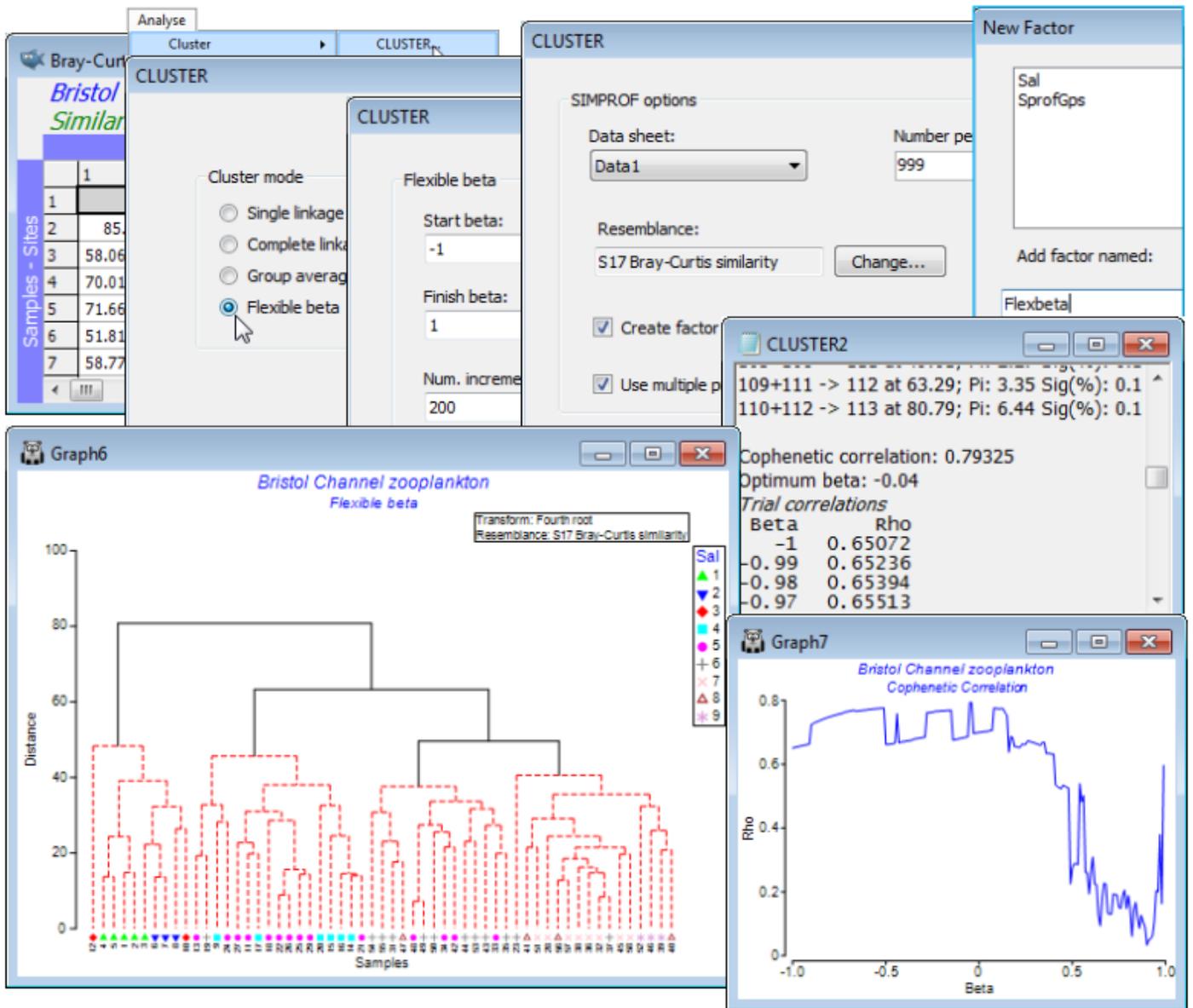


Linkage by flexible beta method

There are four possible Cluster mode choices within the **Analyse>Cluster>CLUSTER** dialog box, distinguished by the way they redefine the among-group dissimilarities at each proposed step of the agglomerative process. The *linkage options* are: •Single (/nearest neighbour) linkage, which has a tendency to produce unhelpful 'chaining' of groups, with many steps adding just a single sample to an existing group; •Complete (/furthest neighbour) linkage, which tends to have the opposite 'over-grouped' effect; •Group average (Unweighted Pair Group Method with Arithmetic mean UPGMA) which is the option shown in all the above plots and is widely used; and •Flexible beta, introduced by Lance GN & Williams WT 1967, *Comp J* 9: 373-380, a generalisation of a WPGMA method in which a range of options is controlled by choice of a parameter β . Chapter 3 of CiMC gives precise definitions of all these options, e.g. for flexible beta see the footnote on p3-4. Choice of β is made automatically to maximise the *cophenetic correlation* ρ between the dissimilarities/distances in the resemblance matrix and distances through the dendrogram between the matching pairs of samples – this idea was met near the beginning of this section – and a plot of ρ vs. β displayed.

Remove the selection on the fourth-root transformed data matrix **Data1**, by **Select>All** (and **Edit>Clear Highlight**, though this is not essential) then with the active sheet as the similarity matrix calculated from **Data1**, take **Analyse>Cluster>CLUSTER>**(SIMPROF test) & (Cluster mode • Flexible beta)>(Start beta: **-1**) & (Finish beta: **1**) & (Num. increments: **200**). These are the defaults, meaning that the cophenetic correlation is computed and graphed for β in increments of 0.01, with the optimum β (maximum ρ) given in the Cluster results window, and this value used to calculate the dendrogram. Note that β does need to be in the range (-1, 1) but negative values (or zero) make better sense theoretically, as is seen here in the line plot of the cophenetic correlation ρ vs. β , so there is a case for restricting to (Start beta: **-1**) & (Finish beta: **0**) & (Num. increments: **100**). If a fixed value of β is preferred (Lance & Williams suggest $\beta = -0.25$), as it might be for repeated clustering, then take, for example (Start beta: **-0.25**) & (Finish beta: **-0.25**) & (Num. increments: **1**). You will also need to specify a factor for the SIMPROF groups, e.g. Add factor named: **Flexbeta**, which gives a Multi-plot (see next section) of the dendrogram and the line plot of ρ vs. β .



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