1 Installation

Some functions of WeightedCluster require the free GraphViz program (Gansner and North, 1999). It needs to be installed before launching R for these functions to work properly. You can download it here: http://www.graphviz.org.

The WeightedCluster library can be installed and loaded using the following commands:

R> install.packages("WeightedCluster")
R> library(WeightedCluster)

2 An illustrative example

In this preview, we use the dataset from McVicar and Anyadike-Danes (2002) which is distributed with the TraMineR library (Gabadinho et al., 2011). This dataset contains sequences of school-to-work transitions in Northern Ireland. The dataset is loaded using:

R> data(mvad)

wcAggregateCases allows us to identify and aggregate identical state sequences (which are in columns 17:86). We print out the basic information about the aggregation and create the uniqueMvad object which contains only unique sequences.

R> aggMvad <- wcAggregateCases(mvad[, 17:86])
R> print(aggMvad)

Number of disaggregated cases: 712
Number of aggregated cases: 490
Average aggregated cases: 1.45
Average (weighted) aggregation: 1.45

R> uniqueMvad <- mvad[aggMvad$aggIndex, 17:86]

Using the unique sequence dataset, we build a sequence object and compute dissimilarities between sequences (see Gabadinho et al., 2011 for more on this topic). The vector aggMvad$aggWeights store the number of replication of each unique sequence. It is thus used as unique sequence weight.

R> mvad.seq <- seqdef(uniqueMvad, weights=aggMvad$aggWeights)
R> ## Computing Hamming distance between sequence
R> diss <- seqdist(mvad.seq, method="HAM"
3 Hierarchical clustering

We can regroup similar sequences using hierarchical clustering with "average" method using weights (aggMvad$aggWeights) (any method may be used).

\[
\text{R} > \text{averageClust} <- \text{hclust(}\text{as.dist(diss)}, \text{ method="average"}, \text{ members=aggMvad$aggWeights})
\]

The agglomeration schedule can be represented graphically as a tree using:

\[
\text{R} > \text{averageTree} <- \text{as.seqtree(averageClust, seqdata=mvad.seq, diss=diss, nclus-
}\text{ter=6})
\]

\[
\text{R} > \text{seqtreedisplay(averageTree, type="d", border=NA, showdepth=TRUE})
\]

4 Cluster quality

We can automatically compute several clustering quality measures (presented in table 1) for a range of numbers of groups: 2 until ncluster=10.

\[
\text{R} > \text{avgClustQual} <- \text{as.clustrange(averageClust, diss, weights=aggMvad$aggWeights, nclus-
}\text{ter=10})
\]

The results can be plotted and used to identify the best number of groups (you can also print them).

\[
\text{R} > \text{plot(avgClustQual)}
\]
Table 1: Cluster Quality Measures Available in WeightedCluster

<table>
<thead>
<tr>
<th>Name</th>
<th>Abbr.</th>
<th>Range</th>
<th>Min/Max</th>
<th>Interpretation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Point Biserial Correlation</td>
<td>PBC</td>
<td>[-1;1]</td>
<td>Max</td>
<td>Capacity of the clustering to reproduce the original distance matrix.</td>
</tr>
<tr>
<td>Hubert's Gamma</td>
<td>HG</td>
<td>[-1;1]</td>
<td>Max</td>
<td>Capacity of the clustering to reproduce the original distance matrix (Order of magnitude).</td>
</tr>
<tr>
<td>Hubert’s Somers D</td>
<td>HGSD</td>
<td>[-1;1]</td>
<td>Max</td>
<td>Same as above, taking into account ties in the distance matrix.</td>
</tr>
<tr>
<td>Hubert’s C</td>
<td>HC</td>
<td>[0;1]</td>
<td>Min</td>
<td>Gap between the current quality of clustering and the best possible quality for this distance matrix and number of groups.</td>
</tr>
<tr>
<td>Average Silhouette Width</td>
<td>ASW</td>
<td>[-1;1]</td>
<td>Max</td>
<td>Coherence of the assignments. A high coherence indicates high between groups distances and high intra group homogeneity.</td>
</tr>
<tr>
<td>Calinski-Harabasz index</td>
<td>CH</td>
<td>[0;+∞]</td>
<td>Max</td>
<td>Pseudo F computed from the distances.</td>
</tr>
<tr>
<td>Calinski-Harabasz index</td>
<td>CHsq</td>
<td>[0;+∞]</td>
<td>Max</td>
<td>Idem, using the squared distances.</td>
</tr>
<tr>
<td>Pseudo $R^2$</td>
<td>R2</td>
<td>[0;1]</td>
<td>Max</td>
<td>Share of the discrepancy explained by the clustering.</td>
</tr>
<tr>
<td>Pseudo $R^2$</td>
<td>R2sq</td>
<td>[0;1]</td>
<td>Max</td>
<td>Idem, using the squared distances.</td>
</tr>
</tbody>
</table>

It is usually easier to choose the number of groups based on standardized scores. Here, five groups seems to be a good solution.

R> plot(avgClustQual, norm="zscore")
Alternatively, we can retrieve the two best solutions according to each quality measure:

R> summary(avgClustQual, max.rank=2)

<table>
<thead>
<tr>
<th>Stat</th>
<th>N groups 1.</th>
<th>stat 1.</th>
<th>N groups 2.</th>
<th>stat 2.</th>
</tr>
</thead>
<tbody>
<tr>
<td>PBC</td>
<td>10</td>
<td>0.7616</td>
<td>9</td>
<td>0.761</td>
</tr>
<tr>
<td>HG</td>
<td>10</td>
<td>0.8939</td>
<td>9</td>
<td>0.893</td>
</tr>
<tr>
<td>HGSD</td>
<td>10</td>
<td>0.8910</td>
<td>9</td>
<td>0.890</td>
</tr>
<tr>
<td>ASW</td>
<td>5</td>
<td>0.3966</td>
<td>3</td>
<td>0.393</td>
</tr>
<tr>
<td>ASWw</td>
<td>5</td>
<td>0.4010</td>
<td>6</td>
<td>0.396</td>
</tr>
<tr>
<td>CH</td>
<td>2</td>
<td>181.9886</td>
<td>3</td>
<td>126.780</td>
</tr>
<tr>
<td>R2</td>
<td>10</td>
<td>0.3980</td>
<td>9</td>
<td>0.396</td>
</tr>
<tr>
<td>CHsq</td>
<td>2</td>
<td>338.5174</td>
<td>5</td>
<td>262.451</td>
</tr>
<tr>
<td>R2sq</td>
<td>10</td>
<td>0.6145</td>
<td>9</td>
<td>0.613</td>
</tr>
<tr>
<td>HC</td>
<td>10</td>
<td>0.0598</td>
<td>9</td>
<td>0.060</td>
</tr>
</tbody>
</table>

5 PAM clustering

The WeightedCluster library also provides an optimized PAM algorithm. We can automatically compute PAM cluster for a range of numbers of groups using:

R> pamClustRange <- wcKMedRange(diss, kvals=2:10, weights=aggMvad$aggWeights)

As before, we can plot the quality measures of each solution (not shown here) or retrieve the two best solutions according to each quality measure using:

R> summary(pamClustRange, max.rank=2)

<table>
<thead>
<tr>
<th>Stat</th>
<th>N groups 1.</th>
<th>stat 1.</th>
<th>N groups 2.</th>
<th>stat 2.</th>
</tr>
</thead>
<tbody>
<tr>
<td>PBC</td>
<td>2</td>
<td>0.619</td>
<td>4</td>
<td>0.618</td>
</tr>
<tr>
<td>HG</td>
<td>10</td>
<td>0.845</td>
<td>9</td>
<td>0.845</td>
</tr>
<tr>
<td>HGSD</td>
<td>10</td>
<td>0.842</td>
<td>9</td>
<td>0.842</td>
</tr>
<tr>
<td>ASW</td>
<td>2</td>
<td>0.411</td>
<td>9</td>
<td>0.370</td>
</tr>
<tr>
<td>ASWw</td>
<td>2</td>
<td>0.412</td>
<td>9</td>
<td>0.378</td>
</tr>
<tr>
<td>CH</td>
<td>2</td>
<td>200.286</td>
<td>3</td>
<td>151.245</td>
</tr>
<tr>
<td>R2</td>
<td>10</td>
<td>0.590</td>
<td>9</td>
<td>0.576</td>
</tr>
<tr>
<td>CHsq</td>
<td>2</td>
<td>394.893</td>
<td>4</td>
<td>310.881</td>
</tr>
<tr>
<td>R2sq</td>
<td>10</td>
<td>0.786</td>
<td>9</td>
<td>0.774</td>
</tr>
<tr>
<td>HC</td>
<td>9</td>
<td>0.100</td>
<td>10</td>
<td>0.104</td>
</tr>
</tbody>
</table>

6 Keeping a solution

The objects returned by as.clustrange or wcKMedRange contain a data.frame with cluster membership (named clustering). For instance, we can plot the sequences
according to PAM clustering in 5 groups using:

\[
\text{R\> seqdplot(mvad.seq, group=pamClustRange$clustering$cluster5, border=NA)}
\]

\[
\begin{array}{cccccc}
\text{Sep.93} & \text{Jun.94} & \text{Mar.95} & \text{Dec.95} & \text{Sep.96} & \text{Jun.97} & \text{Mar.98} & \text{Dec.98} \\
0.0 & 0.4 & 0.8 & & & & & \\
\end{array}
\]

7 Disaggregating data

Once the sequences have been regrouped, it is often useful to “disaggregate” the data. For instance, we may want to add the cluster membership in the original data set (i.e. before unique sequences were identified). This allows us to cross-tabulate cluster membership and father unemployment (variable funemp). This operation is performed using \texttt{aggMvad$disaggIndex} which stores the index of each unique sequence in the original dataset.

\[
\text{R\> uniqueCluster5 <- avgClustQual$clustering$cluster5} \\
\text{R\> mvad$cluster5 <- uniqueCluster5[aggMvad$disaggIndex]} \\
\text{R\> table(mvad$funemp, mvad$cluster5)}
\]

\[
\begin{array}{cccccc}
1 & 2 & 3 & 4 & 5 \\
\text{no} & 134 & 348 & 70 & 24 & 19 \\
\text{yes} & 14 & 69 & 10 & 16 & 8 \\
\end{array}
\]

References
