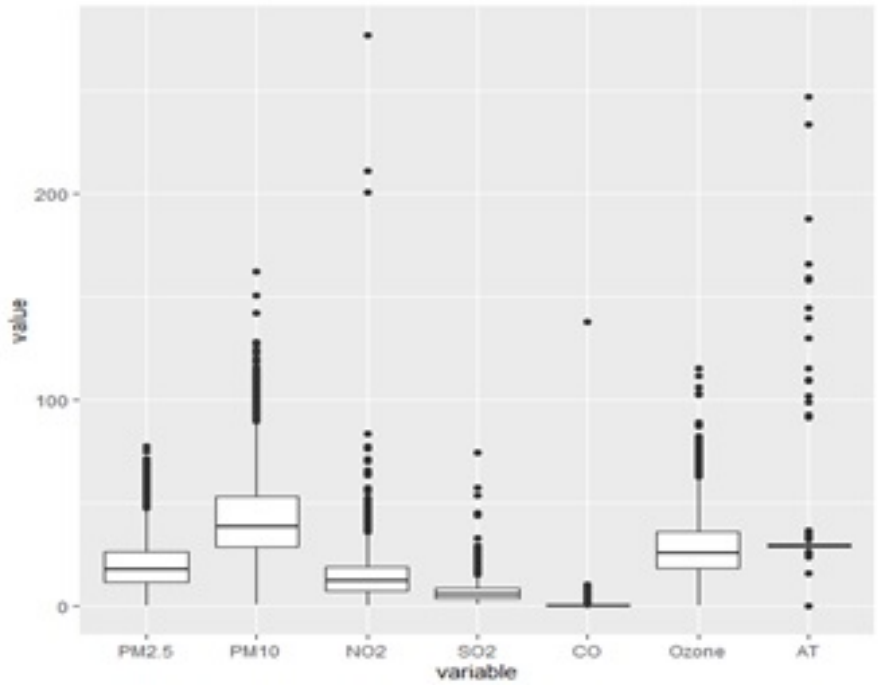

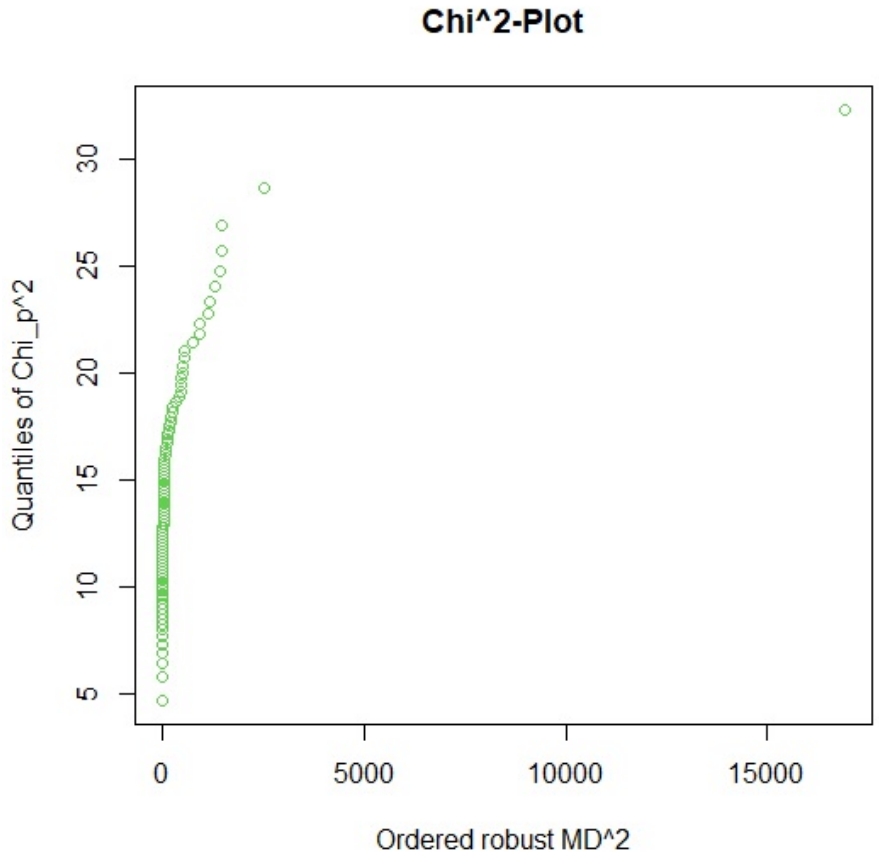

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Fat tailed distributions are characterized by larger values of skewness or kurtosis relative to a Gaussian or Exponential-family distributions. Some common fat-tailed distributions include:

- Cauchy
- Pareto
- Levy

All of these characterize the Non-Gaussian setup. While assuming "Gaussian" or "Gaussian-mixture" models/noise the tail of them must be investigated else once can expect more hallucinating results.

"The best thing about being a Statistician is that you get to play in everyone's backyard".
- Prof. John W. Tukey

Thank You!!!