Clustering methods & choice of linkage

PRIMER 7 now carries out a wider range of clustering methods than previously: a) hierarchical agglomerative clustering using one of four linkage methods – single, complete, group average (UPGMA) and flexible beta (a standard WPGMA extension); b) hierarchical (binary) divisive clustering – a new unconstrained form (*UNCTREE*) of the previously offered constrained binary divisive routine (*LINKTREE*, covered in Section 13); and c) a new flat-form, i.e. non-hierarchical, method (*kRCLUSTER*) which is a development of *k*-means clustering. Both the *UNCTREE* and *kRCLUSTER* algorithms are designed to fit with the non-parametric approach which is central to the PRIMER package, e.g. by optimising the *ANOSIM R* statistic (see Section 9) as a measure of group separation based only on the ranks of the resemblance matrix. These new (and old) clustering methods, all accessed by **Analyse>CLUSTER**, are described in detail in Chapter 3 of CiMC. For most methods the output is a dendrogram, i.e. tree diagram, displaying a hierarchical grouping of samples (or sometimes of species, see Section 10), with a divisive hierarchy being differentiated visually from an agglomerative one by a slight change in the way the final pairings are displayed. The main output of the non-hierarchical *kRCLUSTER* method(s) is simply a factor (or indicator) specifying the group to which each of the samples (or species) is allocated. All routines can be applied directly to any of the triangular matrices produced by the **Analyse>Resemblance** menu.

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