Introduction

Hierarchical clustering organizes data into a nested tree of clusters without predefining the number of groups. It suits exploratory analysis when you want a multiresolution view of structure in the data, and it works directly from a distance matrix so it accepts many distance measures and linkage rules. This discussion describes a concrete implementation plan for agglomerative hierarchical clustering, explains the role of dendrograms in the method, and highlights practical choices such as linkage, distance metric, and stopping rules. (Singh, Bhatia, & Sangwan, 2007).

Overview of the algorithm

Agglomerative hierarchical clustering is a bottom-up algorithm. Start with each observation as its own cluster. At each step, find the two clusters with the smallest inter-cluster dissimilarity and merge them. Repeat until all items join a single cluster or until a stopping rule halts the process. The inter-cluster dissimilarity is defined by two things: the pairwise distance metric between observations (for example, Euclidean or Manhattan) and the linkage criterion that converts pairwise distances into distances between clusters (for example, single, complete, average, or Ward). Different linkage choices produce different cluster shapes, and they influence sensitivity to noise and outliers. (Singh et al., 2007).

Step-by-step implementation plan

- 1. **Data preparation.** Clean missing values, encode categorical variables if needed (e.g., one-hot), and standardize numeric features so that scale differences do not bias distances.
- **2.** Choose distance metric. For continuous features, use Euclidean distance; for mixed data types consider Gower distance or dedicated mixed-data distances.
- **3.** Compute the distance matrix. Compute pairwise distances for all observations; this yields an n-by-n symmetric matrix.
- **4. Select linkage.** Decide on single, complete, average (UPGMA), or Ward linkage. Ward minimizes within-cluster variance and often gives compact, spherical clusters; single linkage can produce chaining.
- 5. Perform agglomeration. Use a standard library implementation (for example, scikit-learn's AgglomerativeClustering or SciPy's hierarchical clustering utilities) to iteratively merge clusters until the stopping criterion is met. These libraries compute the linkage efficiently and return either labels for a chosen number of clusters or a full linkage matrix for visualization (scikit-learn developers, n.d.).
- **6.** Choose the cut. Decide where to cut the tree to form final clusters. You can pick a fixed number of clusters k, a distance threshold, or inspect the dendrogram for large vertical jumps in linkage distance that indicate natural cluster splits.
- 7. Validate clusters. Use internal validation indices such as silhouette score or external labels when available. For stability, repeat with bootstrapped samples or with different linkage/distance choices (Espinoza, 2011).

The role of dendrograms

A dendrogram is the tree diagram that records the sequence of merges and the distances at which they occurred. It serves three practical functions. First, it is a diagnostic: by plotting cluster merges vs. distance you can visually inspect where large increases in merge distance occur and therefore select a natural cut point. Second, it preserves the full hierarchy so you can produce clusterings at multiple resolutions without re-running the algorithm. Third, dendrograms help explain results to stakeholders because they show which observations or subclusters joined together and at what dissimilarity level. For implementation, produce the linkage matrix and render a dendrogram using SciPy or matplotlib; then mark candidate cut heights to derive cluster labels programmatically (SciPy developers, n.d.).

Practical considerations and limitations

Hierarchical clustering scales as roughly $O(n^2)$ in memory and $O(n^2 \log n)$ or worse in time depending on implementation, so it becomes impractical for very large data sets. Presampling, feature reduction, or approximate nearest neighbor preclustering can help. Choice of linkage and metric materially affects result interpretability; document and test alternatives. Finally, dendrograms become cluttered for large n; in those cases use heatmaps of reordered distance matrices or summarize clusters instead (Espinoza, 2011).

Conclusion

Implementing hierarchical clustering means making clear choices about preprocessing, distance, and linkage, then producing and interpreting a dendrogram to select cluster cuts and explain structure. The dendrogram is central: it records the full hierarchical solution, enables multiresolution analysis, and guides the cut that produces the final clustering. Proper validation and scalability strategies complete a robust workflow. (Singh et al., 2007).

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