



# Assessing similarity of $n$ -dimensional hypervolumes: Which metric to use?

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## Abstract

**Aim:** The  $n$ -dimensional hypervolume framework (*Glob. Ecol. Biogeogr.* [2014] 23:595–609) implemented through the R package 'hypervolume' is being increasingly used in ecology and biogeography. This approach offers a reliable means for comparing the niche of two or more species, through the calculation of the intersection between hypervolumes in a multidimensional space, as well as different distance metrics (minimum and centroid distance) and niche similarity indexes based on volume ratios (Sørensen–Dice and Jaccard similarity). However, given that these metrics have conceptual differences, there is still no consensus on which one(s) should be routinely used in order to assess niche similarity. The aim of this study is to provide general guidance for constructing and comparing  $n$ -dimensional hypervolumes.

**Location:** Virtual study site.

**Taxon:** Virtual species.

**Method:** First, the literature was screened to verify the usage of the different metrics in studies (2014–2018) relying on this method. Subsequently, a comparative analysis based on simulated morphological and bioclimatic traits was performed, taking into consideration different analytical dimensions, sample sizes and algorithms for hypervolume construction.

**Results:** Literature survey revealed that there was no clear preference for one metric over the others in current studies relying on the  $n$ -dimensional hypervolume method. In simulated data, a high correlation among similarity and distance metrics was found for all datatypes considered. For most analytical scenarios, using at least one overlap and one distance metric would be therefore the most appropriate approach for assessing niche overlap. Yet, when hypervolumes are fully disjunct, similarity metrics become uninformative and calculating the two distance metrics is recommended. The sample size and the choice of algorithm and dimensionality can lead to significant variations in the overlap of hypervolumes in the hyperspace, and therefore should be carefully considered.

**Main conclusions:** Best practise for constructing  $n$ -dimensional hypervolumes and assessing their similarity are drawn, representing a practical aid for scientists using the 'hypervolume' R package in their research. These recommendations apply to most datatypes and analytical scenarios. The R scripts published alongside this methodological study can be modified for performing large-scale analyses of species niches



or automatically assessing pairwise similarity metrics among multiple hypervolume objects.

#### KEYWORDS

bioclimatic variables, centroid distance, Hutchinson, Jaccard similarity, morphospace, multidimensional space, niche overlap, simulation, Sorensen similarity, species distribution modelling, traits

## 1 | INTRODUCTION

The idea that species occupy a set of specific environmental conditions within their habitats, loosely an ecological niche, has old roots in ecology and evolution (Colwell & Rangel, 2009; Martins, 2017; Soberón, 2007). Since the first introduction of the niche concept (e.g. Elton, 1927; Grinnell, 1917, 1924), different conceptual frameworks for representing species niches have been proposed in the ecological literature (Chase & Leibold, 2003). More than 60 years ago, Hutchinson (1957) theorized that the niche of a species could be approximated as an  $n$ -dimensional hypervolume, namely an abstract Euclidean space defined by a set of independent axes corresponding to, for example, environmental factors that affect organismal performance, its physiological limits or morphological traits. Although the Hutchinsonian hypervolume has so far proved to be one of the most important conceptual ideas in niche-based ecology (Colwell & Rangel, 2009; Courchamp & Bradshaw, 2018; Holt, 2009), up to now its practical application in real-world ecological data has been delayed by the objective challenges of working with a hyperspace using multidimensional mathematics.

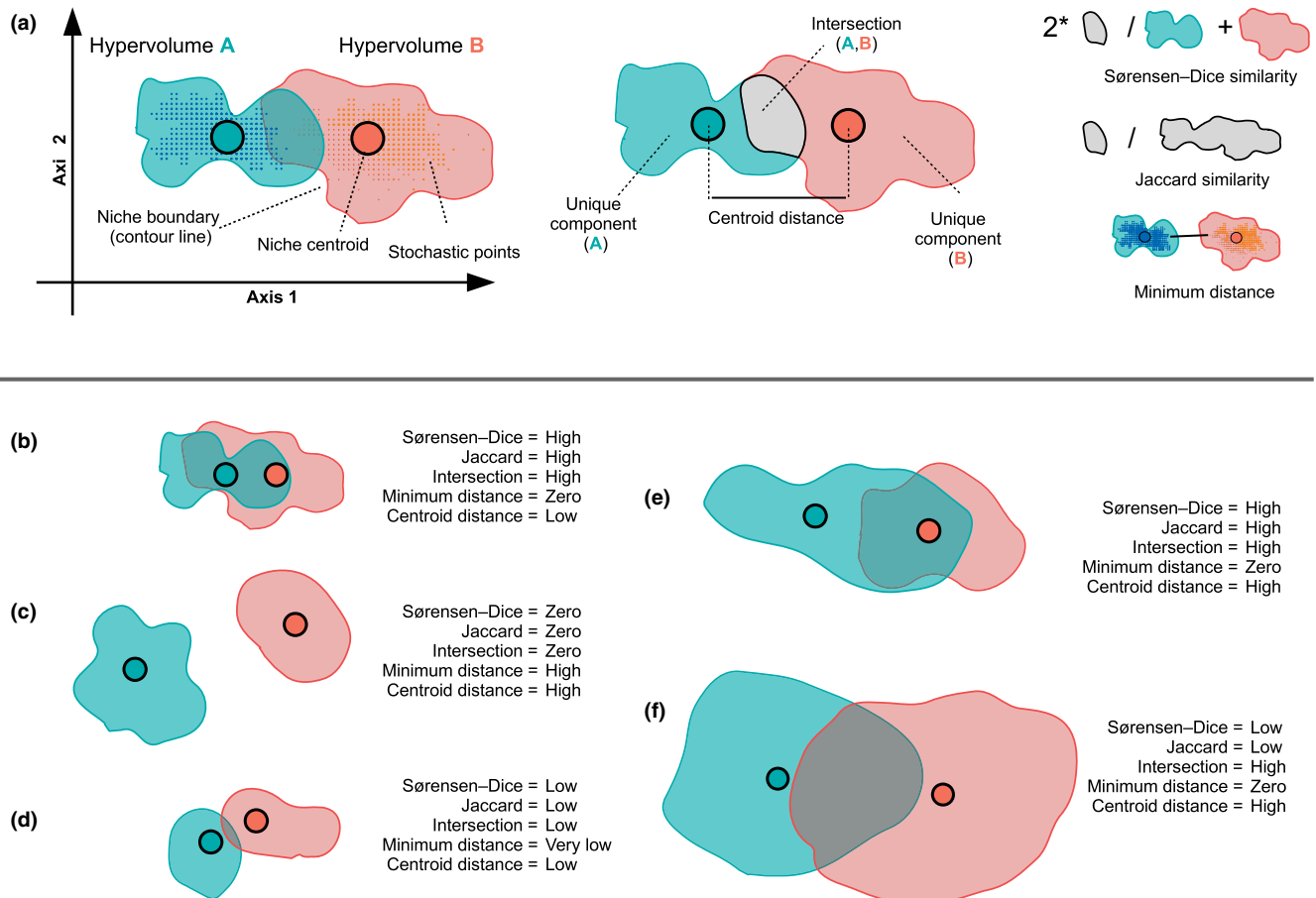
However, the Hutchinsonian niche concept recently gained new momentum, thanks to the publication of a (relatively) simple and computationally fast statistical framework for constructing and visualizing geometrical  $n$ -dimensional hypervolumes (Blonder, Lamanna, Violle, & Enquist, 2014; Blonder et al., 2018). The  $n$ -dimensional hypervolume method, implemented through the 'hypervolume' R packages (Blonder, 2018a), relies on high-dimensional kernel density estimation (Blonder et al., 2014), support vector machine delineation or convex hull generation procedures (Blonder et al., 2018) to delineate the shape and volume of the niche hyperspace (Figure 1a). In just a few years, this method has become popular among ecologists, biogeographers and evolutionary biologists, extensively applied in niche- and trait-based studies (Table S1 in Appendix S1) and the subject of different theoretical and technical discussions (Blonder, 2016a, 2016b; Blonder et al., 2017; Carmona, de Bello, Mason, & Lepš, 2016; Carvalho & Cardoso, 2018; Qiao, Escobar, Saupe, Ji, & Soberón, 2017a, 2017b). For instance,  $n$ -dimensional hypervolumes are being increasingly used to explore the bioclimatic niches of species in space and time (Duque-Lazo, Navarro-Cerrillo, & Ruíz-Gómez, 2018; Greve et al., 2017; Krehenwinkel, Rödder, & Tautz, 2015; Mammola & Isaia, 2017; Tingley, Vallinoto, Sequeira, & Kearney, 2014), to address

the question of the functional diversity of populations and communities (Barros, Thuiller, Georges, Boulangeat, & Münkemüller, 2016; Bittebiere, Saiz, & Mony, 2019; Bourgeois et al., 2019; Díaz et al., 2016; Enrique et al., 2018; Papuga, Gauthier, Pons, Farris, & Thompson, 2018), to tackle behavioural processes (Pruitt et al., 2017), and to assist species delimitations and taxonomical descriptions (Koch et al., 2016; Mammola et al., 2018; Onn, Abraham, Grismer, & Grismer, 2018; Simó-Riudalbas, Tarroso, Papenfuss, Al-Sariri, & Carranza, 2018). Furthermore, this method has been conveniently adapted to specific research questions (Irl et al., 2017) and/or used to analyse non-biological types of data (e.g. Gonzalez-Granadillo, Garcia-Alfaro, & Debar, 2017; Kudła & Pawlak, 2018).

The  $n$ -dimensional hypervolume is greatly appreciated because it provides a simple means for comparing the niche of one or more species in a multidimensional space. This is done by calculating different metrics ranging from the intersection between hypervolumes to different distance metrics and niche similarity indices based on volume ratios (Table 1). These metrics allow the researcher to quantify shared niche volume in the multidimensional space as well as the hypervolume relatedness, and thus to indirectly assess competition dynamics, niche convergence or displacement and phylogenetic niche conservatism. However, given that, on one hand, these metrics have subtle conceptual differences and, on the other, a comprehensive comparison is lacking between their performance in relation to varying analytical scenarios, there is still no consensus on which one(s) should be routinely calculated in order to compare two or more hypervolumes.

The goal of this study is to systematically test the inherent effects of different sources of variability in the construction of hypervolumes and assessment of their similarity, in order to deliver a first guideline on how to build robust and unbiased analyses based on the R package 'hypervolume'. Initially, the literature was screened to verify the usage of the different overlap and distance indexes in current research studies (2014–2018) relying on this method. Subsequently, based on simulations (Zurell et al., 2010), I explored the following questions:

- What are the optimal metrics for assessing similarity between  $n$ -dimensional hypervolumes?
- What is the influence of the sample size on the assessment of the similarity between hypervolumes?
- Which other parameters (algorithm, bandwidth) influence the assessment of the similarity between hypervolumes?



**FIGURE 1** Representation of two hypervolumes A and B in a two-dimensional space and different theoretical configurations of two 2-dimensional hypervolumes. (a) Using the method by Blonder et al. (2014, 2018), the two-dimensional hypervolumes for two species A and B can be constructed and visualized as a pair plot. The stochastic coloured points for each species reflect the real description of each hypervolume, that is, random points sampled from the inferred hypervolume (mathematical details in Blonder et al., 2014: p. 598 Box 1; p. 599 Box 2). The contour lines bounding the niches are used for a more intuitive visual presentation. Once two hypervolumes are generated, different geometrical operations can be computed (see Table 1) to estimate hypervolume distance (Centroid distance, Minimum distance) and shared volume (Intersection, Sørensen–Dice similarity, Jaccard similarity). (b) Typical configuration of overlapping hypervolumes, in which all similarity and distance metrics are highly correlated or anticorrelated. (c) Configuration of two disjunct hypervolumes. In this case, all similarity metrics reach values of zero and only distance metrics can be used to quantify the extent to which the two hypervolumes are dissimilar. (d) Configuration of two hypervolumes in which, on one hand, similarity metrics are low due to a limited volume intersection and, on the other, niche centroids are relatively close. (e) Configuration of two hypervolumes in which intersection and similarity is high, but also the distance between niche centroids. (f) Configuration of two hypervolumes in which intersection is high, but simultaneously similarity indexes are not, because the two hypervolumes have conspicuous unique components [Colour figure can be viewed at [wileyonlinelibrary.com](http://wileyonlinelibrary.com)]

For each one of these three questions, the nature of the input data (morphological traits or climatic variables) was furthermore taken into account, as well as the effect of the number of axes used to construct the hypervolume (i.e. analytical dimensionality).

## 2 | MATERIALS AND METHODS

### 2.1 | Literature overview

The usage of the different overlap and distance metrics (see Table 1) in research studies relying on the  $n$ -dimensional hypervolume method was verified via a survey of the recent literature. All Journal articles citing the method by Blonder et al. (2014) were searched for in Google Scholar (<https://scholar.google.it/>), considering a time range

from the first online publication of the method to 6 August 2018 (i.e. the first draft of this paper). Only peer-reviewed international articles were considered, that is, excluding articles not in English, preprints, conference papers, book chapters, theses and dissertations. Assembled papers were screened to verify which of the five standard metrics (Table 1) was used by the authors to compare the generated hypervolumes (see Table S1 in Appendix S1). Additional non-default metrics employed by the authors to compare hypervolumes were classified as 'Others' metrics. To verify whether the usage of metrics varied according to the type of study, the nature of the data employed in each paper was also assessed, that is, either 'Environmental variables' (e.g. bioclimatic variables), 'Functional traits' (e.g. size), a combination of both or 'Other' datatypes (e.g. differential type of indexes).



**TABLE 1** Metrics for assessing similarity and distance between  $n$ -dimensional hypervolumes currently implemented in the 'hypervolume' R package (Blonder, 2018a). Note that two hypervolumes can be compared via these metrics only if they are constructed using the same axes, both in term of number of axes (dimensionality) and their identity (type of data). See Figure 1 for some examples of hypervolume configurations

Metric	R command	Definition	Notes
Intersection ( $\cap$ )	hypervolume_set()	The intersection of the two hypervolumes in the multidimensional space, calculated as the fraction of points falling within the boundaries of both hypervolumes	A positive value always lower than the total volume of the two input hypervolumes. Note that the computation is performed on a random sample of points from both hypervolumes
Centroid distance	hypervolume_distance()	The Euclidean distance between the centroids of two hypervolumes	A positive value that tends to zero as the distance between centroids decreases
Minimum distance	hypervolume_distance()	The pairwise minimum Euclidean distance between two sets of random points comprising two hypervolumes	Note that, by definition, the minimum distance is smaller than the centroid distance
Sørensen–Dice similarity (S)	hypervolume_overlap_statistics()	Given two hypervolumes A and B, $S(A,B)=2* A \cap B /( A  +  B )$	Both indices range from 0 (both input hypervolumes are fully disjunct) to 1 (both input hypervolumes are identical)
Jaccard similarity (J)	hypervolume_overlap_statistics()	Given two hypervolumes A and B, $J(A,B)= A \cap B / A \cup B $	

Notes: A = a hypervolume; B = a hypervolume;  $\cap$  = intersection between two hypervolumes, as calculated via the *hypervolume\_set* R function;  $\cup$  = union between two hypervolumes as calculated via the *hypervolume\_set* R function.

## 2.2 | Simulation experiments

For each simulation, two independent sets of morphological traits and bioclimatic variables were used to generate virtual species. These variables were chosen as they are the most common type of data currently studied in  $n$ -dimensional hypervolume studies (Blonder, 2018b). Furthermore, for each simulation three distinct analytical dimensions were tested, that is, varying from three to five the number of input variables (axes) to generate from three- to five-dimensional hypervolumes. All simulations were performed in R (R Core Team, 2017).

Simulations based on morphological data represent hypothetical studies of species traits in a multidimensional morphospace (Blonder, 2018b). Morphological traits were generated using the R packages 'phytools' (Revell, 2012) and 'APE' (Paradis, Claude, & Strimmer, 2004), whereby pure birth trees with 30 tips each were generated and combined in an ultrametric tree from which Brownian characters were extracted (Appendices S2–S4). Note that an initial exploratory analysis of additional types of virtual traits drawn from standard distributions was conducted. In particular, normal, lognormal, gamma and bimodal distributions were considered, as long as these represent alternative proxies for the distribution of real biological traits. Although simulations based on different distributions of data yielded different  $n$ -dimensional geometries, comparable results in terms of Pearson correlations among similarity and distance metrics were obtained—divergence in the correlation among metrics of maximum  $\pm 0.15$ .

Simulations based on bioclimatic data represent typical studies of a climatic niche of species in a multidimensional bioclimatic space (Blonder, 2018b), a topic which is typically explored in the context of modelling studies on the geographical distribution of species (for a discussion see Blonder et al., 2017; Qiao, Escobar, Saupe, Ji, & Soberón, 2017a; Qiao, Escobar, Saupe, Ji, & Soberón, 2017b). For simulating bioclimatic data the R package 'virtualspecies' was used

(Leroy, Meynard, Bellard, & Courchamp, 2016), whereby virtual species' environmental suitability was generated from a spatial set of bioclimatic conditions.

### 2.2.1 | What are the optimal metrics for assessing similarity between $n$ -dimensional hypervolumes?

To answer the first question, the performance of the standard metrics to assess hypervolume similarity was compared to determine their reciprocal correlation. The R script to generate this set of simulations is available in Appendix S2.

For the first simulations, random sets of five virtual species were generated based on simulated morphological traits which, in turn, were used to construct morphological  $n$ -dimensional hypervolumes and to calculate overlap and distance metrics. For each analysed dimensionality, 999 random replicates were run, sampling 30 individuals of the virtual species from the generated functional trees. The virtual species simulation was constrained so that the first two species had the same range of distribution of all traits (1–10, uniform distribution), one species had a range approximately 0.5 times smaller (1–5), one approximately 2 times larger (1–20) and the last species approximately 3 times larger (1–30) than the first species—thus likely to have a significantly divergent hypervolume with respect to the other species for most simulations. Given that high correlation between the hypervolume axes can lead to biased results (Blonder et al., 2014, 2018), multicollinearity among simulated traits was explored at each run with Pearson  $r$  correlations. Whenever the Pearson  $r$  correlation between any of the generated traits was  $>|0.8|$ , the specific dataset was discarded and a new set of virtual species was generated. All generated traits for the five virtual species were standardized (Blonder et al., 2014). Hypervolumes were constructed using the box method, given that it is computationally faster, and choice of bandwidth was



automated using a Silverman estimator (Silverman, 1992). To compare the morphospace of the five virtual species, triangular matrixes of pairwise volume intersections, niche centroid distances and Jaccard and Sørensen–Dice similarity indexes were generated. All these metrics were calculated using the relevant functions of the 'hypervolume' R package (Blonder, 2018a; Table 1). Afterwards, triangular matrixes were converted to arrays (excluding the diagonal and all symmetrical duplicate values in the top parts of the matrixes) in order to calculate pairwise Pearson  $r$  correlations among the metrics.

For the second simulation, standard bioclimatic variables at a resolution of 10 min were used as input data (WorldClim; Hijmans, Cameron, Parra, Jones, & Jarvis, 2005). The variables used were: Annual Mean Temperature (Bio1), Temperature Seasonality (Bio4), Annual Precipitation (Bio12), Precipitation Seasonality (Bio15) and Mean Temperature of Driest Season (Bio9). For each analysed dimensionality, 999 random replicates were run. At each replica, three virtual species were generated using the *formatfunction* R command (Leroy et al., 2016), that is, simulating the species response to the different climatic gradients listed above and combining these responses to define the virtual environmental suitability. Specifically, a unimodal response curve—quadratic function—was assumed for each environmental variable, using a random mean within the range of the environmental gradient and a random noise. The simulation was designed to account for multicollinearity, by discarding simulated datasets in which the Pearson  $r$  correlation between any of the generated bioclimatic axes was  $>|0.8|$ . Moreover, to ensure that the results were not influenced by the choice of a specific geographical range and the environmental peculiarities therein, at each permutation, virtual species were generated into a random region of the world (here intended as different model calibration areas; Barve et al., 2011), namely either a primarily tropical area (South America), a temperate region (Europe) or an oceanic island system (Oceania). Once the three virtual species were generated, 30 geographical occurrence localities for each virtual species were randomly sampled from their area of environmental suitability via the *sampleOccurrences* R function (Leroy et al., 2016). The selection of occurrences was not constrained by any sampling bias, and was carried out using the threshold method and a randomly sampled beta between 0.4 and 0.7, that is, within a typical range of thresholds used in species distribution modelling (Liu, Berry, Dawson, & Pearson, 2005). The values of the environmental predictors were extracted for each of these localities and used to construct the bioclimatic  $n$ -dimensional hypervolumes of the three virtual species and to compare their multidimensional spaces. The hypervolumes were generated via the same methodological protocol as the simulation experiment based on morphological data and, in turn, the pairwise correlations among similarity and distance metrics were calculated.

## 2.2.2 | What is the influence of the sample size on the assessment of the similarity between hypervolumes?

To answer this second question, the influence of the sample size (i.e. the number of observations used to construct the hypervolumes)

on the assessment of the hypervolumes' similarity was evaluated. The same simulation protocol described for addressing question A was used, but this time hypervolumes were constructed based on different number of observations (10, 20, 50, 100, 200, 500, 750 and 1,000), each time sampled from the same generated random distribution of 3,000 observations. Note that to speed up the simulation, for both datatypes only two virtual species were generated, the second virtual species having a range for the distribution of all traits either 0.5 times smaller, equal, 1.5 or 2 times larger than the first species (randomized at each permutation). The values of similarity and distance metrics and the variation in overall volume dimension for each sample size were compared through analysis of variance (ANOVA), using as baseline the sample size of 10. The R script to generate this set of simulations is available in Appendix S3.

## 2.2.3 | Which parameters have the greatest influence on the assessment of the similarity between hypervolumes?

In the last simulation experiment, the influence of the method used to construct the hypervolumes was explored. The same general simulation protocol described for addressing question A was used; also, in this case, only 2 virtual species and 30 observations each were generated to reduce computational time. For each replica, the hypervolumes of the two species were constructed using three distinct algorithms, namely box (hereinafter Box), Gaussian (hereinafter Gaus) and Support Vector Machine (SVM), fitted with default settings (Blonder, 2018a). For the box and Gaussian methods, three distinct bandwidths were further considered, by multiplying the bandwidth values estimated via the Silverman estimator (Silverman, 1992) by 2, 3 and 4 respectively. The values of similarity and distance metrics for each method, as well as the overall volume dimension, were compared with ANOVA. The R script to generate this set of simulations is available in Appendix S4.

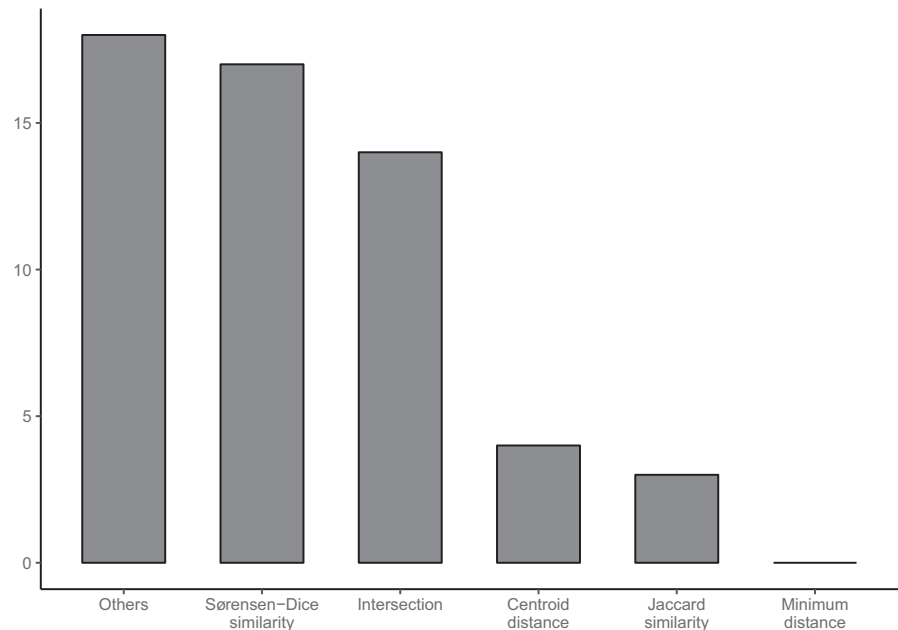
# 3 | RESULTS

## 3.1 | Literature overview

A total of 124 papers were assembled and analysed (Appendix S1). Of these, 64 were theoretical papers (e.g. reviews, opinions, methodological papers) or primary research articles citing the paper by Blonder et al. (2014) but not employing the 'hypervolume' method itself. These papers were not considered further. The usage of the overlap and distance indexes varied significantly in the remaining research studies analysed ( $n = 60$ , Figure 2). The most frequently used metrics to assess niche similarity were the Sørensen–Dice similarity (24% of the studies,  $n = 17$ ) and the intersection (20%,  $n = 14$ ). Conversely, the use of Jaccard similarity occurred sporadically (4%,  $n = 3$ ). Distance metrics were also rarely used: centroid distance was employed in four studies (5%), whereas minimum distance was never used. Eighteen studies (26%) used different types of metrics not implemented in



**FIGURE 2** Usage of the different metrics in the research studies relying on the  $n$ -dimensional hypervolume method. Studies not calculating any metric ( $n = 17$ ) are not visualized in the barplot



the 'hypervolume' R package, and 17 studies (19%) did not compare the niche of species at all, that is, they did not calculate any of these metrics. Of the 43 studies using overlap and distance metrics, 30 relied on a single metric to assess shared volume, 10 used 2 metrics and only 2 relied on 3 metrics. There was no clear preference for one metric over the others, depending on the datatype on which the study was based ( $\chi^2[4, N = 57] = 6.23$ ,  $p = 0.18$ )—either environmental variables or functional traits; other datatypes were not considered.

### 3.1.1 | Empirical correlation between indexes

Simulations based on different input data yielded similar correlation values among the different metrics considered (Figure 3). The values of the Pearson  $r$  correlations were in general lower for the simulations at higher dimensions; the absolute value of the correlation decreased at an increasing dimensionality of the analysis between similarity metrics and intersection and increased between distance metrics. As expected, correlation among all similarities and all distance metrics was high. In all simulations, the Jaccard and Sørensen–Dice similarity were the two metrics displaying the highest correlation (Pearson  $r \sim 1$  for all simulations). Both indexes showed a minor, although still  $>0.6$ , correlation with the intersection, with lower correlation values at the highest dimensionality.

The two distance metrics were significantly correlated for both datatypes considered and the three dimensionality (all Pearson  $r > 0.6$ ). Compared to the correlation values among similarity metrics, the minimum distance was not always highly correlated with centroid distance (values between 0.6 and 0.7), because this metric approaches zero when two hypervolumes are highly overlapping (exemplified in Figure 1b,e,f).

The Pearson  $r$  correlations between distance metrics and similarity metrics showed a more erratic pattern. The correlations between

similarity and distance metrics were generally lower than those obtained when confronting similar types of metrics (Pearson  $r < 0.6$ ;  $< |0.5|$  for bioclimatic data in four and five dimensions). In general, a minimum distance showed the lowest values of correlation with similarity metrics. These general lower correlation values can be explained considering that, when two hypervolumes are disjunct, similarity metrics reach values of 0 (no intersection), at which point only distance metrics are quantitatively informative for assessing niche similarity (exemplified in Figure 1c). Moreover, this can also be due to specific hypervolume configurations (exemplified in Figure 1e).

### 3.1.2 | The influence of sample size

For all datatypes and analytical dimensions, the sample size had a significant influence on the calculated overlap and distance metrics. In general, variability in the simulation results decreased with increasing sample size (Figure 4b–f). Larger sample sizes also yielded more similar hypervolumes in terms of overall volume (Figure 4a). There was a general decrease in the minimum and centroid distance values at increasing sample sizes (Figure 4b,c; ANOVA; all  $p$ -values  $< 0.01$ ) and a parallel increase in Jaccard, intersection and Sørensen–Dice similarity metrics (Figure 4g–f; ANOVA; all  $p$ -values  $< 0.01$ ).

### 3.1.3 | The influence of algorithm and parameters

For all datatypes and analytical dimensions, the choice of the algorithm had a significant influence on the overall hypervolume volume and the calculated overlap and distance metrics (Figure 5). Compared to the other methods, SVM delineation always yielded the least voluminous (Figure 5a) and least overlapping hypervolumes (Figure 5b–f) for both datatypes and the three dimensionalities tested (ANOVA; all  $p$ -values  $< 0.05$ ). Box and Gaussian approaches generated more comparable

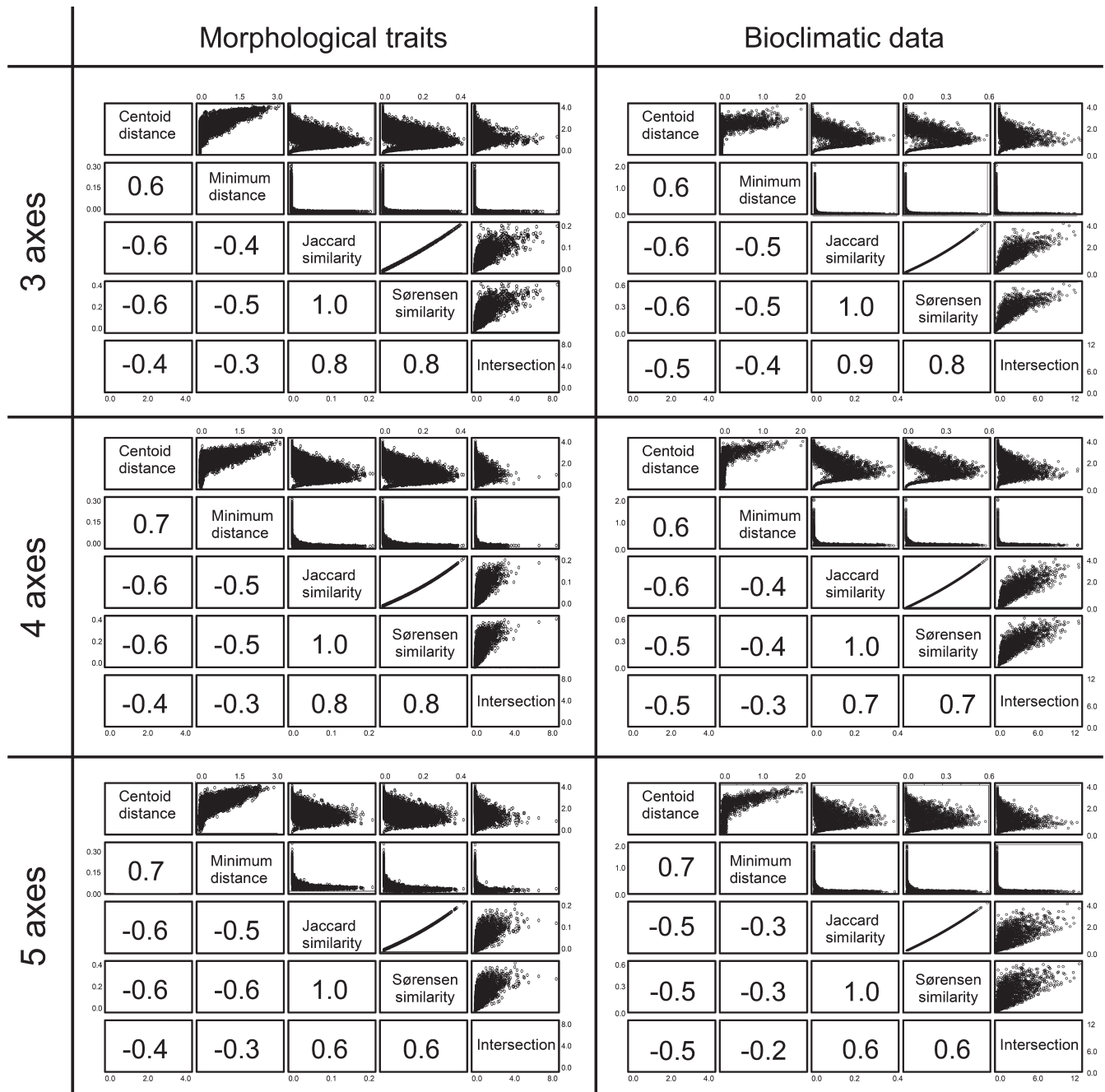




hypervolumes, yet still significantly different from one another. Specifically, hypervolumes generated via the Gaussian method were more overlapping (Figure 5b–f) and more voluminous (Figure 5a) for both datatypes and the three dimensionality tested (ANOVA; all  $p$ -values < 0.05). When generating hypervolumes via both these methods, increasing the bandwidth lead to more voluminous and overlapping hypervolumes, having at the same time a greater distance between centroids (ANOVA; all  $p$ -values < 0.05).

## 4 | DISCUSSION

By means of simulations based on different datatypes, analytical dimensions, sample sizes and input parameters, it was possible to show some patterns of empirical correlation between metrics used to assess the shared volume and distance between  $n$ -dimensional hypervolumes. Methodological implications and suggestions for real case analyses are discussed, also in light of the emerging trend in  $n$ -dimensional hypervolume studies published so far (Appendix S1).



**FIGURE 3** Correlation charts for the five metrics used to assess hypervolume similarity in the simulations. Each panel reports the correlation chart relative to an individual simulation, that is, with a fixed dimensionality (number of axes) and input data (morphological traits or bioclimatic gradients). At the top, bivariate scatterplots. At the bottom, Pearson  $r$  correlation coefficients rounded to the first decimal

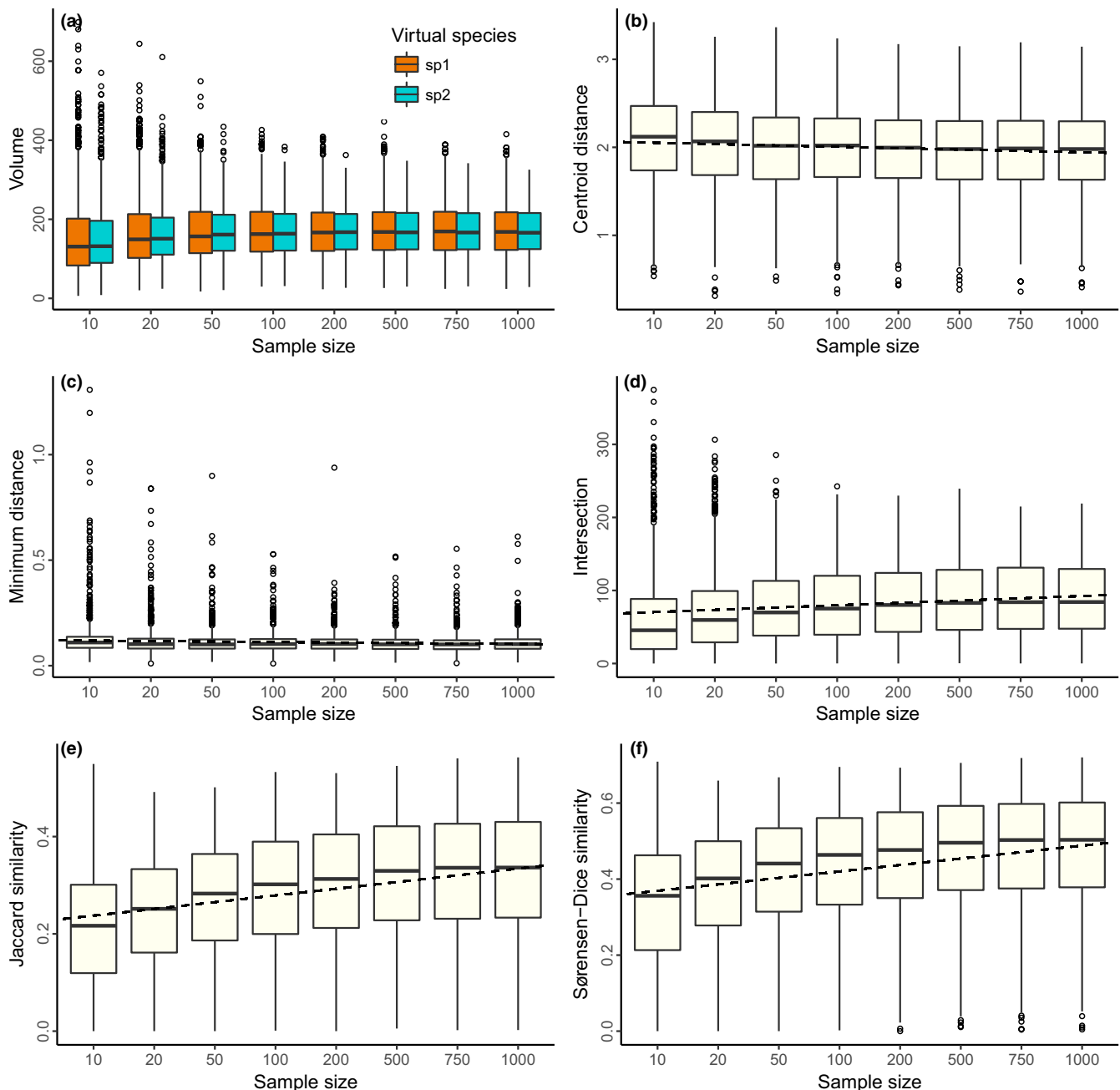


#### 4.1 | Distance metrics

Distance metrics provide empirical information about the general spatial relatedness of two hypervolumes, that is, how far the hypervolumes are in the multidimensional space. Indirectly, this information can be used to assess niche dissimilarity. From this perspective, the distance between centroids provides information about the intrinsic distance between the niches of two species, and it would be recommended to routinely report this metric. Yet, this metric has seldom been used in studies published so far (Figure 2). Possibly, this could be a

consequence of the fact that this metric is not stable under scale transformations. Indeed, the hypervolume construction requires all axes to be on coordinates with the same (or no) units (Blonder et al., 2014) and all axis to be orthogonal. To overcome this problem, one should always specify the type of scale transformation used, and eventually report variance or range to be able to interpret this metric better.

The minimum distance provides empirical information about the distance between the boundaries of two hypervolumes. This metric approaches zero when two hypervolumes are highly overlapping (exemplified in Figure 1b,e,f); therefore, a minimum distance of zero



**FIGURE 4** Boxplots showing the variation of volume (a), distance metrics (b, c) and similarity metrics (d–f) according to the eight tested sample sizes. Dotted lines represent general trends as recovered through ANOVA test between sample size levels. Given that trends for both datatypes and the three dimensionality tested were similar, only the plots relative to one simulation are arbitrarily shown (morphological traits, three dimensions, 999 replicas) [Colour figure can be viewed at [wileyonlinelibrary.com](http://wileyonlinelibrary.com)]

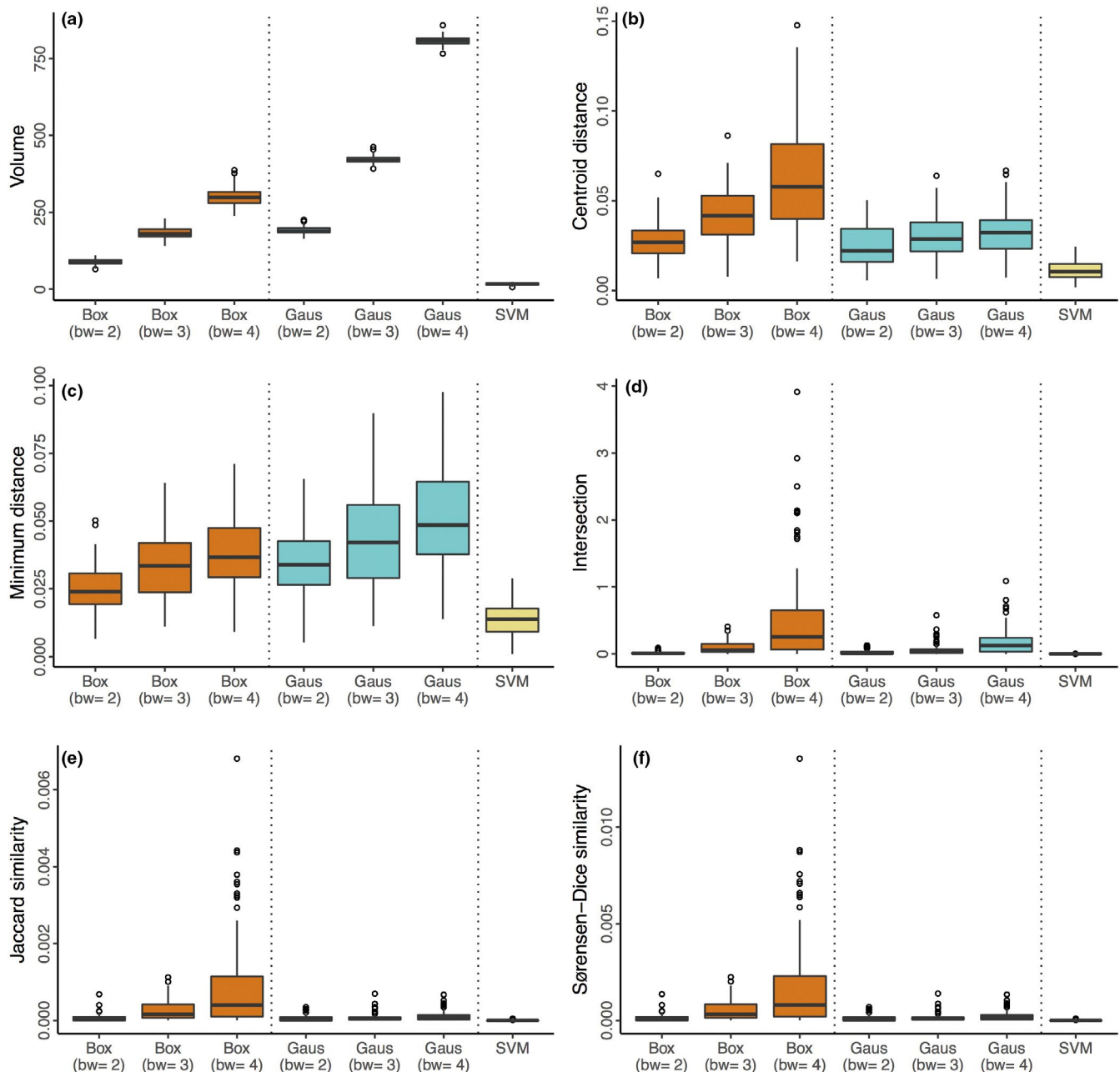


exclusively provides the information that two hypervolumes are highly overlapping. From a computational point of view, the calculation of the minimum distance is slower than the centroid distance, especially with large datasets (Blonder, 2018a). Accordingly, it is suggested to rely on the minimum distance only in specific cases. For example, a strong spatially biased set of occurrences might make the centroid distance a less-reliable estimate of similarity than the minimum distance. Also, it would be useful to calculate both centroid and minimum distance when comparing disjunct hypervolumes (Figure 1c), as in a similar case the two distance metrics would carry

slightly different information—the distance between the centre of the two niches and the distance between the boundaries.

## 4.2 | Similarity metrics

Similarity metrics allow the user to quantify shared niche volume in the multidimensional space and thus to indirectly assess niche overlap and to answer general questions on competition dynamics (Blonder, 2018b). In the simulation experiments, it was found that for both datatypes, the Jaccard and Sørensen–Dice similarities were the indexes



**FIGURE 5** Boxplots showing the variation in volume (a), distance metrics (b, c) and similarity metrics (d–f) according to the method used to construct the hypervolumes. Given that trends for both datatypes and the three dimensionalities tested were similar, only the plots relative to one simulation are arbitrarily shown (morphological traits, 3 dimensions, 999 replicas). Box = Box method; bw = bandwidth multiplier; Gaus = Gaussian method; SVM = Support Vector Machine method [Colour figure can be viewed at [wileyonlinelibrary.com](https://onlinelibrary.wiley.com)]



showing the highest reciprocal correlation (approaching Pearson  $r$  values of 1). Therefore, using either of those for assessing the overlap makes no apparent difference. Note also the identical behaviour of these two indexes at different sample sizes (cf. Figures 4e,f) and when comparing different algorithms and parameters (cf. Figure 5e,f). Yet the majority of recent studies (2014–2018) relying on the 'hypervolume' R packages used either the hypervolume intersection or the Sørensen–Dice similarity index rather than the Jaccard similarity index (Figure 2). This is possibly an artefact due to the fact that Sørensen–Dice was the first overlap index implemented in the 'hypervolume' R package (in Blonder et al., 2014), whereas the Jaccard similarity index was only later included within the set of default metrics.

In the simulation experiments, both indexes were also highly correlated with the hypervolume intersection (Figure 3). On one hand, this is not surprising given that the intersection value is used in the formula for constructing these indexes; on the other, some caution should be exercised in generalizing this correlative pattern to real-world data. Indeed, while similarity and intersection metrics may seem to carry the same information (Figure 1b), this is not always true. For instance, two hypervolumes may not only have a high intersection but also high unique components (i.e. non-shared volumes), resulting in higher values of intersection and smaller Jaccard and Sørensen–Dice similarity indexes (Figure 1f). As such, it is not recommended to rely solely on the intersection metric to assess niche similarity—as is found to occur in 5 out of 14 studies calculating the intersection. Although in most analytical scenarios this will be just a slight inaccuracy, in some peculiar cases (exemplified in Figure 1f) a similar approach would lead to an incorrect quantification of the similarity between two hypervolumes.

It is worth noting that all these similarity metrics reach values of zero as soon as the hypervolumes are disjunct, at which point they become uninformative for comparing the hypervolumes. In other words, a value of zero in the intersection and overlap provides only the self-evident information that two hypervolumes are fully disjunct (i.e. highly divergent). To compare disjunct hypervolumes using similarity metrics, one could either try to change the algorithm and parameters for hypervolume construction (Figure 5) or increase the sample size (Figure 4), in order to achieve a greater intersection of the hypervolumes in the hyperspace and non-zero values in these metrics. However, when hypervolumes are disjunct, distance metrics might still be the most appropriate metrics (see previous section).

Also note that the explored range of dimensionalities (from three to five) is potentially low for detecting mathematical phenomena that manifest in high-dimensional settings, the so-called 'curse of dimensionality' (after Bellman, 1957). As dimensionality gets high, most overlap scores will progressively become smaller due to the geometric scalings inherent to the hypervolume approach and to the fact that most volumes of the hypervolumes will shift towards their boundaries. Although so far analyses based on the  $n$ -dimensional hypervolume framework were primarily performed within low dimensional settings (five dimensions or so; see Appendix S1), this is a potential issue to take into consideration and that requires further investigations. For

example, it might be a relevant issue if hypervolume methods will be applied in palaeobiology, where >200 characters are oftentimes used (e.g. Close, Friedman, Lloyd, & Benson, 2015; Deline et al., 2018; Flannery Sutherland, Moon, Stubbs, & Benton, 2019).

### 4.3 | Alternative overlap indexes

The scope of this study was limited to analysis of similarity and distance metrics currently implemented in the 'hypervolume' R package (Blonder, 2018a). Eighteen studies considered in the literature overview, however, relied on other metrics as an alternative to (or in parallel to) the default ones. The metrics were either designed ad hoc for the purposes of the specific research or derived from the literature. Indeed, depending on the type of data at hand, there are several valuable alternatives for assessing niche similarity and overlap (e.g. Junker, Kuppler, Bathke, Schreyer, & Trutschig, 2016; Peterson, Soberón, & Sánchez-Cordero, 1999; Warren, Glor, & Turelli, 2008), such as methods based on simulations (Stockman, Danell, & Bond, 2008) or resampled geographical species distributions (Broennimann, Di Cola, & Guisan, 2017; Broennimann et al., 2012; Godsoe & Case, 2015). Although these other approaches certainly represent valuable alternatives to the default ones, it may be useful to calculate and report the default metrics too, to enhance and facilitate future meta-analyses and comparisons.

### 4.4 | Best practices and recommendations

Based on the results of this study, it is possible to draw some best practices for constructing and comparing  $n$ -dimensional hypervolumes, with a special reference to the method by Blonder et al. (2014, 2018):

- As long as the correlation between overlap and distance metrics can be low for both datatypes considered (Figure 3), the most diligent approach would be to routinely calculate and report at least one overlap and one distance metric;
- When two hypervolumes are fully disjunct, overlap metrics become uninformative in assessing niche similarity. Calculating and reporting both distance metrics (minimum and centroid distance) would be the most appropriate approach in this specific case.
- Even when relying on other metrics not provided in the 'hypervolume' R packages, good practice would be to routinely report at least one overlap and one distance metric, as this would facilitate comparisons between studies;
- In parallel to reporting the similarity and distance metrics, it would be useful to produce a graphical representation of the hypervolumes, allowing a reader to appreciate the spatial relatedness among generated hypervolumes. This recommendation applies for analyses in low dimensions, insofar as it became virtually impossible to rely on graphical representations as the number of dimensions gets high;
- To facilitate replicability of the analyses, the publication of hypervolume objects themselves is also recommended—for example, as an RDS file, using the basic R function 'saveRDS' (R Core Team, 2017).

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## DATA AVAILABILITY STATEMENT

This study is based on simulated data which can be generated by using the R codes provided as appendices (Appendices S2–S4). Papers analysed in the literature survey are listed in Appendix S1.

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## REFERENCES

- Blonder, B. (2016a). Pushing past boundaries for trait hypervolumes: A response to Carmona et al. *Trends in Ecology & Evolution*, 31(9), 665–667. <https://doi.org/10.1016/j.tree.2016.07.001>
- Blonder, B. (2016b). Do hypervolumes have holes? *The American Naturalist*, 187(4), 93–105. <https://doi.org/10.1086/685444>
- Blonder, B. (with contributions from Harris, D. J.) (2018a). Hypervolume: High dimensional geometry and set operations using Kernel Density Estimation, Support Vector Machines, and Convex Hulls. R Package Version, 2, 8. Retrieved from <https://CRAN.R-project.org/package=hypervolume>
- Blonder, B. (2018b). Hypervolume concepts in niche- and trait-based ecology. *Ecography*, 41, 1441–1455. <https://doi.org/10.1111/ecog.03187>
- Blonder, B., Lamanna, C., Violle, C., & Enquist, B. J. (2014). The n-dimensional hyper-volume. *Global Ecology and Biogeography*, 23, 595–609.
- Blonder, B., Lamanna, C., Violle, C., & Enquist, B. (2017). Using n-dimensional hypervolumes for species distribution modeling: A response to Qiao et al. (2016). *Global Ecology and Biogeography*, 26, 1071–1075.
- Blonder, B., Morrow, C. B., Maitner, B., Harris, D. J., Lamanna, C., Violle, C., ... Kerkhoff, A. J. (2018). New approaches for delineating n-dimensional hypervolumes. *Methods in Ecology and Evolution*, 9(2), 305–319.
- Barros, C., Thuiller, W., Georges, D., Boulangeat, I., & Münkemüller, T. (2016). N-dimensional hypervolumes to study stability of complex ecosystems. *Ecology Letters*, 19, 729–742.
- Barve, N., Barve, V., Jiménez-Valverde, A., Lira-Noriega, A., Maher, S. P., Peterson, A. T., ... Villalobos, F. (2011). The crucial role of the accessible area in ecological niche modeling and species distribution modeling. *Ecological Modelling*, 222(11), 1810–1819. <https://doi.org/10.1016/j.ecolmodel.2011.02.011>
- Bellman, R. E. (1957). *Dynamic programming*. Princeton, NJ: Princeton University Press.
- Bittebiere, A. K., Saiz, H., & Mony, C. (2019). New insights from multidimensional trait space responses to competition in two clonal plant species. *Functional Ecology*, 33(2), 297–307. <https://doi.org/10.1111/1365-2435.13220>
- Bourgeois, B., Munoz, F., Fried, G., Mahaut, L., Armengot, L., Denelle, P., ... Violle, C. (2019). What makes a weed a weed? A large-scale evaluation of arable weeds through a functional lens. *American Journal of Botany*, 106(1), 90–100. <https://doi.org/10.1002/ajb.1213>
- Broennimann, O., Di Cola, V., & Guisan, A. (2017). ecospat: Spatial Ecology Miscellaneous Methods. R Package Version, 2(2). Retrieved from <http://CRAN.R-project.org/package=ecospat>
- Broennimann, O., Fitzpatrick, M. C., Pearman, P. B., Petitpierre, B., Pellissier, L., Yoccoz, N. G., ... Guisan, A. (2012). Measuring ecological niche overlap from occurrence and spatial environmental data. *Global Ecology and Biogeography*, 21(4), 481–497. <https://doi.org/10.1111/j.1466-8238.2011.00698.x>
- Carmona, C. P., de Bello, F., Mason, N. W. H., & Lepš, J. (2016). The density awakens: A reply to Blonder. *Trends in Ecology and Evolution*, 31, 667–669. <https://doi.org/10.1016/j.tree.2016.07.003>
- Carvalho, J. C., & Cardoso, P. (2018). Decomposing the causes for niche differentiation between species using hypervolumes. *BioRxiv*, <https://doi.org/10.1101/485920>
- Chase, J. M., & Leibold, M. A. (2003). *Ecological niches: Linking classical and contemporary approaches*. Chicago, IL: University of Chicago Press.
- Close, R. A., Friedman, M., Lloyd, G. T., & Benson, R. B. (2015). Evidence for a mid-Jurassic adaptive radiation in mammals. *Current Biology*, 25(16), 2137–2142. <https://doi.org/10.1016/j.cub.2015.06.047>
- Colwell, R. K., & Rangel, T. F. (2009). Hutchinson's duality: The once and future niche. *Proceedings of the National Academy of Sciences*, 106(2), 19651–19658. <https://doi.org/10.1073/pnas.0901650106>
- Courchamp, F., & Bradshaw, C. J. A. (2018). 100 articles every ecologist should read. *Nature Ecology & Evolution*, 2, 395–401. <https://doi.org/10.1038/s41559-017-0370-9>
- Deline, B., Greenwood, J. M., Clark, J. W., Puttick, M. N., Peterson, K. J., & Donoghue, P. C. (2018). Evolution of metazoan morphological disparity. *Proceedings of the National Academy of Sciences*, 115(38), 8909–8918. <https://doi.org/10.1073/pnas.1810575115>
- Díaz, S., Kattge, J., Cornelissen, J. H., Wright, I. J., Lavorel, S., Dray, S., ... Garnier, E. (2016). The global spectrum of plant form and function. *Nature*, 529(7585), 167–171.
- Duque-Lazo, J., Navarro-Cerrillo, R. M., & Ruiz-Gómez, F. J. (2018). Assessment of the future stability of cork oak (*Quercus suber* L.) afforestation under climate change scenarios in Southwest Spain. *Forest Ecology and Management*, 409, 444–456. <https://doi.org/10.1016/j.foreco.2017.11.042>
- Elton, C. (1927). *Animal ecology*. London, UK: Sedgwick and Jackson.
- Enrique, G., Violle, C., Pérez-Ramos, I. M., Marañón, T., Navarro-Fernández, C. M., Olmo, M., & Villar, R. (2018). A multidimensional functional trait approach reveals the imprint of environmental stress in Mediterranean woody communities. *Ecosystems*, 21(2), 248–262. <https://doi.org/10.1007/s10021-017-0147-7>
- Flannery Sutherland, J. T., Moon, B. C., Stubbs, T. L., & Benton, M. J. (2019). Does exceptional preservation distort our view of disparity in the fossil record? *Proceedings of the Royal Society B*, 286(1897), 20190091. <https://doi.org/10.1098/rspb.2019.0091>
- Godsoe, W., & Case, B. S. (2015). Accounting for shifts in the frequency of suitable environments when testing for niche overlap. *Methods in Ecology and Evolution*, 6, 59–66. <https://doi.org/10.1111/2041-210X.12307>
- Gonzalez-Granadillo, G., Garcia-Alfaro, J., & Debar, H. (2017). A polytope-based approach to measure the impact of events against critical infrastructures. *Journal of Computer and System Sciences*, 83(1), 3–21. <https://doi.org/10.1016/j.jcss.2016.02.004>
- Greve, C., Haase, M., Hutterer, R., Rödder, D., Ihlow, F., & Misof, B. (2017). Snails in the desert: Species diversification of *Theba* (Gastropoda: Helicidae) along the Atlantic coast of NW Africa. *Ecology and Evolution*, 7(14), 5524–5538.
- Grinnell, J. (1917). The niche-relationships of the California Thrasher. *The Auk*, 34, 427–433. <https://doi.org/10.2307/4072271>
- Grinnell, J. (1924). Geography and evolution. *Ecology*, 5, 225–229. <https://doi.org/10.2307/1929447>
- Hijmans, R. J., Cameron, S. E., Parra, J. L., Jones, P. G., & Jarvis, A. (2005). Very high resolution interpolated climate surfaces for global land areas. *International Journal of Climatology*, 25(15), 1965–1978. <https://doi.org/10.1002/joc.1276>
- Holt, R. D. (2009). Bringing the Hutchinsonian niche into the 21st century: Ecological and evolutionary perspectives. *Proceedings of*



- the National Academy of Sciences, 106, 19659–19665. <https://doi.org/10.1073/pnas.0905137106>
- Hutchinson, G. E. (1957). Concluding remarks. *Cold Spring Harbor Symposia on Quantitative Biology*, 22, 415–427. <https://doi.org/10.1101/SQB.1957.022.01.039>
- Irl, S. D. H., Schweiger, A. H., Medina, F. M., Fernández-Palacios, J. M., Harter, D. E. V., Jentsch, A., ... Beierkuhnlein, C. (2017). An island view of endemic rarity - Environmental drivers and consequences for nature conservation. *Diversity and Distributions*, 23(10), 1132–1142. <https://doi.org/10.1111/ddi.12605>
- Junker, R. R., Kuppler, J., Bathke, A. C., Schreyer, M. L., & Trutschnig, W. (2016). Dynamic range boxes—a robust nonparametric approach to quantify size and overlap of n-dimensional hypervolumes. *Methods in Ecology and Evolution*, 7(12), 1503–1513.
- Koch, C., Flecks, M., Venegas, P. J., Bialke, P., Valverde, S., & Roedder, D. (2016). Applying n-dimensional hypervolumes for species delimitation: Unexpected molecular, morphological, and ecological diversity in the Leaf-Toed Gecko *Phyllodactylus reissii* Peters, 1862 (Squamata: Phyllodactylidae) from northern Peru. *Zootaxa*, 4161(1), 41–80. <https://doi.org/10.11646/zootaxa.4161.1.2>
- Krehenwinkel, H., Rödder, D., & Tautz, D. (2015). Eco-genomic analysis of the poleward range expansion of the wasp spider *Argiope bruennichi* shows rapid adaptation and genomic admixture. *Global Change Biology*, 21(12), 4320–4332.
- Kudła, P., & Pawlak, T. P. (2018). One-class synthesis of constraints for Mixed-Integer Linear Programming with C4. 5 decision trees. *Applied Soft Computing*, 68, 1–12. <https://doi.org/10.1016/j.asoc.2018.03.025>
- Leroy, B., Meynard, C. N., Bellard, C., & Courchamp, F. (2016). Virtualspecies, an R package to generate virtual species distributions. *Ecography*, 39(6), 599–607. <https://doi.org/10.1111/ecog.01388>
- Liu, C., Berry, P. M., Dawson, T. P., & Pearson, R. G. (2005). Selecting thresholds of occurrence in the prediction of species distributions. *Ecography*, 28(3), 385–393. <https://doi.org/10.1111/j.0906-7590.2005.03957.x>
- Mammola, S., Arnedo, M. A., Pantini, P., Piano, E., Chiappetta, N., & Isaia, M. (2018). Ecological speciation in darkness? Spatial niche partitioning in sibling subterranean spiders (Araneae: Linyphiidae: Troglohyphantes). *Invertebrate Systematics*, 32(5), 1069–1082. <https://doi.org/10.1071/IS17090>
- Mammola, S., & Isaia, M. (2017). Rapid poleward distributional shifts in the European cave-dwelling Meta spiders under the influence of competition dynamics. *Journal of Biogeography*, 44(12), 2789–2797.
- Martins, R. P. (2017). To what degree are philosophy and the ecological niche concept necessary in the ecological theory and conservation? *European Journal of Ecology*, 3(1), 42–54. <https://doi.org/10.1515/eje-2017-0005>
- Onn, C. K., Abraham, R. K., Grismer, J. L., & Grismer, L. (2018). Elevational size variation and two new species of torrent frogs from Peninsular Malaysia (Anura: Ranidae: *Amolops* Cope). *Zootaxa*, 4434(2), 250–264. <https://doi.org/10.11646/zootaxa.4434.2.2>
- Papuga, G., Gauthier, P., Pons, V., Farris, E., & Thompson, J. D. (2018). Ecological niche differentiation in peripheral populations: A comparative analysis of eleven Mediterranean plant species. *Ecography*, 41(10), 1650–1664. <https://doi.org/10.1111/ecog.03331>
- Paradis, E., Claude, J., & Strimmer, K. (2004). APE: Analyses of phylogenetics and evolution in R language. *Bioinformatics*, 20(2), 289–290. <https://doi.org/10.1093/bioinformatics/btg412>
- Peterson, A. T., Soberón, J., & Sánchez-Cordero, V. (1999). Conservatism of ecological niches in evolutionary time. *Science*, 285(5431), 1265–1267.
- Pruitt, J. N., Howell, K. A., Gladney, S. J., Yang, Y., Lichtenstein, J. L. L., Spicer, M. E., ... Pinter-Wollman, N. (2017). Behavioral hypervolumes of predator groups and predator-predator interactions shape prey survival rates and selection on prey behavior. *The American Naturalist*, 189(3), 254–266. <https://doi.org/10.1086/690292>
- Qiao, H., Escobar, L. E., Saupe, E. E., Ji, L., & Soberón, J. (2017a). A cautionary note on the use of hypervolume kernel density estimators in ecological niche modelling. *Global Ecology and Biogeography*, 26, 1066–1070. <https://doi.org/10.1111/geb.12492>
- Qiao, H., Escobar, L. E., Saupe, E. E., Ji, L., & Soberón, J. (2017b). Using the KDE method to model ecological niches: A response to Blonder et al. (2017). *Global Ecology and Biogeography*, 26(9), 1076–1077.
- R Core Team. (2017). *R: A language and environment for statistical computing*. Vienna, Austria: R Foundation for Statistical Computing. Retrieved from <https://www.R-project.org/>
- Revell, L. J. (2012). phytools: An R package for phylogenetic comparative biology (and other things). *Methods in Ecology and Evolution*, 3(2), 217–223. <https://doi.org/10.1111/j.2041-210X.2011.00169.x>
- Silverman, B. W. (1992). *Density estimation for statistics and data analysis*. London, UK: Chapman and Hall.
- Simó-Riudalbas, M., Tarroso, P., Papenfuss, T., Al-Sariri, T., & Carranza, S. (2018). Systematics, biogeography and evolution of *Asaccus gallagheri* (Squamata, Phyllodactylidae) with the description of a new endemic species from Oman. *Systematics and Biodiversity*, 16(4), 323–339.
- Soberón, J. (2007). Grinnellian and Eltonian niches and geographic distributions of species. *Ecology Letters*, 10(12), 1115–1123. <https://doi.org/10.1111/j.1461-0248.2007.01107.x>
- Stockman, A. K., Danell, R. M., & Bond, J. E. (2008). D-NOVL: A program to simulate overlap between two niche-based distribution models. *Molecular Ecology Resources*, 8, 290–294.
- Tingley, R., Vallinoto, M., Sequeira, F., & Kearney, M. R. (2014). Realized niche shift during a global biological invasion. *Proceedings of the National Academy of Sciences*, 111(28), 10233–10238. <https://doi.org/10.1073/pnas.1405766111>
- Warren, D. L., Glor, R. E., & Turelli, M. (2008). Environmental niche equivalency versus conservatism: Quantitative approaches to niche evolution. *Evolution*, 62(11), 2868–2883. <https://doi.org/10.1111/j.1558-5646.2008.00482.x>
- Zurell, D., Berger, U., Cabral, J. S., Jeltsch, F., Meynard, C. N., Münkemüller, T., ... Grimm, V. (2010). The virtual ecologist approach: Simulating data and observers. *Oikos*, 119(4), 622–635. <https://doi.org/10.1111/j.1600-0706.2009.18284.x>

## BIOSKETCH

**Stefano Mammola** is an ecologist whose scientific activity focuses primarily on the use of caves and other subterranean habitats as model systems in which to investigate an array of ecological processes.

## SUPPORTING INFORMATION

Additional supporting information may be found online in the Supporting Information section at the end of the article.

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