Using traj Package to Identify Clusters of Longitudinal Trajectories

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Abstract

The traj package implements the 3-step procedure proposed by Leffondre et al. (2004) to identify clusters of longitudinal trajectories. The first step calculates 24 summary measures that describes features of the trajectories. The second step performs a factor analysis on these 24 measures to select measures that best describenthe main features of the trajectories. The third step classifies the trajectories into clusters based on the previously selected factors. The traj package also offers a wide variety of plotting function used to visualize the results.

This vignette illustrates the use of the traj package using simulated data. A more detailed description of the methods can be found in Sylvestre et al. (2006) or Leffondre et al. (2004).

1 Data

Data consist in two dataframes. The first dataframe, example.data\$data, contains the values for each individual trajectory. Each row correspond to a trajectory.

```
library(traj)
head(example.data$data)
```

| | ID | X1 | X2 | X3 | X4 | X5 | Х6 |
|---|----|--------|--------|--------|--------|--------|--------|
| 1 | 1 | 5.659 | 9.340 | 3.770 | 17.361 | 8.824 | 9.281 |
| 2 | 2 | 23.593 | 11.752 | 7.684 | 12.830 | 13.002 | 9.665 |
| 3 | 3 | 15.469 | 8.756 | 6.493 | 11.261 | 10.420 | 17.405 |
| 4 | 4 | 7.312 | 11.688 | 12.476 | 8.890 | 6.522 | 7.701 |
| 5 | 5 | 12.844 | 11.088 | 7.650 | 10.269 | 12.453 | 11.557 |
| 6 | 6 | 3.522 | 15.285 | 7.860 | 7.114 | 17.954 | 4.168 |

The second dataframe, example.data\$time, contains the time points at which the corresponding values for each individual trajectory were measured. Both dataframes must be of the same dimension.

head(example.data\$time)

| | ID | time.1 | time.2 | time.3 | time.4 | time.5 | time.6 |
|---|----|--------|--------|--------|--------|--------|--------|
| 1 | 1 | 1 | 2 | 3 | 4 | 5 | 6 |
| 2 | 2 | 1 | 2 | 3 | 4 | 5 | 6 |
| 3 | 3 | 1 | 2 | 3 | 4 | 5 | 6 |
| 4 | 4 | 1 | 2 | 3 | 4 | 5 | 6 |
| 5 | 5 | 1 | 2 | 3 | 4 | 5 | 6 |
| 6 | 6 | 1 | 2 | 3 | 4 | 5 | 6 |

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2 Analysis

The first step in the analysis consists of the computing 24 measures of each trajectory.

The 24 measures are:

- 1. Range
- 2. Mean-over-time
- 3. Standard deviation (SD)
- 4. Coefficient of variation (CV)
- 5. Change
- 6. Mean change per unit time
- 7. Change relative to the first score
- 8. Change relative to the mean over time
- 9. Slope of the linear model
- 10. R^2 : Proportion of variance explained by the linear model
- 11. Maximum of the first differences
- 12. SD of the first differences
- 13. SD of the first differences per time unit
- 14. Mean of the absolute first differences
- 15. Maximum of the absolute first differences
- 16. Ratio of the maximum absolute difference to the mean-over-time
- 17. Ratio of the maximum absolute first difference to the slope
- 18. Ratio of the SD of the first differences to the slope
- 19. Mean of the second differences
- 20. Mean of the absolute second differences
- 21. Maximum of the absolute second differences
- 22. Ration of the maximum absolute second difference to the mean-over-time
- 23. Ratio of the maximum absolute second difference to mean absolute first difference
- 24. Ratio of the mean absolute second difference to the mean absolute first difference

The 24 measures can be computed using the step1measures function.

s1 = step1measures(example.data\$data, example.data\$time, ID = TRUE)

- [1] "Correlation of m5 and m6 : 1"
- [1] "Correlation of m12 and m13 : 1"
- [1] "Correlation of m17 and m18 : 0.999"

head(s1\$measurments)

ID m1m2mЗ m4m5 m6 m7m8m91 13.590 9.039 4.661 51.57 3.6225 0.60376 0.64015 0.40076 0.861616 1 2 2 15.909 13.088 5.534 42.28 -13.9279 -2.32131 -0.59035 -1.06421 -1.735574 3 3 10.912 11.634 4.107 35.30 1.9365 0.32275 0.12519 0.16645 0.555447 4 9.098 2.447 26.90 0.3893 0.06488 0.05324 0.04279 -0.489632 4 5.955 5 5 5.194 10.977 1.875 17.08 -1.2863 -0.21438 -0.10015 -0.11718 0.008112 6 6 14.432 9.317 5.955 63.91 0.6457 0.10761 0.18333 0.06930 0.299663 m14m10m11 m12m13m15 m16m17m18 m19 1 1.196e-01 13.590 8.656 8.656 6.367 13.590 1.5035 15.773 10.047 - 0.8066.237 4.913 11.841 0.9047 2 3.442e-01 5.146 6.237 -6.822 -3.5942.126 5.515 4.314 3 6.402e-02 6.985 5.515 6.985 0.6004 12.576 9.929 3.425 4 1.401e-01 4.376 3.146 3.146 2.460 4.376 0.4809 -8.936 -6.426 -0.799 5 6.549e-05 2.619 2.598 2.598 2.179 3.438 0.3132 423.805 320.306 0.215 6 8.864e-03 11.763 11.197 11.197 8.912 13.786 1.4797 46.006 37.367 -6.387 m22m23 m20 m21 m24 1 14.883 22.127 2.4479 3.475 2.338 6.367 9.214 0.7040 1.876 1.296 2 3 6.229 7.826 0.6727 1.814 1.444 4 3.182 4.374 0.4808 1.778 1.294 5 2.813 6.057 0.5518 2.780 1.291 6 15.520 24.626 2.6431 2.763 1.741

Each row in the dataframe returned by step1measures corresponds to the trajectory on the same row in the input data (example.data\$data). For each trajectory, the 24 measures have been calculated and correspond to columns m1 to m24.

In the second step of the analysis, a factor analysis is performed to select a subset of measures that describes the main features of the trajectories. The function step2factors is used to perform the factor analysis.

s2 = step2factors(s1)

[1] "m6 is removed because it is perfectly correlated with m5"
[2] "m13 is removed because it is perfectly correlated with m12"
[1] "Computing reduced correlation e-values..."

head(s2\$factors)

TD m21 m24m4 m51 1 51.57 3.6225 22.127 2.338 2 42.28 -13.9279 2 9.214 1.296 3 3 35.30 1.9365 7.826 1.444 4 4 26.90 0.3893 4.374 1.294 5 5 17.08 -1.2863 6.057 1.291 6 6 63.91 0.6457 24.626 1.741

In this example, the step2factors has identified measures 4, 5, 21 and 24 as the main factors of this set of trajectories. Measures 6, 13 and 18 were not considered because they were too correlated with other measures (measures with a correlation higher than 0.95 are omitted from the factor analysis).

Once this step is done, the third step of the procedure consists in clustering the trajectories based on the measures identified in the factor analysis. This step is implemented in the step3clusters function. Two options are available to select the number of clusters. First, the user can a priori decide on the number of clusters, such as in the following example in which the number of clusters is set to 4.

s3 = step3clusters(s2, nclusters = 4)

Alternatively, the number of clusters can be left blank in which case the step3clusters function will rely on the NbClust function from the NbClust package to determine the optimal number of clusters based on one of the criteria available in NbClust. Please see NbClust documentation for more details.

The function step3clusters assigns each trajectory to one and only one cluster and returns a dataframe that identifies cluster membership.

head(s3\$clusters)

The traj object returned by the function step3clusters can be plotted by an array of plotting functions, as described in the next section.

3 Plotting the traj object

The traj object created by step3clusters can be plotted by an array of plotting functions.



Cluster plots of data vs. time of 10 samples

This function selects 10 random trajectories from each cluster and plots them using randomly selected colours. The user can specify the number of trajectories to plot, the colours or any other generic plotting parameter. The user can request that trajectories from only one cluster be plotted.



Mean for Every Cluster

The plotMeanTraj function plots the mean trajectory of every cluster. The user can request that trajectories from only one cluster be plotted.



Median, 10% and 90% for Every Cluster

The plotMedTraj function plots the median trajectory of every cluster with 10th and 90th percentiles. The user can request that trajectories from only one cluster be plotted.



Boxplots for Every Cluster







The plotBoxplotTraj function will plot the box-plot distribution of every time point in each cluster. The user can request that trajectories from only one cluster be plotted.



Mean Trajectory of all Clusters

The plotCombTraj function will plot the mean or median of all the clusters on one single graph. Different colours can be selected as well as different line styles.

References

- (a) Sylvestre MP; et al. (2006). Classification of patterns of delirium severity scores over time in an elderly population. International Psychogeriatrics; 18(4); 667-680. doi:10.1017/S1041610206003334.
- (b) Leffondree; K. et al. (2004). Statistical measures were proposed for identifying longitudinal patterns of change in quantitative health indicators. Journal of Clinical Epidemiology; 57; 1049-1062. doi: 10.1016/j.jclinepi.2004.02.012.