

differences, i.e. the sum of squared differences between the individual distance values and their average.

Another choice that one can make concerning the NMDS algorithm was also described in the original Kruskal (1964) paper and concerns how to handle tied values among the input distances: in the *primary* approach, different occurrences of the same distance value might be matched with different fitted values, while in the *secondary* approach, tied values must be matched with the identical fitted value (see section 3.12 and Legendre & Legendre 2012, pp. 514-514).

Finally, after the NMDS helper applied the method to a distance matrix calculated from a data-table and an additional step was assigned to it, the original variables (columns) of the input data-table can be related to the resulting NMDS space as supplementary variables. This allows one to project the response variables either as linear vectors (when biplot scores of supplementary variables are graphed) or as centroids. Note, however, than unlike the ordination diagrams in other ordination methods (CA, DCA, CCA, PCA, or RDA), this has no theoretical basis, because the NMDS method, usable with any type of dissimilarity measure, cannot postulate any explicit model of response-variable relationship to the ordination axes.

NMDS does not produce any standard Canoco 5 scores, but it does produces specialized NMDS.* scores that can be plotted as standard case scores.

Canoco 5 maximizes the variation of case scores along NMDS axes by applying a principal component rotation to the scores resulting from the NMDS optimization process. This is achieved in a subsequent PCA step of the NMDS analyses generated by the Canoco Adviser and this rotation is also advisable for customized analyses.

4.4.3.7 Principal Coordinates Analysis (PCO) and PCNM

PCO inserts a custom page at the beginning of the Analysis Setup Wizard page sequence. The page contents (in the basic version, without PCNM-related options) is illustrated below.

Setup principal coordinate analysis of sample dissimilarities

Input Data Table

Table 'Table 1' contains:

data for calculating sample distances square matrix of (dis)similarities and the actual values are:

using this distance measure: distances

SQRT(Bray-Curtis distance) distances

Export distances into TSV file: Browse

PCO Results Use

From Principal Coordinate Analysis results use:

all axes with positive eigenvalues

axes with 1 largest positive eigenvalues

all axes with non-zero eigenvalues

Project plant species as supplementary data

The *Input Data Table* area allows you to specify how the matrix of distances will be obtained. See the NMDS custom page (section 4.4.3.6) for a detailed description, including the 11 available distance measures.

PCO is applied to the distance matrix by transforming the distances (D_{ij}) to a $\{-0.5 D_{ij}^2\}$ matrix, which is then double-centred (see e.g. Jongman et al. 1995; equation 5.17) and