cutTreeBalanced: Balanced cuts for dendrograms

Cutting dendrograms to achieve hierarchical clustering with balanced cluster sizes.

1 Abstract

Hierarchical (a.k.a. agglomerative) linkage techniques are common in a wide range of fields such as economics, bioinformatics, (some fields). The output of these techniques are dendrograms, which are directed acylic graphs (note: not just DAGs - they have tree structure) that define the linkage between input data. Generating clusters requires some method of cutting the dendrogram to separate groups of points from each other. Many existing cutting techniques, such as a straight cut along a constant height, lead to clusters with highly imbalanced sizes. This paper presents and demonstrates balancedCut for Python - a method of cutting dendrograms with balanced cluster sizes.

2 Introduction

- What is hierarchical clustering, dendrogram, tree cut.
- Straight cut (i.e. constant height cut).
- hdbscan: [1], dynamicTreeCut [2]
- High-dimensional data have reduced contrast [3], and often high 'hubness' [4], as a result of curse of dimensionality. In these cases, similarity by usual distance metrics is not well defined. Single-linkage, Ward linkage, or other linkages may result in dendrograms that are impossible to cut while preserving underlying structure. In these cases, variable cutting distance is required.
- Example of hubness causing bad hierarchical clustering results: [5] (a reference to the abstract: Abstract).

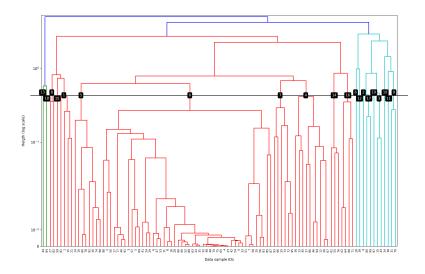


Figure 1: A dendrogram generated by single-linkage clustering, showing a straight cut at height XYZ. Straight cuts at any height generate clusters with imbalanced sizes (can we add a histogram of cluster sizes at multiple heights? LJM)

3 Algorithm and Results

[algorithm explanation]

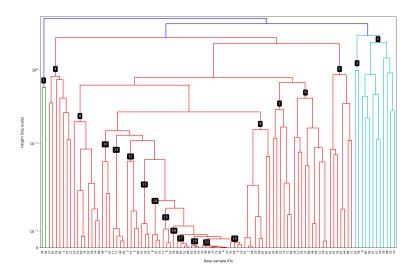


Figure 2: The same dendrogram as in 1, but demonstrating a balanced cut of size XYZ

References

- [1] L. McInnes, J. Healy, and S. Astels, "Hdbscan: Hierarchical density based clustering," *Journal of Open Source Software*, vol. 2, no. 11, p. 205, 2017.
- [2] P. Langfelder, B. Zhang, and S. Horvath, "Defining clusters from a hierarchical cluster tree: The dynamic tree cut package for r," *Bioinformatics*, vol. 24, no. 5, pp. 719–720, 2008.
- [3] K. Beyer, J. Goldstein, R. Ramakrishnan, and U. Shaft, "When is 'nearest neighbor' meaningful?" in *International conference on database theory*, 1999, pp. 217–235.
- [4] M. Radovanovic, A. Nanopoulos, and M. Ivanovic, "Hubs in space: Popular nearest neighbors in high-dimensional data," *Journal of Machine Learning Research*, vol. 11, no. sept, pp. 2487–2531, 2010.

[5] J. MacCuish, C. Nicolaou, and N. E. MacCuish, "Ties in proximity and clustering compounds," *Journal of Chemical Information and Computer Sciences*, vol. 41, no. 1, pp. 134–146, 2001.