Hierarchical agglomerative clustering

Lots of data sets have structure at different scales, to a certain extent we saw that with the Hawk dataset, there were two properties that separated the data into clusters in the wing length and weight space, one was species and the other was probably sex. The difficulty in clustering the data arose from the overlapping of the two scales, the difference between the two genders for the RT hawks matched the species difference between the SS and CH hawks. Of course, in the case of k-means clustering we dealt with the number of clusters, rather than the scale of clusteriness, though the two are roughly reciprocally related. Here though we will talk about scale and the idea is that it might be hard to see what scale is appropriate for examining clusters in a dataset, or we might be interested in different scales, or different sizes of cluster at the same time.

This is where hierarchical cagglomerative clustering, or HAC, is useful; it is a map of the entire clustering structure of the data, up to the usual sort of caveats that it only reliably finds simple, glob-shaped, structures. The idea is to start with all the data and identify the two closest data points. These are then joined together to form a cluster, once they are clustered they are treated as a single data point. Of course that means working out the distance of this new point, representing the small cluster, and all the other data points, there are various ways to do that and we will discuss that, the most straight forward is the average, so if \bf{a} and \bf{b} are the two points added to make the cluster $\{\bf{a}, \bf{b}\}$ then the distance from this to a point \bf{c} is

$$d(\mathbf{c}, \{\mathbf{a}, \mathbf{b}\}) = \frac{1}{2} [d(\mathbf{c}, \mathbf{a} + d(\mathbf{c}, \mathbf{b}))]$$
(1)

Now we just keep going, at every step merging the two closest points to make a cluster, or a bigger cluster, and then recalculating distances and iterating again until at the very end there is one big cluster with all the points in.

An example - the DKB data

This is easiest to see from an example; we will look at the DKB data set [?], this gives a set of distances between different languages. We will describe how these distances are calculated soon but first of, this is a very satisfying sort of example because languages clearly have a multi-scale clustering structure, even if people attempt to create clusters by calling one set of languages

'English' and another 'Norwegian', it is clear this is entirely artificial; as an Irish-English speaker the language I speak is clearly different from other Englishes spoken in Bath where I live and in my house my children use a young peoples English which is different from mine, even some very basic words are different, I eat my dinner, my daugher scrans hers. In the case of Norwegian, there are two very different sorts of Norwegian, Bokmøal and Nynorsk, both of which are called Norwegian even if are not much less different from each other as they from other nearby language like Danish. At a larger scale, Norwegian, like English, is a Germanic language, French a Romance language and Irish, the language spoken in Ireland along with Irish-English is a Celtic language and all these clusters can be further grouped in Indo-European languages.

The other nice thing about doing HAC on languages is that you might expect that languages diverge at a roughly fixed rate so the clustering describes their evolutionary history.

The DKB dataset uses a set of standard words, called a Swadesh set after a linguist called Morris Swadesh, which contains words for basic actions, like eating and sleeping, and common objects like the obvious body parts and things like fire and water. The most common equivalents of these words are found for 84 different Indo-European languages. Next, for any pair of these words, for example, sleep and schlafen, words with the same meaning in English and German, the word origins are studied to see if they have the same etymology. In the case of sleep and schlafen the answer is yes, they both come from the same Proto-Germanic word, they are cognate. Ihe Irish for sleep, however, is coladh which is not related to the German or English word; French, dormir, Italian, dormire, Spanish, dormir, Portuguese, dormir and Romanian, dormi all have cognate words with the same Latin origin. The distance between two languages is then defined as the number of noncognate pairs divided by the total number of pairs. In the DKB dataset a 200 word Swadesh list is used, so generally the number of pairs of words for each pair of languages is 200, though, in a few cases the translated list was incomplete.

Anyway, the upshot is that the DKB dataset is a matrix of distances between 84 languages. We can apply HAC to this using a standard library; we can also plot the resulting *dendrogram*, the clustering libraries tend to have nice graphing commands that show a tree of the clusters merging in a way that matches the separation of the points being merged. Again, this is more obvious from a graph, the HAC for all 84 languages is shown in Fig. 1.

This dendrogram has been coloured to show some of the clusters, for this the number of clusters was specified.

It is clear that HAC has succeeded in discovering something interesting in the data, the coloured groups largely represent recognizable language families. The olive green are mostly Slavic languages, though Latvian and Lithuanian aren't Slavic, the grey are Germanic, the magenta are Romance, brown is Indo-Aryan, purple is Iranian, red is just Albanian and green is Celtic; the orange is confusing since Greek and Armenian are not normally thought of as closely related languages. At a lower level, Dutch, Flemish and Afrikaans are close to each other, for example, as are the two dialects of Irish.

Clearly this graph doesn't match evolution, the Celtic languages, for example, did not diverge from Greek more recently than they diverged from Latin. Indeed, the idea that language evolution is a tree is wrong, languages have multiple influences, they are not just the isolated descendants of a parent language; indeed, they may have more than one parent. The creoles are a particularly important example of that and the HAC approach does not work well with creoles. The location of Haitian Creole doesn't put it any closer to French than to the other Romance languages, the complex history of Haitian Creole is beyond anything that this approach can detect. The other creole, Sranan Tongo, called here Taki-Taki, is placed in a similar way relative to its closest Indo-European languages.

Distances

Above we glossed over the question of how we work out new distances as we merge clusters; the example was given of using the average, so the distance between any two clusters is the average distance between each pair of one point from one cluster and one point from the other:

$$d(C_1, C_2) = \frac{1}{|C_1||C_2|} \sum_{x \in C_1} \sum_{y \in C_2} d(x, y)$$
 (2)

This is one way to proceed, another would be to pick the smallest distance:

$$d(C_1, C_2) = \min[d(x, y) | x \in C_1, y \in C_2]$$
 (3)

This is known as single linkage, if the largest distance is used

$$d(C_1, C_2) = \text{maximum}[d(x, y)|x \in C_1, y \in C_2]$$

$$\tag{4}$$

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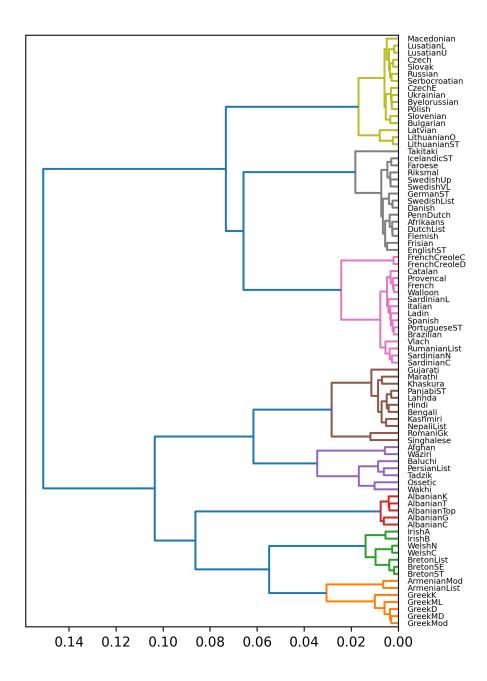


Figure 1: A dendrogram for the DKB language data; the languages are merged into larger and larger clusters, with the merge points placed on the x-axis at a distance between the two points or clusters when they merge.

this is called *complete linkage*.

The most common approach, Ward linkage, the one used for the figure, is more complicated than the merge-the-nearest-clusters strategy we have discussed so far. It is sometimes phrased in a different way as an attempt to minimize an objective function, typically the variance of the clusters as they are formed. This means that it assesses clusters by calculating the within-cluster variance:

$$V(C) = \frac{2}{|C|(|C|-1)} \sum y \neq x, y \in C \sum_{x \in C} d(x,y)^2$$
 (5)

of the potential new clusters; this allows the increase in within-cluster variance to be calculated: if $C = C_1 \cup C_2$ the increase in variance is

$$\Delta V = V(C) - V(C_1) - V(C_2) \tag{6}$$

and the merger with the smallest ΔV is the one that is performed.

References

[1] Dyen, I., Kruskal, J. B., & Black, P. (1992). An Indoeuropean classification: A lexicostatistical experiment. *Transactions of the American Philosophical Society*, 82(5), iii–132.