Comparison of nMDS and PCoA

— Point of view of P. Legendre

In PCoA, the solution is found using eigen decomposition of the transformed dissimilarity matrix. In nMDS, the solution is found by an iterative approximation algorithm.

Nonmetric multidimensional scaling (**nMDS**)

1. The iterative algorithm may find different solutions depending on the starting point of the calculation, which, in most instances, is a randomly chosen configuration.

2. The dissimilarities are distorted (stretched or squeezed) during nMDS calculation. That is an acknowledged property of the method. The distances in the ordination solution do not exactly correspond to the starting dissimilarities.

3. The solution may differ depending on the criterion that one (or R function) chooses to optimise: Stress.formula1, Stress.formula2, Sstress, or Strain. These different criteria are available in different nMDS functions. Except for highly experienced users, it is difficult to determine which option is best for a particular data set.

4. In some nMDS functions, several parameters are available, which can produce different ordination solutions. It is difficult for users to determine which option is best for a particular data set. For that reason, users usually choose the default option of the R function or program.

5. Users must determine the number of dimensions of the ordination solution. If a user asks to produce all ordination axes, the solution is not exact since the distances are distorted.

6. The stress statistic does not indicate the proportion of the variance of the data represented in the ordination solution.

=> nMDS is useful, for example, when it is necessary, for a figure drawn for publication, to squeeze in two dimensions a PCA or PCoA solution that requires 3 or 4 dimensions to represent well the main distance relationships among the sites.

Principal coordinate analysis (**PCoA**)

1. PCoA finds the optimal solution by eigenvalue decomposition. The PCoA solution is unique.

2. In a PCoA ordination, the dissimilarities are not distorted in the ordination solution.

3. PCoA can be used to find the first few ordination axes for a given dissimilarity matrix. These axes are those that maximize the variance of the observations.

4. PCoA allows one to find **all** ordination axes corresponding to a given dissimilarity matrix. The matrix of PCoA ordination axes allows one to precisely reconstruct the distances among objects. Reason: the matrix of Euclidean distances among objects computed from the PCoA axes is strictly equal to the dissimilarity matrix subjected to PCoA, whatever the dissimilarity function that has been used. Proof of that property is found in Gower (1966) and in Legendre & Legendre (2012). The ordination solution is unique and exact.

5. Hence, the set {dissimilarity function, ordination method} produces a unique transformation of the data, and it is reproduced exactly if one runs PCoA again on the same data. That solution can be used as starting point for new analyses, for example for *K*-means partitioning.

6. The pseudo-R^2 statistic, computed as the sum of the eigenvalues of the axes of interest (for example the first 2 axes) divided by the sum of all eigenvalues, indicates the fraction of the variance of the data represented in the ordination. This is a useful statistic to assess the ordination result.