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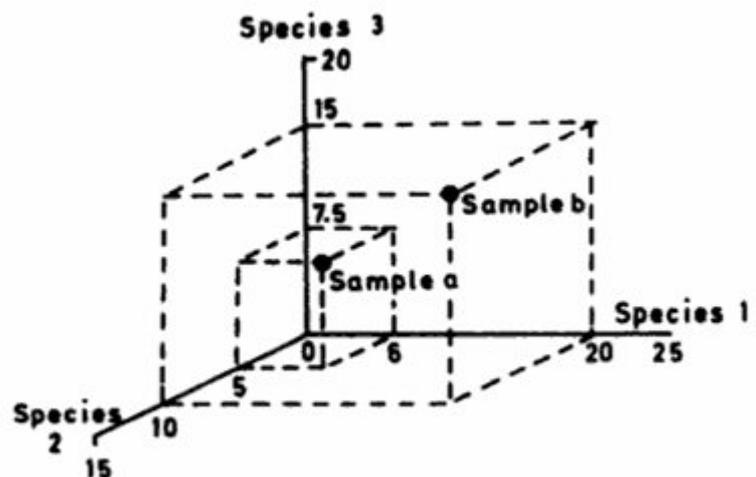
Ordination analysis

Theory

Ordination (from Latin *ordinatio*, putting things into order, or German *die Ordnung*, order) is a multivariate analysis, which searches for a continuous pattern in multivariate data, usually the data about species composition of community samples (sample \times species matrix). We can imagine such multivariate data as samples located in multidimensional hyperspace, where each dimension is defined by an abundance of one species (example for a community of two samples with three species is on [Figure 1](#)). The use of ordination in ecology was pioneered by English-born Australian botanist and ecologist [David Goodall](#), whose first paper using ordination (PCA) was published in 1954 ([Goodall 1954](#)).

The main assumption of ordination is that analyzed data are redundant, i.e. they contain more variables than is necessary to describe the information behind, and we can reduce the number of these variables (and dimensions) without losing too much information. For example, in the case of species composition data, often some of the species are ecologically similar (e.g. species which prefer to grow in wet instead of dry habitat), meaning that the dataset contains several redundant variables (species) telling the same story. Or, to explain the redundancy in another way, from occurrence (or absence) of one species we can often predict occurrence (or absence) of several other species (e.g. if the sample includes species of wet habitats, we may expect that species preferring dry habitats will not be present, while other wet-loving species may occur).

Fig. 1: Multivariate species space defined by three species, with two samples located according to abundance of the three species. From Zuur et al. (2007).



Since multidimensional space is not easy to display, describe or even just imagine, it is worth to reduce it into few main dimensions, while preserving maximum information. This also means that if the individual variables are completely independent of each other (e.g. each species have entirely different preferences), then ordination is not likely to find some reasonable reduction of the multidimensional space since each dimension (species) has its meaning.

What ordination method does can be formulated in two alternative ways:

1. it searches for gradients in species composition (represented by ordination axes) and attempts to explain these gradients by environmental variables; or
2. it searches for distribution of samples in reduced ordination space which maximally reflects the

dissimilarity between samples in terms of their species composition.

Types of ordination methods

Table 1 summarizes individual ordination methods.

	(a) Raw-data-based (classical approach)		(b) Transformation-based	(c) Distance-based
	Linear	Unimodal		
(1) Unconstrained (indirect) Shiny app (how to use, blog)	PCA Principal Component Analysis	CA & DCA Correspondence Analysis & Detrended Correspondence Analysis	tb-PCA Transformation-based Principal Component Analysis	PCoA, NMDS Principal Correspondence Analysis, Non-metric Multidimensional Scaling
(2) Constrained (direct, canonical) Shiny app	RDA Redundancy Analysis	CCA Canonical Correspondence Analysis	tb-RDA Transformation-based Redundancy Analysis	db-RDA Distance-based Redundancy Analysis

Tab. 1: Summary of ordination methods. Based on Lepš & Šmilauer (2003), extended for other methods from Legendre & Legendre (2012).

Ordination methods in Table 1 can be divided according to two criteria: **whether their algorithm includes also environmental variables** along to the species composition data: unconstrained do not, constrained do, and **what type of species composition data is used for analysis**: raw data (sample-species matrix of species composition), pre-transformed raw data (e.g. using Hellinger transformation), or distance matrix (sample-sample symmetric matrix of distances between samples).

Does the ordination algorithm include also environmental variables?

(1) Unconstrained ordination (indirect gradient analysis)

Ordination axes are not constrained by environmental factors. The method aims to uncover the main gradients (directions of changes) in species composition data, and returns unconstrained ordination axes, which corresponds to the directions of greatest variability within the dataset. Optionally, these gradients can be *post hoc* (after the analysis) interpreted by environmental variables (if these are available). Environmental variables do not enter the ordination algorithm. Unconstrained ordination is primarily an exploratory analytical method, used to explore the pattern in multivariate data; it generates hypotheses, but does not test them.

(2) Constrained ordination (direct gradient analysis, canonical ordination)

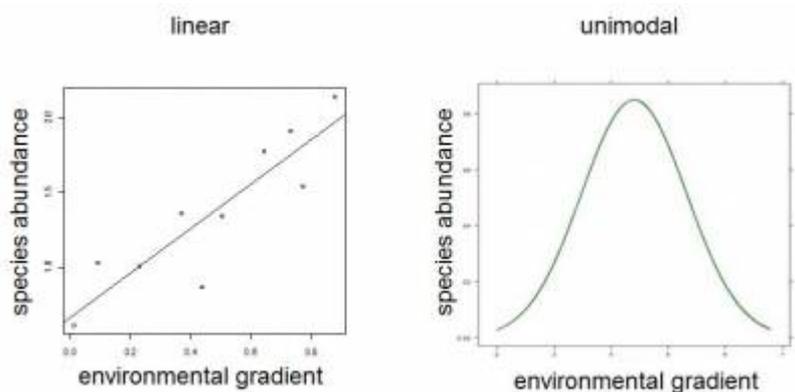
Ordination axes are constrained by environmental factors. It relates the species composition directly to the environmental variables and extracts the variance in species composition which is directly related to the environment. Environmental variables directly enter the algorithm, and the constrained ordination axes corresponds to the directions of the variability in data which is explained by these environmental variables. The method is usually used as confirmatory analysis, i.e. it is able to test the

hypotheses about the relationship between environmental factors on species composition (unlike unconstrained ordination, which is exploratory). It decomposes the total variance in species composition data into a fraction explained by environmental variables (related to constrained ordination axes) and not explained by environmental variables (related to unconstrained ordination axes). It offers several interesting opportunities when it comes to explanatory variables: **forward selection** (the selection of important environmental variables by excluding those which are not relevant for species composition), **Monte Carlo permutation test** (a test of significance of the variance explained by environmental factors) and **variance partitioning** (partitioning of the variance explained by different groups of environmental variables).

What type of species composition data is used for analysis?

(a) Raw-data-based methods (classical approach)

Fig. 2: An assumption of linear (left) vs unimodal (right) response of species fitness/abundance along environmental gradient distinguishes the use of linear vs unimodal ordination method.

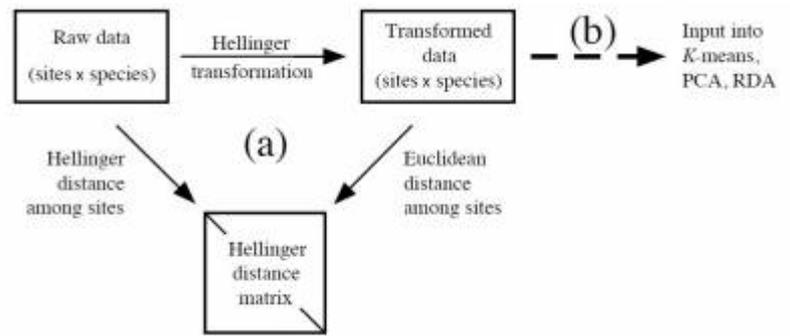


Methods based on analysis of raw sample-species matrices with abundance or presence/absence data. Within these methods, two categories are traditionally recognized, differing by an assumption of species response along the environmental gradient:

- **linear** (Figure 2, the left figure) – assume that species response linearly along environmental gradient, which could be true for rather homogeneous ecological data, where ecological gradients are rather short (Figure 4 left);
- **unimodal** (Figure 2, the right figure) – species response unimodally along gradient, having its optima at certain gradient position; this model is more close to the reality of ecological data and is more suitable for heterogeneous datasets (structured by a strong or long ecological gradient, with high species turnover and many zeroes in the species matrix) with rather long environmental gradients (Figure 4 right).

(b) Transformation-based methods (tb-PCA and tb-RDA)

Fig. 3: (a) Hellinger distance can be calculated either directly from raw species composition data, or by first transforming species composition data by Hellinger transformation (standardization) and then applying Euclidean distance on these transformed data. (b) Hellinger transformed data could be used in ordination methods using Euclidean distance (e.g. PCA, RDA, K-means clustering), in which case these methods use Hellinger distances (Hellinger transformed data + Euclidean distance = Hellinger distance). From Legendre & Legendre (2012), modified from Legendre & Gallagher (2001).



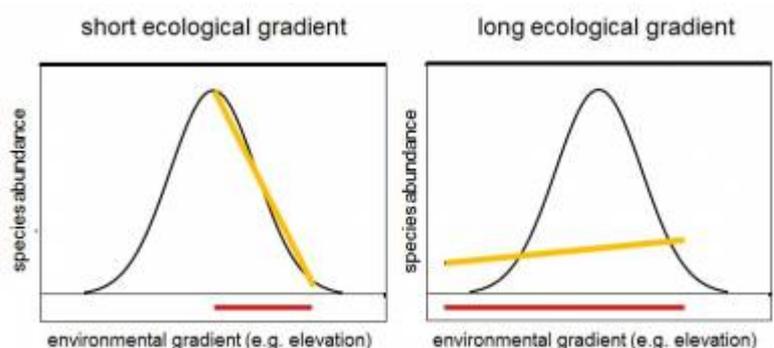
This category includes linear raw-data-based ordination methods (PCA, RDA), applied on sample x species data transformed by Hellinger (or one of several other) transformations. The Euclidean distance (implicit for PCA/RDA (Figure 3) when applied on Hellinger-transformed species composition data results into Hellinger distance, which is more suitable for ecological data, because (contrary to Euclidean distance) it is asymmetric (ignores double zeros). Legendre & Gallagher (2001) consider this as a preferable way how to analyse heterogeneous data (otherwise not suitable for linear methods) using linear ordinations¹. Additionally to Hellinger transformation, the other suitable transformation is chord transformation, and other possible (but less suitable) transformations are species profile transformation, chi-square distance and chi-square metric transformations.

(c) Distance-based methods

Methods using the matrix of distances between samples measured by distance coefficients, and projecting these distances into two- or more-dimensional ordination diagrams. **Distance-based RDA (db-RDA)** is the combination of PCoA, applied on raw data using selected distance measure, and RDA applied on eigenvectors resulting from PCoA. It offers an alternative to RDA (based on Euclidean distances) and tb-RDA (based on Hellinger distances if transformed by Hellinger transformation), with a freedom to choose distance measure suitable for investigated data².

Linear or unimodal ordination method?

Fig. 4: Hypothetical species response along environmental gradient. Red line indicates the segment of the gradient actually sampled, and yellow line indicates how would the species response look like if fitted by linear model. According to Lepš & Šmilauer (2003).



In the case that we sampled rather a short fraction of the environmental gradient (short red line

segment at the left figure of [Figure 4](#)), we may assume that species response (although fundamentally unimodal) can be modeled as linear (yellow line segment). In the case of the long gradient (figure at right), to model species response as linear would be wrong (right figure of [Figure 4](#)).

To decide whether to apply **linear or unimodal ordination method** on your data, you can use the rule of thumb introduced by [Lepš & Šmilauer \(2003\)](#): first, calculate DCA (detrended by segments) on your data, and check the length of the *first* DCA axis (which is scaled in units of standard deviation, S.D.). The length of first DCA axis > 4 S.D. indicates heterogeneous dataset on which unimodal methods should be used, while the length < 3 S.D. indicates homogeneous dataset for which linear methods are suitable (see [Figure 5](#)). In the gray zone between 3 and 4 S.D., both linear and unimodal methods are OK. Note that while linear methods should not be used for heterogeneous data, unimodal methods can be used for homogeneous data, but linear methods, in this case, are more powerful and should be preferred. Alternatively, if your data are heterogeneous, but you still want to use linear ordination methods (PCA, RDA), apply them on Hellinger transformed species composition data to calculate ordination based on Hellinger distances (as recommended e.g. by [Legendre & Gallagher \(2001\)](#)).

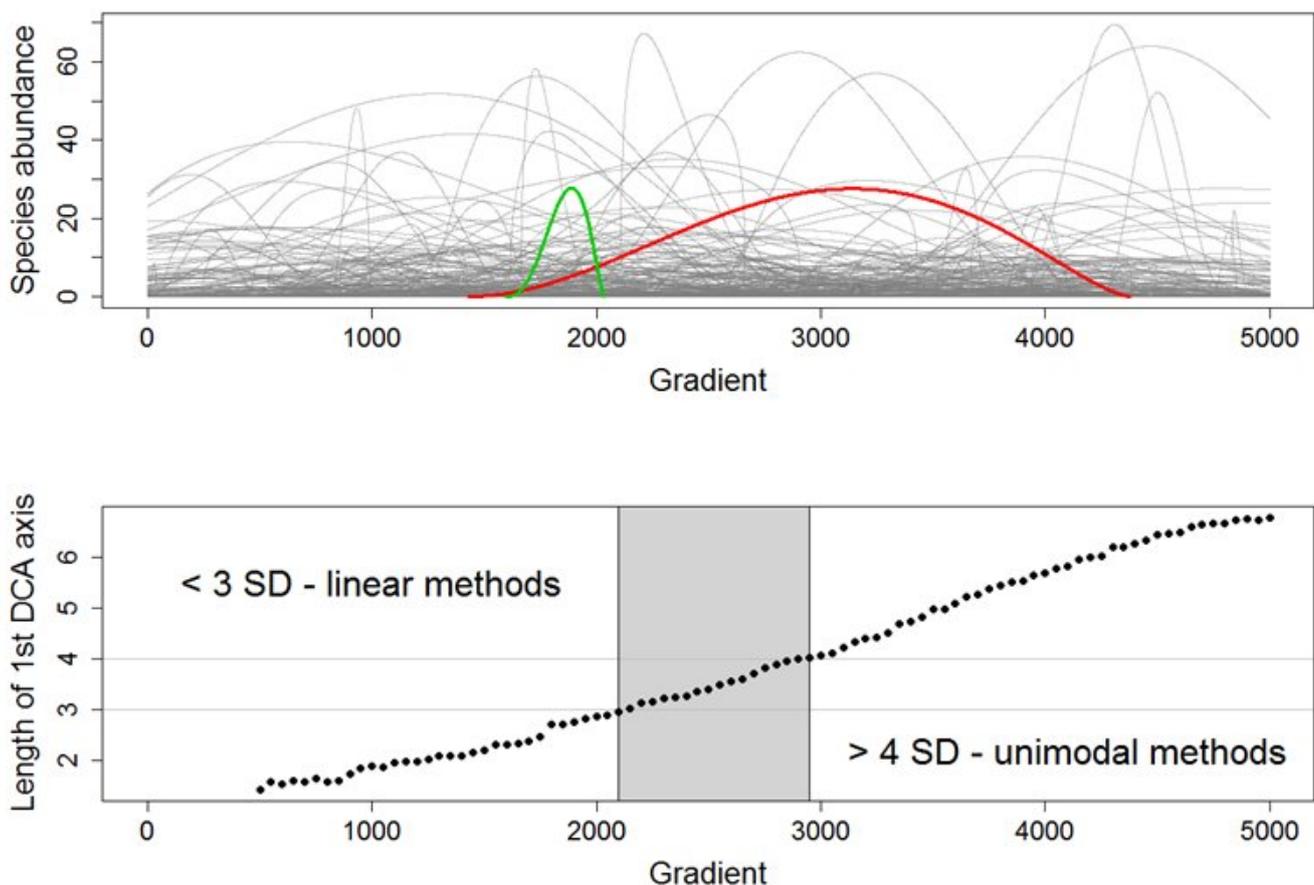
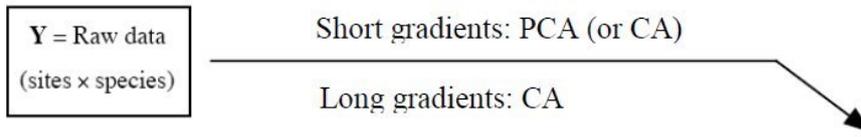


Fig. 5: Illustration of the rule how to select whether to use linear ordination methods (like PCA or RDA) or unimodal (CA, DCA or CCA) on the data. Upper diagram shows simulated community structured by a single environmental gradient, with number of species response curves. The diagram below shows the relationship between the length of the gradient sampled in the simulated community on the //x/-axis (in arbitrary units), and length of the first DCA ordination axes (in units of S.D.). The dataset which according to DCA is rather homogeneous (< 3 S.D.) has environmental gradient up to 2000 units long; the longer gradient results into heterogeneous dataset for which linear methods are not suitable.

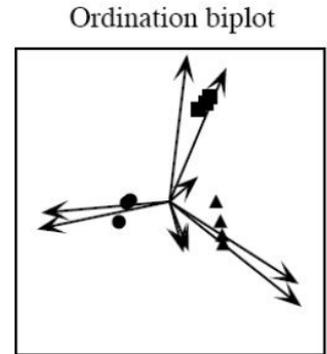
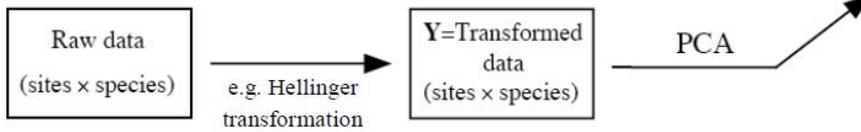
Summary: Three alternative approaches for ordination

(1) Unconstrained ordination analysis

(a) Classical approach

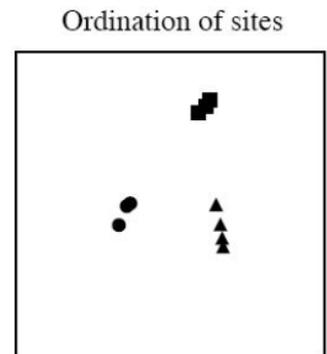
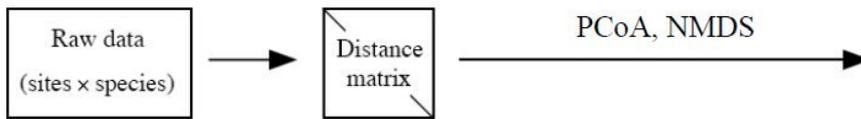


(b) Transformation-based approach (tb-PCA)



Representation of elements:
Species = arrows (for linear methods) or centroids (for unimodal)
Sites = symbols

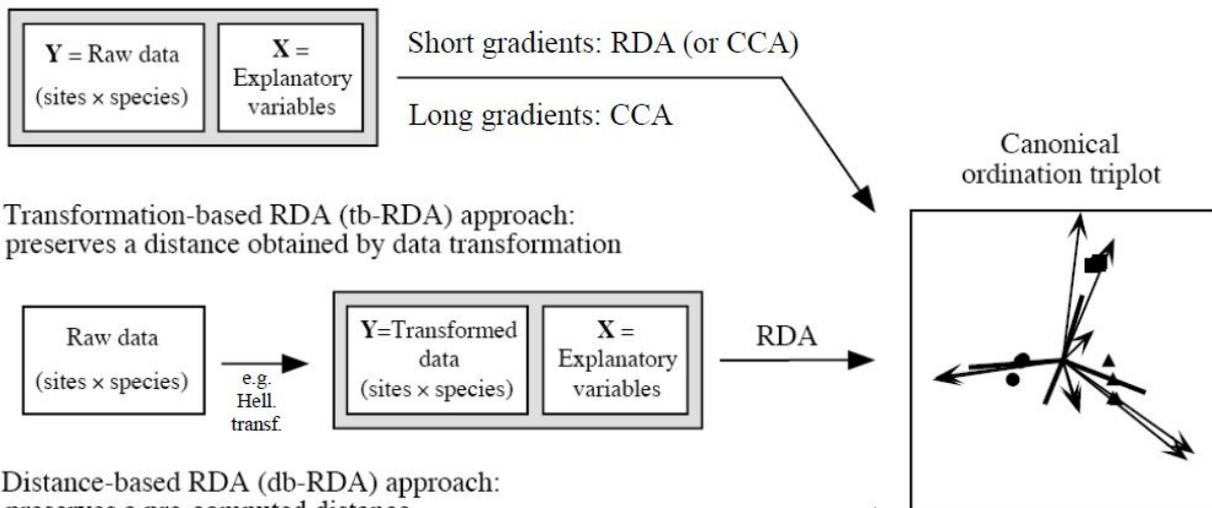
(c) Distance-based approach (PCoA)



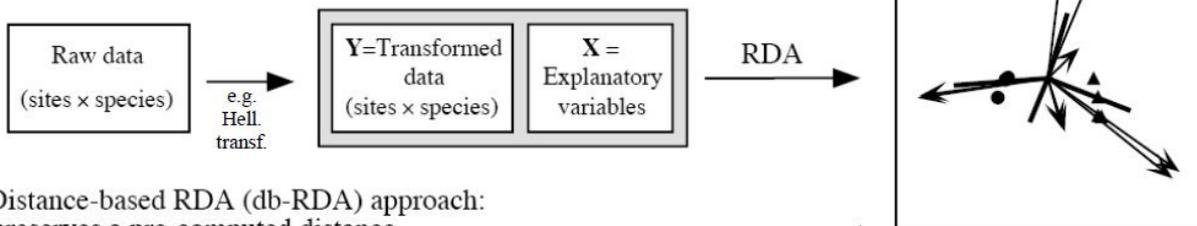
Representation of elements:
Sites = symbols
(Species could be added e.g. as weighted averages)

(2) Constrained ordination analysis

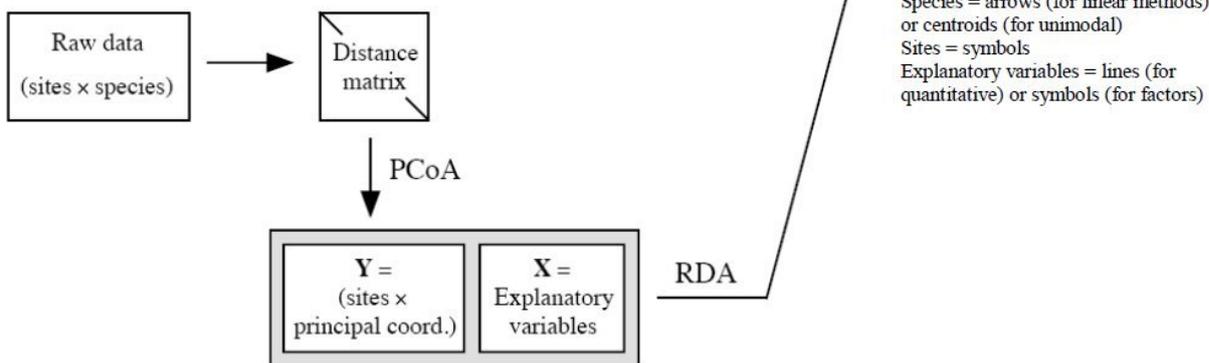
(a) Classical approach: RDA preserves the Euclidean distance, CCA preserves the chi-square distance



(b) Transformation-based RDA (tb-RDA) approach: preserves a distance obtained by data transformation



(c) Distance-based RDA (db-RDA) approach: preserves a pre-computed distance



Representation of elements:
 Species = arrows (for linear methods) or centroids (for unimodal)
 Sites = symbols
 Explanatory variables = lines (for quantitative) or symbols (for factors)

(slightly) modified from Legendre & Legendre (2012)

Fig. 6: Three alternative approaches to unconstrained (above) and constrained (below) ordination analysis. From Legendre & Legendre (2012), slightly modified by D. Zelený.

Further reading

- [Ordination methods - an overview \(Mike Palmer\)](#)

1) Oposite opinion, however, was presented by [Minchin & Rennie at the ESA conference in 2010](#).
 2)

Distance measure used in PCoA and db-RDA must be Euclidean, i.e. it must obey triangle inequality principle, otherwise it will produce negative eigenvalues, which in db-RDA may result in unrealistically high explained variation.

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<https://www.davidzeleny.net/anadat-r/> - **Analysis of community ecology data in R**

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