Use and misuse of discrete character data for morphospace and disparity analyses

Sylvain Gerber

► To cite this version:

Sylvain Gerber. Use and misuse of discrete character data for morphospace and disparity analyses. Palaeontology, 2019, 62 (2), pp.305-319. 10.1111/pala.12407 . hal-02340296

HAL Id: hal-02340296

<https://hal.sorbonne-universite.fr/hal-02340296>

Submitted on 30 Oct 2019

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

1 **USE AND MISUSE OF DISCRETE CHARACTER DATA FOR MORPHOSPACE AND**

2 **DISPARITY ANALYSES**

3

4 Sylvain Gerber

5

6 Institut Systématique Evolution Biodiversité (ISYEB), Muséum national d'Histoire naturelle, CNRS, Sorbonne

7 Université, EPHE, 45 rue Buffon, CP 50, 75005 Paris, France; sylvain.gerber@mnhn.fr

8

9

10 **Running head:** Discrete character data in disparity analyses

11

12 **Abstract**

13

14 The measurement of morphological variation in macroevolutionary studies is increasingly

15 based on morphospaces constructed from discrete character data. This trend mostly results

16 from the appropriation of phylogenetic data matrices as character spaces for carrying out

17 disparity analyses. Phylogenetic matrices provide morphological descriptions of taxa as

18 combinations of character states and thus appear – if not conceptually, at least mathematically

19 – comparable to discrete character datasets found in numerical taxonomy or built for disparity

20 purposes. Hence, phylogenetic matrices seem to constitute an abundant source of data readily

21 available for morphospace analyses. Discrete character spaces have been generally described

22 as more flexible than morphospaces capturing continuous shape variation. The discrete coding

23 of morphology allows morphospaces to accommodate more disparate morphologies and the

24 ability of discrete character schemes to handle missing data is also often emphasized. This

25 flexibility comes at a cost, however. Multivariate ordinations of such spaces often provide

deceptive visualizations and may invite the use of inappropriate methodologies for their exploration. The high amount of missing data that typifies many phylogenetic datasets is also problematic for the measurement of dissimilarity among taxa and can therefore be detrimental to the assessment of morphological disparity. In the present contribution, the properties of discrete character spaces are described and common pitfalls discussed. Graphical and methodological approaches are suggested to circumvent or limit their impact, and greater caution is recommended when using discrete character data for morphospace and disparity inferences.

Key words: character space, phylogenetic data matrices, disparity, macroevolution, missing data, morphological hypercube.

The morphological disparity of a clade can be defined as a measure of the degree of morphological distinctness exhibited by its constitutive taxa (for reviews, see Foote 1997; Wills 2001; Erwin 2007; Wagner 2010; Hopkins and Gerber 2017). Its study has been pioneered by palaeobiologists in the 90's (e.g. Gould 1991; Foote 1993), but the concept has since reached prominence as a macroevolutionary measure of morphological variation in both palaeontological and neontological contexts (e.g. Neige 2003; Ricklefs 2004; Chartier et al. 2017). Methodologically, morphological disparity is estimated from the quantitative description of the distribution of taxa in morphospace, the space spanned by the set of morphological variables used to describe and compare the taxa studied.

Diverse kinds of morphospaces can be built depending on the descriptors used to characterise the sample of morphologies considered. In what follows, I focus on discrete character spaces. These morphospaces have recently risen in popularity in palaeobiology, particularly among vertebrate specialists, as a consequence of the idea of co-opting phylogenetic data matrices as a source of morphological data for disparity analysis (e.g. Brusatte et al. 2008, 2011; Prentice et al. 2011; Thorne et al. 2011; Butler et al. 2012; Ruta et al. 2013; Heterington et al. 2015; Romano 2017). Lloyd (2016) provided a recent account of the strengths and challenges associated with the use of discrete character data in studies of disparity and rates of morphological evolution. The theoretical and empirical features of discrete character spaces do not seem to have been much discussed however, and how these features affect morphospace and disparity studies has therefore been largely overlooked. In the present contribution, I describe and illustrate some properties of discrete character spaces and highlight potential pitfalls with the use of such spaces in disparity studies within current analytical frameworks. Although some of these issues do not seem to have ideal solutions for now, some suggestions are made to lower their impact on the interpretation of morphospace patterns and on estimates of morphological disparity.

The discussion mostly revolves around two points in need of further attention: the use of reduced-space ordination methods to visualize discrete character spaces and the large amount of missing data that typifies many phylogenetic datasets. Regarding the first point, it is often tempting to try to visualize the morphospaces we are working with. The use of ordination methods on discrete character spaces however leads to visualizations that can be prone to misinterpretations. It also tends to cause confusions between the morphospace itself and its ordination, inviting the use of inappropriate methods for analysing morphospace patterns. A hypercube graph example is developed to illustrate these aspects. The second point on missing data reflects a pressing concern given the widespread use of phylogenetic datasets for disparity analyses. Abundant missing entries have a substantial and detrimental effect on the assessment of morphological dissimilarity among specimens and can therefore strongly bias disparity estimates, in particular if those are calculated from ordinations of deficient pairwise distance matrices. Graphical options and weighting approaches are suggested to account for the uneven quality of specimen scoring.

DISCRETE CHARACTER DATA AND PHYLOGENETIC DATA MATRICES

Discrete character data have long been used as a means of quantifying morphological variation, including in the early years of the disparity research program (e.g. Foote 1992; Thomas and Reif 1993). Discrete coding corresponds to the morphological description of each specimen in a sample as a sequence of character states. The characters can possess two or more states, corresponding to binary and multistate characters respectively. In the latter case, the different states can be treated as ordered or unordered depending on the underlying mode of variation that is assumed.

101 One of the main advantages of discrete character schemes compared to other descriptors lies
102 in their ability to accommodate a broader range of morphologies within a single analysis.
103 Indeed, fairly disparate morphological structures, which can be challenging for morphometric
104 approaches, can usually be more easily analysed within a discrete character framework.
105 Discrete coding also offers the possibility of including morphological features that are only
106 present in a subset of the sample of specimens (a context that also precludes many alternative
107 morphometric methods). The study of evolutionary novelties is an important research
108 program in macroevolution (e.g. Wagner and Lynch 2010; Erwin 2017) and the ability to
109 account for the origination of novel morphological features (e.g. via a presence/absence
110 coding scheme) is thus central to disparity. Discrete character data therefore appear especially
111 relevant for studies at high taxonomic ranks where morphological variation is expected to be
112 substantial and homology difficult to define uniformly across the taxa sampled. Discrete data
113 are also useful if the morphological phenotypes considered include articulated or
114 disconnected structures, such as the different bones of a skeleton. This flexibility generally
115 comes at the expense of relatively cruder descriptions of morphologies, but careful coding
116 schemes can still allow informative accounts of the morphological traits deemed relevant for a
117 study.

118 Phylogenetic data matrices are instances of discrete character data and as such they have been
119 increasingly considered as the basis for morphospace and disparity analyses in recent years.
120 One could nevertheless expect them to differ from the discrete character datasets that are
121 specifically assembled for the purpose of disparity analyses. Phylogenetic data matrices are
122 built for phylogenetic purposes and this has logical implications for the definition and coding
123 of characters (e.g. Estabrook et al. 1975), notably regarding homoplasy (convergence and
124 reversal) and autapomorphies (derived character state restricted to a unique terminal taxon).
125 The aim of phylogenetics is to establish branching orders and group taxa into evolutionarily

coherent clades. Therefore, morphological features that would be known or anticipated to be highly homoplastic would not in principle be considered as suitable characters and included in a phylogenetic dataset. An opposite view on homoplasy is generally held in the field of disparity (Gould 1991; Foote 1996). Far from being nuisances, convergences and reversals are seen as important evolutionary phenomena in studies of morphological disparity (see Foote 1996 for a discussion on total versus net changes) and their consideration, in conjunction with a phylogenetic hypothesis, improve the interpretations of evolutionary patterns. Autapomorphic characters are uninformative in parsimony analysis, which is still the most widespread approach in morphology-based phylogenetic inference (autapomorphies are nonetheless informative in maximum likelihood and Bayesian approaches; Lewis 2001). One should therefore expect them to be rarely found in phylogenetic datasets. The view of their role in disparity studies ranges from central importance (Gould 1991) to negligible (Cisneros and Ruta 2010; Ruta and Wills 2016) but for distinct conceptual and methodological reasons (see below).

Hence, phylogenetic and disparity datasets, respectively aiming at grouping and distinguishing taxa, in principle reflect two different modes of character matrix construction. In a hypothetical phylogenetic dataset with no homoplasy and no autapomorphies, two terminal sister taxa (OTUs) share the same sequence of character states. They are, as scored, morphologically undistinguishable, which is not pertinent from a disparity viewpoint. The use of phylogenetic datasets for disparity purposes thus implicitly relies on the expectation of some erroneous assessments of character state homology and/or on the presence of parsimony-uninformative characters.

Empirically, it appears that discrete character datasets built for phylogenetic and disparity purposes do not in fact greatly differ from each other regarding the nature of the characters that they include. Based on measures of HER (Homoplasy Excess Ratio), Hughes et al.

151 (2013) showed that phylogenetic and disparity datasets on average exhibit comparable
152 degrees of homoplasy, even though the small sample of datasets investigated did not allow
153 further comparison of the statistical distributions of HER for the two kinds of datasets.
154 Studies of rates of character change in various groups have also shown that rate distributions
155 are better fitted by gamma and lognormal models rather than by uniform (single-rate) models
156 (Wagner et al. 2006; Wagner 2012; Harrison and Larsson 2015). These non-uniform
157 distributions indicate significant rate heterogeneities among characters and suggest that
158 phylogenetic data matrices commonly include homoplastic characters. Phylogenetic and
159 disparity datasets also appear comparable with respect to the presence of autapomorphic
160 characters. Most phylogenetic data matrices include autapomorphic characters indicating that
161 phylogeneticists do not deliberately exclude them regardless of their relevance to the method
162 of phylogenetic inference subsequently used (P. Wagner, pers. comm., based on a meta-
163 analysis of 188 matrices of invertebrate clades showing that most matrices have at least one
164 autapomorphic binary character, and nearly all have at least one autapomorphic character
165 state on either a binary or multistate character).

166 Whether the two distinct research questions underlying the construction of phylogenetic and
167 disparity datasets lead to comparable matrices or not, the use of the former as a surrogate for
168 the latter still implies a series of reformatting steps. A phylogenetic data matrix cannot be
169 directly co-opted without at least a few changes (see Hughes et al. 2013). For instance, the
170 row corresponding to the outgroup needs to be removed in most cases. The question that
171 motivated the construction of the phylogenetic data matrix might also have had an influence
172 on the taxonomic coverage and (sub)sampling effort carried out, and it is important to assess
173 the representativeness of the sampled OTUs for a disparity analysis meant to characterize the
174 clade they belong to. Besides, it is also not uncommon for OTUs in a phylogenetic data
175 matrix to represent different taxonomic ranks and some matrix rows might need to be

176 amalgamated to level these differences and homogenise the dataset. Finally, phylogenetic data
177 matrices conducive to phylogenetic trees with low level of homoplasy might indicate a
178 stringent selection of characters and the possibility of expanding the character set in the
179 prospect of a disparity analysis.

180 Hence, a phylogenetic data matrix can form a basis for the elaboration of a discrete character
181 space, but the taxa and characters enclosed generally need critical re-evaluation. The
182 characters eventually gathered generate a set of possibilities for morphological variation
183 (“possibilities” in a combinatorial but not necessarily biological sense). This set can be finite
184 or infinite depending on the definition of characters and their implied number of states (e.g.,
185 Hoyal Cuthill 2015). The next step is to define relationships among these possible
186 morphological options, traditionally based on measures of morphological (dis)similarity, in
187 order to generate a morphological space.

190 **MEASURING DISSIMILARITY AND THE MORPHOLOGICAL HYPERCUBE**

191
192 Hereafter, only binary characters are considered. This allows a simpler derivation of the
193 observations and conclusions that are equally valid for geometrically more complex
194 morphospaces built from datasets that include multistate characters. For convenience, it is
195 also assumed that there is no missing data (this issue is dealt with in a following section) and
196 that all characters can be treated equally. This last point means that all characters are given
197 the same weight when estimating pairwise dissimilarity. Note that this equal weighting of
198 characters is unlikely to be biologically meaningful given the anatomical diversity of
199 characters typically combined, but this is the approach usually taken in empirical studies (see
200 “CONCLUDING REMARKS AND PERSPECTIVES”).

201 With discrete character data, the measurement of dissimilarity between two taxa is based on
202 the number of matches and mismatches between their scored character states. For binary
203 characters, this is equivalent to measuring the Hamming distance between the two sequences
204 of character states. For instance, for a set of $p=6$ binary characters, the OTUs A (1, 0, 0, 1, 0,
205 1) and B (1, 1, 0, 0, 0, 1) have 4 matches (characters 1, 3, 5, and 6) and 2 mismatches
206 (characters 2 and 4). The Hamming distance between A and B is thus 2. The distance between
207 any possible pairs of morphologically distinct OTUs ranges from 1 to p . The Hamming
208 distance satisfies the properties of equality, positivity, symmetry, and triangle inequality, and
209 it is therefore a metric on the set of all sequences of binary character states of length p . The
210 resulting discrete character space is a Hamming cube. If one considers the p states of all
211 possible sequences as coordinates in $\mathbb{R}^p$, one obtains a Euclidean representation of the discrete
212 character space as a p -dimensional unit hypercube. A hypercube is the generalization of the
213 concept of cube to higher dimensions. Each sequence occupies one of the vertices of the
214 hypercube, and the distance between two sequences is the sum of unit-length edges separating
215 their vertices (as opposed to the Euclidean distance between vertices). In this context, the
216 morphospace is the spatial representation of taxa relative to an underlying set of possibilities
217 for morphological variation. With p binary characters, this set of possibilities is the 2^p
218 combinations of the character states corresponding to the 2^p vertices of the hypercube.
219 Some geometric properties of such morphospaces can be easily inferred. For instance, adding
220 an autapomorphic character to a dataset adds one dimension to the morphological hypercube,
221 but it doubles the set of options for morphological variation: $p+1$ binary characters give $2^{(p+1)}$
222 sequences, that is, 2×2^p possible combinations of characters. The $(p+1)$ -hypercube has now
223 twice the number of vertices, but only one of these extra 2^p vertices is (and can be) occupied.
224 This is not necessarily problematic but it must be kept in mind if one uses quantitative
225 approaches whose performances are sensitive to morphospace dimensionality. Geometrically,

an autapomorphy adds a dimension that separates the taxon that possesses it from all the other taxa of the clade. If autapomorphies are uniformly distributed across OTUs, their overall effect is to increase pairwise distances by pushing OTUs away from each other in orthogonal directions (in the Euclidean representation of the hypercube). In this case, their interest is limited for autapomorphies will not qualitatively affect the morphospace structure and relative measures of disparity extracted from it (Cisneros and Ruta 2010). A more restricted and informative distribution of autapomorphies might also have a limited effect on overall disparity patterns inasmuch as their individual contributions to dissimilarity measures is relative to the total number of characters, but their interest rests upon their ability to single-out remarkable taxa and document the structure of morphospace occupation (Gould 1991; Foote 1997).

Many other geometric features of discrete character spaces are not as easily grasped and high-dimensional objects can be challenging to our intuition (e.g. Abbott 1884). Visualisation techniques such as projections onto lower-dimensional spaces are therefore frequently employed and it is important to assess the effect of such approaches on our understanding and interpretation of morphospace patterns.

MORPHOSPACE ORDINATION AND VISUALIZATION

Morphospace visualization is often considered as an important step for illustrating and discussing morphological patterns. Like most morphospaces however, discrete character spaces have a high number of dimensions and two- or three-dimensional representations of morphospaces consequently offer only a partial view of the amount and structure of morphospace occupation. Great care is therefore required when describing morphospace

patterns from a reduced number of axes. This is especially true for discrete character spaces for which usually only a very small fraction of the variation is captured by the first axes of the multivariate ordination.

For discrete character data, it is customary to visualize a morphospace by carrying out a Principal Coordinate Analysis (PCoA) on the pairwise dissimilarity matrix **D** (an alternative not discussed here is Non-Metric Multidimensional Scaling, but the method aims at preserving ordering relations rather than distances among the objects it ordines). PCoA provides a Euclidean representation of a dissimilarity matrix (Gower 1966), here analogous to the hypercube geometry described above. The principal coordinates generated (at most $n-1$ where n is the number of OTUs) are functions of the original variables (the morphological characters), as conveyed by the choice of the distance measure. If **D** is not Euclidean, because of the distance measure chosen (or because of missing data), negative eigenvalues will be produced. A transformation of **D** is therefore recommended prior to its ordination (e.g. square root transformation).

The resulting depiction of the morphospace is the set of taxa displayed as points in the space of the ordination, a generic representation common to all types of morphological descriptors. Importantly however, this ordination is an embedding of the true discrete character space (morphological hypercube or similar but more complex discrete spaces) in a continuous Cartesian coordinate system, that of the principal coordinate axes. Unfortunately, this discrete structure is difficult to represent and is therefore often overlooked. Yet, conflating the geometric properties of the morphospace with those of its ordination has non-trivial consequences for the interpretation of morphological patterns and for the choice of methods employed to explore morphospaces.

A small example is presented in Figure 1 to illustrate these points. It is based on a subset of the archosaur dataset from Brusatte et al. (2008). For the sake of the example, a stringent

selection of characters had to be carried out in order to obtain a dataset where the OTUs retained are scored using only binary characters and without missing data. The culling of rows and columns from the original phylogenetic data matrix undoubtedly leads to an uninformative dataset, but it remains relevant for the present illustrative purpose. The subset considered includes 18 genera of crurotarsans coded for 10 binary characters (characters {2, 3, 4, 9, 19, 21, 22, 24, 25, 45} in Brusatte et al. 2008). As described above, dissimilarity among genera is calculated as the Hamming distance and these pairwise distances are stored in the distance matrix **D**. In the interest of visualization, a multivariate ordination of the morphospace is produced by carrying out a PCoA of the square root of **D**. Figure 1A shows the traditional representation of the morphospace with taxa abstracted as points in the principal coordinate space.

Two related questions are generally investigated or discussed when considering morphospace patterns. One concerns the overall amount of morphospace being occupied by a clade and the reasons for the existence of unoccupied regions. Discussions of this problem arose from Raup's seminal work on the unequal filling of the shell coiling morphospace (Raup 1966) and are central to the field of theoretical morphology (e.g. McGhee 2006). The causes generally invoked include the functional and developmental limits imposed on the variational properties of phenotypes, ecological restrictions, and historical contingency (e.g. Raup 1972, Maynard Smith et al. 1985; Erwin 2007; Oyston et al. 2015). The second research question aims at dissecting the temporal and/or spatial dynamics of morphospace occupation and forms the core of disparity analyses.

If the discrete character space is mistaken for its ordination, both these research questions can be misdirected. A priori unoccupied regions visible on the principal coordinate ordination might correspond to positions that do not belong to the discrete character space and therefore do not call for any biological explanation. Only a finite and non-randomly located (and in fact

quite structured) positions correspond to the hypercube vertices, i.e. to meaningful positions in the actual morphospace. This is illustrated in Figure 1B, where the two-dimensional projection of the entire architecture of the 10-hypercube is displayed, that is, its 1024 vertices and its 5120 unit-length edges. To obtain this representation, all 1024 combinations of character states needs to be enumerated, along with a record of their 10 neighbouring combinations (those differing by only one character state change). With p characters, there are 2^p vertices and $2^{p-1}p$ edges though, and it becomes rapidly difficult to enumerate all possible options and represent the hypercube graphically. Figure 1C shows a simplified representation where only a small subset of vertices and edges are computed and displayed, defined in a way that ensures a complete connectedness of the observed OTUs. It emphasizes the strong visual effect of the two-dimensional projection of a high-dimensional discrete morphospace. All the segments depicted represent edges and have therefore the same unit length despite their drastically variable projected lengths. Also, provided the distance matrix subjected to PCoA is Euclidean, edges are either parallel (if they correspond to the same character) or orthogonal, even if the ordination suggests otherwise. Spatial relationships among vertices inferred from the ordination should therefore be treated with caution since they will be misleading in most cases. This bias typically impacts graphical techniques such as convex hulls. The relative surface areas of these polygons can be poor indicators of the relative disparity of the groups they delineate in the ordination.

A possible way to visually circumscribe the morphospace within the space of principal coordinates could be to consider the hypersphere it is inscribed in (as conveyed by Fig. 1B). By definition, all vertices are at a distance $(\sqrt{p})/2$ from the centroid of the hypercube. Hence, one could draw the circle of radius $(\sqrt{p})/2$ centred on the hypercube centroid to have an idea of the size of the morphospace. The centroid position can be calculated as the average principal coordinate scores of one of the observed vertices and of its diagonally opposite

vertex (i.e. its opposite combination of character states). In practice however, the probability of having a good correlation between the true and the projected maximum distances is low (and decreases as p increases) and the circle drawn will generally largely exceeds the two-dimensional distribution of the vertices. An alternative is proposed below based on the pattern of distribution of vertices.

Figure 1D illustrates the variation of the density of vertices under random orientations of the hypercube along the first principal coordinate axis (here the hypercube is centred at the origin of the principal coordinate system for convenience). It shows a density that decreases as one moves away from the hypercube centroid (this can also be noticed in Fig. 1B). This pattern has important implications: it means that even a uniform filling of the discrete morphospace will lead to a non-uniform distribution of taxa in the two- or three-dimensional visualization supplied by the PCoA (an orthogonal projection of the hypercube). Hence, density contour lines, heatmap representations, and similar approaches found in spatial point pattern analysis which might seem appropriate to document morphospace occupation (e.g. Ruta and Wills 2016) should be avoided or used with caution. More generally any method that relies on the continuous coordinate system of the ordination might be prone to similarly misleading description of morphological patterns.

The density of vertices along any principal coordinate axis is approximately distributed as $N(0,0.25)$ (PCoA considers each binary character as a dimension of the Euclidean space, and their individual variance for the entire population of vertices is 0.25). Frequency ellipses can be used to delineate the bivariate distribution of the vertices in the plane of pairs of principal coordinate axes. In the bivariate case, a circular ellipse of radius ≈ 1.224 centred on the hypercube centroid will on average enclosed 95 percent of the morphospace vertices (with two degrees of freedom, $\chi^2_2(0.95) \approx 5.991$, so the radius of the circular ellipse is indeed $\sqrt{(5.991 \times 0.25)}$; see Fig. 1C).

This sub-circular shape of the morphospace also explains the very low percentage of variance that is usually summarized by the first few principal coordinate axes. Hypercubes and related spaces do not show preferential directions of elongation (hence the smooth decrease of eigenvalues). Nevertheless, some datasets that are more structured and depart from a uniform filling of the hypercube can show a more efficient redistribution of variance following PCoA. Such a structured morphospace occupation can be due to strong phylogenetic signal, clustered sets of character state combinations (morphologically distinct groups of taxa), or, more problematically, non-random distribution of missing data.

PHYLOMORPHOSPACE

phylogenetic datasets naturally encourage the use of their phylogenetic content in the course of disparity analyses, and the usefulness of contrasting patristic and phenetic dissimilarities in disparity studies has been emphasized (e.g. Foote 1996; Wagner 1997). Here I restrict the discussion to the use of phylogenetic information to project the inferred tree onto the morphospace. This construction has been referred to as “phylomorphospace” (Sidlauskas 2008, but see Strelin et al. 2018 for a warning regarding the use of this term). It has been used to infer the placement of “ancestors” in the morphospace, assess the strength of the phylogenetic signal contained in a morphological dataset, and test for patterns of convergence (e.g. Klingenberg and Gidaszewski 2010; Stayton 2015).

Producing a phylomorphospace visualization implies determining the location of the internal nodes of the tree in the morphospace, i.e., estimating their phenotypic trait values, and therefore requires a model of trait evolution. Importantly, the meaningfulness of these estimates depends on the adequacy of the model chosen. Different methods are employed for

inferring ancestral trait values depending on whether the phenotypic traits considered show discrete or continuous modes of variation. In the case of discrete character spaces, it is therefore again critical to properly distinguish the discrete architecture of the morphospace from its ordination in a space equipped with a continuous coordinate system. Only methods devised for discrete traits (e.g. maximum parsimony or posterior probabilities calculated from the likelihoods of ancestral states in Mk models; Cunningham et al. 1998; Hunt and Slater 2016) are appropriate for estimating ancestral character states in this context. Use of methods for continuous traits (e.g., squared-change parsimony, maximum likelihood models based on Brownian motion) applied to the principal coordinate scores of OTUs will lead to the incorrect placement of ancestral nodes in the ordination (e.g. Ruta et al. 2013; Hopkins and Smith 2015). Their positions will be undefined locations in the discrete morphospace and subsequent analyses and interpretations relying on them will be flawed.

Figure 2 provides a simple theoretical illustration of this problem. Five OTUs (labelled A to E) are coded with 8 binary characters. These include 3 parsimony informative characters that support the phylogenetic reconstruction (Fig. 2A) and 5 autapomorphic characters that distinguish the OTUs from each other. Character states at internal nodes are estimated using maximum parsimony. As mentioned earlier, without autapomorphies and in the absence of homoplasy, sister OTUs would be merged with their supporting node. For instance, OTUs A and B and node i would all be described by the sequence (1, 0, 0).

Figure 2B shows the morphological hypercube (8 dimensions) embedded in the Euclidean space. The tips (OTUs) and the reconstructed internal nodes of the tree are located at their respective vertices of the hypercube. The branches of the tree correspond to edges (or sequences of edges in the general case) and are highlighted. This is a phylomorphospace representation that accounts for the discrete nature of the characters. Figure 2C shows the same hypercube and the same OTUs, but the distribution of internal nodes has been estimated

using squared-change parsimony from the principal coordinate scores of the OTUs. The resulting depiction of the tree is substantially different from that of Figure 2B and none of the inferred internal nodes belong to vertices of the hypercube. This representation is invalid because it fails to acknowledge the true, underlying morphospace.

Phylomorphospaces built from continuous traits usually provide easily interpretable bivariate visualizations, with all internal nodes located within the convex hull defined by the OTUs and a degree of branch-crossing indicative of the amount of homoplasy. Conversely, with discrete characters, phylomorphospace visualizations tend to show very complex patterns from which little can be inferred (e.g. Halliday and Goswami 2015). Figure 2D illustrates the geometry of the phylomorphospace representation in the simple case considered. The parsimony informative characters supporting the tree define a subspace within the discrete morphospace. It is also a hypercube but of lower dimensionality (here it is a cube). As described earlier and shown here, the autapomorphies push OTUs away from the subspace of parsimony informative characters in orthogonal directions.

Brusatte et al. (2011) suggested the use of inferred ancestral nodes to derive phylogenetically corrected disparity curves. They described that the addition of reconstructed ancestors leads to an inflation of the morphospace, since these ancestors appear to fall outside the limits drawn by the observed taxa, as outlined by means of convex hulls. This is in fact a misinterpretation of the effect of the bivariate projection of the discrete morphospace and a drawback of the use of convex hulls in a discrete character context. These ancestors do not represent any aberrant or inexplicable combinations of character states but correspond to existing vertices on the discrete morphospace. Their apparent peripheral distribution results from the geometry of the morphospace (see Fig. 2B), the presence of homoplasy, and the distribution of the total set of taxa (observed and reconstructed) from which the ordination plane is defined.

426

427 **THE PROBLEM OF MISSING DATA**

428

429 Unscored entries in discrete character data matrices is problematic both for phylogenetic
430 inference (e.g. Platnick et al. 1991; Maddison 1993; Wilkinson 1995; but see Kearney 2002)
431 and for disparity analyses. They correspond to either missing or inapplicable data, and are
432 traditionally reported as ‘?’ and ‘–’, respectively. Missing and inapplicable character states are
433 handled similarly by phylogenetic software such as PAUP* (Swofford 2003) or TNT
434 (Goloboff et al. 2008), and within standard disparity pipelines. The distinction between the
435 two is not negligible from a morphospace perspective however.

436

437

438 *Inapplicable character states*

439

440 Within current methodological frameworks, it does not seem advisable to retain in a disparity-
441 aimed dataset characters that happen to be inapplicable for one or more taxa in a sample.
442 These taxa do not have definable positions along the dimensions defined by the inapplicable
443 characters but instead occupy the complementary subspace of the morphospace. A distance
444 matrix can still be computed (albeit a deficient one) and ordinated by means of PCoA, but this
445 will artificially enforce the placement of these taxa in a space they do not technically reside
446 in. As it is sometimes done, disparity can even be calculated from this ordination, but the
447 meaning of such measures is questionable on logical grounds. Novel kinds of morphospaces
448 (and morphospace representations) need to be devised to accommodate the problem of
449 inapplicable character states. This would be particularly useful for studies at high taxonomic
450 ranks where OTUs tend to reside in only partially overlapping character spaces.

451

452

453 *The effect of missing data*

454

455 The central problem of missing data for disparity analysis is that it generates inconsistencies
456 in the pairwise distance matrix **D**. If one considers the following three taxa with one missing
457 entry for taxon A for the fifth characters:

458

459 Taxon A: (0, 0, 1, 0, ?)

460 Taxon B: (0, 0, 1, 0, 0)

461 Taxon C: (0, 0, 1, 0, 1)

462

463 Comparison of sequences of B or C with A can only be done for four characters. From this
464 partial information, C is seen as identical to A, B as identical to A, and yet, B and C differ by
465 one mismatch. A taxon with missing data directly affects the $n-1$ distances it is involved in. It
466 does not affect other pairwise comparisons, but it leads to inconsistencies in the overall
467 distance matrix with cases as described above and a proportion of triplets of taxa whose
468 pairwise comparisons do not satisfy the triangle inequality. If so, **D** is not fully metric
469 anymore and its PCoA generates negative eigenvalues and potentially confusing
470 visualizations (e.g. morphologically distinct taxa merged into a unique position). Some
471 methods have been proposed to eliminate negative eigenvalues. These methods either add a
472 specific constant value to the non-diagonal entries of **D** or **D**² (e.g. Lingoes 1971; Cailliez
473 1983) or ‘squeeze’ the eigenvalues of the Gower-centred matrix (e.g., Hayes and Hill 1981;
474 Kirkpatrick and Lofsvold 1992). These corrections however differentially rescale

475 dissimilarities depending on their magnitudes (Legendre and Legendre 1998), and therefore
 476 need to be considered carefully in the context of disparity.

477 Obtaining a precise description of the effect of missing data on the distance matrix is a
 478 difficult task because numerous factors may affect, in interrelated ways, the response of the
 479 distance matrix to missing data. These factors include the shape of the frequency distribution
 480 of the pairwise distances (e.g., mean and variance), the shape of the character matrix $\mathbf{M}$ (n/p
 481 ratio), the distribution of missing data in $\mathbf{M}$ (amount and structure), and the use of scaling
 482 option for dissimilarities (when missing data occur, scaling is employed to make comparisons
 483 of dissimilarities fairer when these have been calculated from sequences of character states of
 484 different lengths. For instance, observed matches and mismatches between two taxa provide a
 485 dissimilarity measure which is then divided by the number of characters involved in its
 486 calculation – “mean character difference”; Sneath and Sokal 1973; Foote 1992).

487 The following simulation can help get a glimpse of the impact of missing data on the distance
 488 matrix. It is again a simplification of most real case studies, but it supplies an intuitive idea of
 489 the average behaviour of $\mathbf{D}$ while leaving aside the idiosyncrasies of empirical datasets. Let $\mathbf{D}$
 490 be the Hamming distance matrix of a complete dataset (taken as a uniform distribution of n
 491 taxa in a p -hypercube), $\mathbf{D}_k$ the distance matrix of the same dataset but plagued with a
 492 proportion k of uniformly distributed missing entries, and $\mathbf{D}_{\text{Euc}}$ the Euclidean distance matrix
 493 calculated from the principal coordinates of $\sqrt{\mathbf{D}_k}$. Results show that the correlations between
 494 $\mathbf{D}$ and $\mathbf{D}_k$, and between $\sqrt{\mathbf{D}}$ and $\mathbf{D}_{\text{Euc}}$, both show a linear decrease with slope -1 as k increases
 495 (correlations measured as Pearson's r and Spearman's ρ). It means for instance that when $k \approx$
 496 10%, r and $\rho \approx 0.9$, and when $k \approx 50\%$, r and $\rho \approx 0.5$. Note that in this example, despite the
 497 changes in the ranking of distances in $\mathbf{D}_k$, morphological disparity measured as the mean
 498 pairwise distance (e.g. Foote 1992; Ciampaglio et al. 2001) would on average be left
 499 unchanged. This does not occur for meaningful reasons however, but results from the uniform

distribution of missing data. This random removal of entries in $\mathbf{M}$ has equal probabilities of increasing or decreasing a pairwise distance compared to its true value. As k increases, it also makes greater departures from the true value easier, leading to an increase in the variance of the distribution of distances (with the same mean) which explains the decrease in r and ρ observed.

Patterns of missing data

Because of the non-random decay and fossilization of organismal characters (e.g. Sansom et al. 2010), missing data tend not to be randomly distributed in the character matrices but instead preferentially affect suites of characters that are generally lost together for anatomical, structural and/or compositional reasons. Smith et al. (2014) developed a linkage algorithm to account for the resulting differential quality of character scoring and showed that disparity estimates do indeed respond differently to random (Poisson distributed in their simulations) and linked missing data. In addition, taphonomic processes and preservational opportunities can also vary in time and space introducing additional heterogeneities in the pattern of missing entries among taxa.

All these factors can artificially inflate or reduce a measure of disparity depending on their particular combination and magnitude for the set of taxa considered. This potentially generates a collection of disparity measures (for instance corresponding to distinct time intervals, geographic areas or taxonomic groups) with reduced commensurability due to the limited overlap of their respective character subspaces. While a small amount of missing data does not seem to prevent reliable measures of disparity, it is unlikely to be the case when the proportion of missing data is significantly higher and heterogeneously distributed.

Unfortunately, the use of phylogenetic data matrices as disparity datasets has been accompanied by a substantial increase in the amount of missing data in disparity studies. Ciampaglio et al. (2001) provided a comparative survey of several disparity indices and investigated their sensitivity to various factors including missing data. At the time, they reported that disparity datasets were typically less than 25% incomplete and showed that the most widely employed disparity indices were relatively stable up to 30% of missing data. With the incorporation of phylogenetic datasets within the pool of disparity datasets, this value of 25% is now regarded as an unrealistic upper bound (Butler et al. 2012; Lloyd 2016). It is not rare to have phylogenetic datasets with more than 50% of missing data, with frequent instances of taxa with more than 80 or 90% of their entries unscored (e.g. Butler et al. 2012). Several approaches have therefore been recently suggested to cope with this intensified problem of missing data.

Suggested approaches

Phylogenetic correction methods to fill in missing data have been proposed and employed in empirical case studies (Brusatte et al. 2011; Butler et al. 2012). One problem with such approaches is that they are dependent on the phylogenetic hypotheses and impose a model of character evolution on the reconstructed dataset. This might obscure the underlying dynamics of the true disparity signal and impede the test of macroevolutionary hypotheses. Smith et al. (2014) recommended that comparisons of disparity estimates among time intervals that involve sets of taxa differentially affected by missing data should account for this discrepancy. They suggested that taxa should be subjected to removal of some of their character entries, based on an adequate linkage pattern, so that all time intervals have as much

missing data as the most incomplete one. While this rarefaction procedure might appear sensible, it is unlikely to improve the quality of disparity curves and may in fact decrease the signal-to-noise ratio. Missing entries are detrimental to the measurement of dissimilarity and increasing their amount is not a desirable option. If there are strong variations in the amount of missing data across time intervals, it is preferable not to artificially deteriorate reliable disparity estimates of well documented time intervals for the sake of comparing them to the low quality (and potentially meaningless) disparity estimates of other time intervals.

Recommendations

What other solutions then? Until new fossil discoveries help filling the gaps in the character matrix, there are options to minimize or at least provide reminders of the negative impact of missing data on the measurement of dissimilarities and the interpretation of morphospace and disparity patterns.

One approach to lower the relative amount of missing data is to work on subsets of characters. If a pattern of character linkage applies to all the taxa investigated, then it means that the whole dataset can be partitioned into distinct subsets of characters with variable degrees of completeness. Reasonably complete subsets can then be combined or treated separately and their disparity patterns inferred. Beyond the preservational reasons underlying their definition, these subsets of characters might also reflect developmentally or functionally driven associations of traits into coherent units of evolutionary transformation (evolutionary modules; e.g. Schlosser and Wagner 2004). The disparity signals of these subsets might therefore be more helpful for identifying the determinants of a clade's disparity than its global

disparity signal, because they are less likely to combine characters with different modes and rates of evolution (Hopkins and Gerber 2017).

If one is interested in a global disparity signal, then approaches are needed to ensure that the missing data will not mislead the discussions of the results. Again, one risk comes from an undue reliance on morphospace ordination. Back to the hypercube example, if a taxon has k entries unscored in its p -length character state sequence, it means that the vertex the taxon truly occupies is one within a set of 2^k vertices, representing a proportion 2^{k-p} of the hypercube. As k increases, this can represent a very large set of possible locations (and a large proportion of the total set of vertices when k gets close to p). Not all possible options are equally likely of course, but still more than one can be expected to be plausible. An increasing proportion of such taxa with high k and high k/p lower the quality of the representation of $\mathbf{D}_k$ in the principal coordinate space, introducing more and more pronounced discordances between disparity estimates measured from $\mathbf{D}_k$ and from the ordination.

In general, despite the uneven quality and completeness of the description of taxa in the character matrix, an equal degree of confidence is implicitly attached to all taxa in the morphospace ordination: All of them contribute equally to the definition of the principal coordinate axes; all of them are depicted in the same way as unique points in the ordination space; all of them are considered equally informative in subsequent analyses carried out from the ordination scores. This uneven scoring quality needs to be documented and taken into account. A simple index $q_i = (p - k_i) / p$ ranging from 0 to 1 (incomplete to complete) can provide a measure of the quality of the morphological description of taxon i .

For visualization purposes, it is possible to use a colour-code based on $\mathbf{q}$ (the column vector storing individual values q_i) in order to convey the degree of reliability one can attribute to a given taxon in the morphospace ordination (although its relative position can still be influenced by other taxa). It could also be possible to normalize $\mathbf{q}$ and use it as a vector of

599 weights to calculate a weighted covariance matrix Σ of the principal coordinate scores. If
600 there is substantial variation in scoring quality among taxa, a principal component analysis of
601 Σ then allows a reorientation of the ordination space improving the representation of spatial
602 relationships among the better-preserved taxa (with the reservations expressed earlier
603 regarding the partial information provided by low-dimensional approximations).
604 For the construction of disparity curves, I do not recommend to carry out analyses from the
605 morphospace ordination (“post-ordination disparity” in Lloyd 2016), but instead to obtain
606 disparity measures directly from the distance matrix $\mathbf{D}_k$ in order to minimize the impact of
607 missing data. Each time interval is characterized by a set of taxa that is a subset of the total
608 number of taxa sampled. The distance matrix of the subset is therefore a submatrix of $\mathbf{D}_k$.
609 Estimating disparity from this submatrix ensures that the estimate is unrelated to the amount
610 and pattern of missing data of taxa occurring in other time intervals. Conversely, a disparity
611 estimate inferred from the principal coordinate scores of the subset of taxa is influenced by all
612 other taxa because the principal coordinate axes are defined from the whole $\mathbf{D}_k$. Hence, the
613 detrimental effect of taxa with large amount of missing data will be spread out over the entire
614 time range studied regardless of their temporal occurrence, and affect all ordination-based
615 disparity estimates. Working with submatrices of $\mathbf{D}_k$ restricts the impact of poorly-preserved
616 taxa to their own time interval (the same argument holds if one is working with different
617 taxonomic groups or geographic regions instead).
618 Disparity is conceived as the spacing and spread of taxa in morphospace. These features are
619 traditionally calculated as the sum of variances and sum of ranges for a morphospace spanned
620 by continuous variables. For discrete character spaces, the average pairwise distance is
621 conceptually equivalent to the sum of variances (the latter can be shown to be proportional to
622 the average squared pairwise Euclidean distance) and maximum pairwise distance indices
623 analogous to range-based measures can be derived as well (Hughes et al. 2013). The number

of character state combinations is also an intuitive measure of the amount of morphospace occupied provided some of its weaknesses are accounted for (sensitivity to sample size and dimensionality. Thomas and Reif 1993; Foote 1994; Ciampaglio et al. 2001). Finally, it appears essential for disparity studies to systematically report the overall proportion of missing data and the average percentages of unscored entries per taxon and per character. Maximum, minimum, and average values of q (or of any other equivalent quality index) should also be calculated for each time interval and plotted alongside disparity curves. This will provide a helpful indication to decide the level of confidence one can put in the disparity values reported.

CONCLUDING REMARKS AND PERSPECTIVES

On phylogenetic datasets as disparity datasets

Discrete character spaces have geometric features that make them quite distinct from other types of morphospaces encountered in evolutionary paleobiology. The discrete coding they allow is particularly relevant for the measurement of morphological variation at high taxonomic level. The co-option of phylogenetic data matrices as bases for morphospace construction has significantly increased the frequency of discrete character spaces in disparity studies. A positive outcome has been the broadening of the taxonomic scope of disparity analyses to include many vertebrate clades whose general morphology is difficult to characterize morphometrically. This rapid increase in the use of phylogenetic data matrices nevertheless calls for a critical assessment of their conceptual and operational value.

While it is often stated in these studies that “well established protocols” of disparity analyses were used, it is important to keep in mind that these protocols were devised for much larger datasets (in terms of number of OTUs). For example, the relative insensitivity to sample size of some disparity indices might need to be reconsidered if the number of taxa sampled in a time interval is very low (a frequent result of the temporal partition of small-size phylogenetic data matrices). Likewise, the often-mentioned ability of PCoA to handle missing data undoubtedly has limits, and obtaining principal coordinate scores does not guarantee their meaningfulness if the input distance matrix is poorly representative of the true pattern of variation. Hence, some aspects of the disparity pipeline need to be adjusted or reconsidered in order to account for the specificities of phylogenetic-based disparity datasets and ensure that their use is not associated with disparity inferences of lower quality.

On the measurement of dissimilarity

Despite the centrality of this problem (the choice of how to relate morphologies underlies the resulting topology of the morphospace), little has been said above on the possible options for measuring dissimilarity between pairs of OTUs. Only a few points are given below (and all assume the validity of a metric topology) but more work and methodological developments are needed in this area (Gerber 2014, 2017).

Lloyd (2016) proposed five criteria defining a good distance measure for disparity analyses:

- (i) distances should be robust against missing data (this property can be assessed by simulations); (ii) the resulting distance matrix should be as Euclidean as possible (leading to no or few negative eigenvalues when carrying out PCoA); (iii) distances should be definable for all possible pairs of OTUs; (iv) their implied spatial pattern should be summarisable with

as few dimensions as possible; (v) the set of distances should be as close to normally distributed as possible (because of the parametric nature of many statistical tests). While points (i) and (iii) are legitimate, points (ii), (iv), and (v) are not justifiable. The choice of the distance measure should be biologically driven and not dictated by the requirements of ordination methods or of any subsequent analyses of the distance matrix. The notion of disparity emerges from the structure of the distribution of distances. Whether the latter departs from normality or does not lend itself to successful ordination in reduced-space should be a secondary concern (patterns of morphospace occupation can be inferred without visualisation). Defining a biologically meaningful measure of distance is a difficult task though given the anatomical diversity of the characters found in phylogenetic and disparity datasets. Weighting approaches might help account for the heterogeneity of characters and of their developmental bases (which invalidates equal weighting and impairs the value of simple measure such as the Hamming distance; see also Mitteroecker and Huttegger 2009). The diverse developmental depth of characters was considered early on as an important issue calling for the differential weighting of characters when measuring dissimilarity between morphologies (Gould 1991). Equal weighting schemes seem to have been preferentially used so far, but treelike representations of development should in principle allow the definition of plausible hierarchies of characters and weighting schemes (Schank and Wimsatt 1986; Arthur 1988). The value of such hierarchical approaches needs to be evaluated.

On the visualization of morphospaces

It has been shown above why a morphospace must be distinguished from its ordination. In the case of discrete character spaces, the ordination consists in a Euclidean embedding of the

morphospace and the ordination space is thus equipped with a coordinate system that differs from that of the morphospace. This distinction is important and both qualitative descriptions and quantitative analyses of the morphospace should not conflate the two spaces. Furthermore, in most empirical instances of discrete character spaces, the depiction of the spatial relationships among taxa supplied by the ordination is deceptive and its reliability can be further deteriorated by abundant missing data. Some graphical options have been suggested above to limit misinterpretations of morphospace patterns, such as the depiction of the connection structure of the vertices or the drawing of frequency ellipses of the distribution of vertices. It is also possible that the developmentally informed weighting schemes recommended above will improve the graphical representation of morphospaces by providing distributions of pairwise distances better summarized by standard ordination methods. A morphological hypercube has been taken as an example throughout, but many datasets depart from this simple case. If multistate characters are present, the discrete space will be geometrically more complex than a hypercube and its architecture will depend on the ordered/unordered status of the character states. While this architecture might be more difficult to visualize, the options described above can be extended to these more complex cases (e.g. visualization of neighbouring vertices). Finally, obtaining informative visualizations of multidimensional spaces is a very general problem (e.g. Abramson and Zarette 2003) and methods developed in different research fields might be fruitfully adapted to the context of morphospaces.

On missing data

Missing data appear to be the most serious problem brought on by the increasing popularity of discrete character data in disparity studies, even though its consequences are often overlooked. Numerous interacting biological and physical factors can be responsible for missing entries in discrete character matrices, making their specific effect on disparity estimates difficult to appreciate. Numerical or, ideally, analytical approaches are needed to better characterize the behaviour of dissimilarity and disparity measures in face of these perturbations. Progresses in this area could also help devise ways to lessen the impact of missing data. Meanwhile, reporting the structure (e.g. row and column distributions) and amount of missing data will allow a critical appraisal of the disparity patterns documented. Combined with the small sample size issue resulting from the temporal partitioning of phylogenetic data matrices, missing data can lead to poorly supported disparity curves and temporal shifts in disparity between successive time intervals might not reflect any biological signal. In such contexts, coarser but more robust descriptions of clade shape seem preferable, for instance through the use of a centre-of-gravity approach (e.g. Foote 1991; Hughes et al. 2013). While not as detailed as standard disparity curves, they will still contribute to our assessment of the relative frequencies of possible disparity patterns, and such assessments remain necessary for detecting potential trends and generalities in morphological macroevolution.

Acknowledgements

I am grateful to Jennifer Hoyal Cuthill and Gunther J. Eble for discussions on some of the topics covered in this contribution and to Zuzana Gerber and Yoland Savriama for comments on an earlier draft. Constructive comments by an anonymous reviewer and a detailed and

insightful review by Peter J. Wagner helped improve and clarify the manuscript. Most of this work was done while holding a research associate position in the Department of Earth Sciences at the University of Cambridge and was funded by a Templeton World Charity Foundation grant (LBAG/143) awarded to Simon Conway Morris.

REFERENCES

ABBOTT, E. A. 1884. *Flatland: A Romance of Many Dimensions*. Seeley & Co, London, 100 pp.

ABRAMSON, G. and ZANETTE, D. H. 2003. Two-dimensional projections of a hypercube. *Physical Review E*, **67**, 057101.

ARTHUR, W. 1988. *A theory of the evolution of development*. John Wiley & Sons Inc., New York, 94 pp.

BUTLER, R. J., BRUSATTE, S. L., ANDRES, B. and BENSON, R. B. 2012. How do geological sampling biases affect studies of morphological evolution in deep time? A case study of pterosaur (Reptilia: Archosauria) disparity. *Evolution*, **66**, 147–162.

BRUSATTE, S. L., BENTON, M. J., RUTA, M. and LLOYD, G. T. 2008. Superiority, competition, and opportunism in the evolutionary radiation of dinosaurs. *Science*, **321**, 1485–1488.

773 –, MONTANARI, S., YI, H. Y. and NORELL, M. A. 2011. Phylogenetic corrections for
774 morphological disparity analysis: new methodology and case studies. *Paleobiology*, **37**, 1–22.
775

776 CAILLIEZ, F. 1983. The analytical solution of the additive constant problem. *Psychometrika*,
777 **48**, 305–308.
778

779 CHARTIER, M., LÖFSTRAND, S., VON BALTHAZAR, M., GERBER, S., JABBOUR, F.,
780 SAUQUET, H. and SCHÖNENBERGER, J. 2017. How (much) do flowers vary? Unbalanced
781 disparity among flower functional modules and a mosaic pattern of morphospace occupation
782 in the order Ericales. *Proceedings of the Royal Society of London, Series B: Biological*
783 *Sciences*, **284**, 20170066.
784

785 CIAMPAGLIO, C. N., KEMP, M. and McSHEA, D. W. 2001. Detecting changes in
786 morphospace occupation patterns in the fossil record: characterization and analysis of
787 measures of disparity. *Paleobiology*, **27**, 695–715.
788

789 CISNEROS, J. C. and RUTA, M. 2010. Morphological diversity and biogeography of
790 procolophonids (Amniota: Parareptilia). *Journal of Systematic Palaeontology*, **8**, 607–625.
791

792 CUNNINGHAM, C. W., OMLAND, K. E. and OAKLEY, T. H. 1998. Reconstructing
793 ancestral character states: a critical reappraisal. *Trends in Ecology & Evolution*, **13**, 361–366.
794

795 CUTHILL, J. F. H. 2015. The morphological state space revisited: what do phylogenetic
796 patterns in homoplasy tell us about the number of possible character states?. *Interface focus*,
797 **5**, 20150049.
798

799 ERWIN, D. H. 2007. Disparity: morphological pattern and developmental context.
800 *Palaeontology*, **50**, 57–73.
801
802 –. 2017. The topology of evolutionary novelty and innovation in macroevolution.
803 *Philosophical Transactions of the Royal Society B*, **372**, 20160422.
804
805 ESTABROOK, G. F., JOHNSON Jr, C. S. and MC MORRIS, F. R. 1975. An idealized
806 concept of the true cladistic character. *Mathematical Biosciences*, **23**, 263–272.
807
808 FOOTE, M. 1991. Morphological and taxonomic diversity in clade's history: the blastoid
809 record and stochastic simulations. *Contributions from the Museum of Paleontology – The*
810 *university of Michigan*, **28**, 101–140.
811
812 –. 1992. Paleozoic record of morphological diversity in blastozoan echinoderms. *Proceedings*
813 *of the National Academy of Sciences*, **89**, 7325–7329.
814
815 –. 1993. Discordance and concordance between morphological and taxonomic diversity.
816 *Paleobiology*, **19**, 185–204.
817
818 –. 1994. Morphology of Ordovician-Devonian crinoids. *Contributions from the Museum of*
819 *Paleontology – The university of Michigan*, **29**, 1–39.
820
821 –. 1996. Perspective: evolutionary patterns in the fossil record. *Evolution*, **50**, 1–11.
822
823 –. 1997. The evolution of morphological diversity. *Annual Review of Ecology and*
824 *Systematics*, **28**, 129–152.

825

826 –. 1999. Morphological diversity in the evolutionary radiation of Paleozoic and Post-
827 Paleozoic crinoids. *Paleobiology*, **25** (S2), 1–115.

828

829 GERBER, S. 2014. Not all roads can be taken: development induces anisotropic accessibility
830 in morphospace. *Evolution & development*, **16**, 373–381.

831

832 –. 2017. The geometry of morphospaces: lessons from the classic Raup shell coiling model.
833 *Biological Reviews*, **92**, 1142–1155.

834

835 GOLOBOFF, P. A., FARRIS, J. S. and NIXON, K. C. 2008. TNT, a free program for
836 phylogenetic analysis. *Cladistics* **24**, 774–786.

837

838 GOULD, S. J. 1991. The disparity of the Burgess Shale arthropod fauna and the limits of
839 cladistic analysis: why we must strive to quantify morphospace. *Paleobiology*, **17**, 411–423.

840

841 GOWER, J. C. 1966. Some distance properties of latent root and vector methods used in
842 multivariate analysis. *Biometrika*, **53**, 325–338.

843

844 HALLIDAY, T. J. D. and GOSWAMI, A. 2016. Eutherian morphological disparity across the
845 end-Cretaceous mass extinction. *Biological Journal of the Linnean Society*, **118**, 152–168.

846

847 HARRISON, L. and LARSSON, H. C. E. 2015. Among-character rate variation distributions
848 in phylogenetic analysis of discrete morphological characters. *Systematic Biology*, **64**, 307–
849 324.

850

851 HAYES, J. F. and HILL, G. W. 1981. Modification of estimates of parameters in the
852 construction of genetic selection indices ('bending'). *Biometrics*, **37**, 483–493.
853

854 HOPKINS, M. J. and GERBER, S. 2017. Morphological Disparity. 1–12. In NUNO DE LA
855 ROSA, L. and MÜLLER, G. (eds). *Evolutionary Developmental Biology: A Reference Guide*,
856 Springer, Cham.
857

858 – and SMITH, A. B. 2015. Dynamic evolutionary change in post-Paleozoic echinoids and the
859 importance of scale when interpreting changes in rates of evolution. *Proceedings of the*
860 *National Academy of Sciences*, **112**, 3758–3763.
861

862 HETHERINGTON, A. J., SHERRATT, E., RUTA, M., WIKINSON, M., DELINE, B. and
863 DONOGHUE, P. C. 2015. Do cladistic and morphometric data capture common patterns of
864 morphological disparity?. *Palaeontology*, **58**, 393–399.
865

866 HUGHES, M., GERBER, S. and WILLS, M. A. 2013. Clades reach highest morphological
867 disparity early in their evolution. *Proceedings of the National Academy of Sciences*, **110**,
868 13875–13879.
869

870 HUNT, G. and SLATER, G. 2016. Integrating paleontological and phylogenetic approaches
871 to macroevolution. *Annual Review of Ecology, Evolution, and Systematics*, **47**, 189–213.
872

873 KEARNEY, M. 2002. Fragmentary taxa, missing data, and ambiguity: mistaken assumptions
874 and conclusions. *Systematic Biology*, **51**, 369–381.
875

876 KIRKPATRICK, M. and LOFSVOLD, D. 1992. Measuring selection and constraint in the
877 evolution of growth. *Evolution*, **46**, 954–971.
878

879 KLINGENBERG, C. P. and GIDASZEWSKI, N. A. 2010. Testing and quantifying
880 phylogenetic signals and homoplasy in morphometric data. *Systematic Biology*, **59**, 245–261.
881

882 LEGENDRE, P. and LEGENDRE, L. 1998. *Numerical Ecology*. Elsevier Science,
883 Amsterdam, 853 pp.
884

885 LEWIS, P. O. 2001. A likelihood approach to estimating phylogeny from discrete
886 morphological character data. *Systematic Biology*, **50**, 913–925.
887

888 LINGOES, J. C. 1971. Some boundary conditions for a monotone analysis of symmetric
889 matrices. *Psychometrika*, **36**, 195–203.
890

891 LLOYD, G. T. 2016. Estimating morphological diversity and tempo with discrete character-
892 taxon matrices: implementation, challenges, progress, and future directions. *Biological*
893 *Journal of the Linnean Society*, **118**, 131–151.
894

895 MADDISON, W. P. 1993. Missing data versus missing characters in phylogenetic analysis.
896 *Systematic Biology*, **42**, 576–581.
897

898 MAYNARD SMITH, J., BURIAN, R., KAUFFMAN, S., ALBERCH, P., CAMPBELL, J.,
899 GOODWIN, B., LANDE, R., RAUP, D. M. and WOLPERT, L. 1985. Developmental
900 constraints and evolution: a perspective from the Mountain Lake conference on development
901 and evolution. *The Quarterly Review of Biology*, **60**, 265–287.

902

903 McGHEE, G. R. 2006. *The geometry of evolution: adaptive landscapes and theoretical*
904 *morphospaces*. Cambridge University Press, Cambridge, 212 pp.

905

906 MITTEROECKER, P. and HUTTEGGER, S. M. 2009. The concept of morphospaces in
907 evolutionary and developmental biology: mathematics and metaphors. *Biological Theory*, **4**,
908 54-67.

909

910 NEIGE, P. 2003. Spatial patterns of disparity and diversity of the Recent cuttlefishes
911 (Cephalopoda) across the Old World. *Journal of Biogeography*, **30**, 1125–1137.

912

913 OYSTON, J. W., HUGHES, M., WAGNER, P. J., GERBER, S. and WILLS, M. A. 2015.
914 What limits the morphological disparity of clades?. *Interface focus*, **5**, 20150042.

915

916 PLATNICK, N. I., GRISWOLD, C. E. and CODDINGTON J. A. 1991. On missing entries in
917 cladistic analysis. *Cladistics*, **7**, 337–343.

918

919 PRENTICE, K. C., RUTA, M. and BENTON, M. J. 2011. Evolution of morphological
920 disparity in pterosaurs. *Journal of Systematic Palaeontology*, **9**, 337–353.

921

922 RAUP, D. M. 1966. Geometric analysis of shell coiling: general problems. *Journal of*
923 *Paleontology*, **40**, 1178–1190.

924

925 –. 1972. Approaches to morphologic analysis. 28–44. In SCHOPF, T. J. M (ed). *Models in*
926 *paleobiology*, Freeman Cooper & Co, San Francisco, 250 pp.

927

928 RICKLEFS, R. E. 2004. Cladogenesis and morphological diversification in passerine birds.
929 *Nature*, **430**, 338.
930
931 ROMANO, M. 2017. Disparity vs. diversity in Stegosauria (Dinosauria, Ornithischia): cranial
932 and post-cranial sub-dataset provide different signals. *Historical Biology*, 1–9.
933
934 RUTA, M., BOTHA-BRINK, J., MITCHELL, S. A. and BENTON, M. J. 2013. The radiation
935 of cynodonts and the ground plan of mammalian morphological diversity. *Proceedings of the*
936 *Royal Society of London, Series B: Biological Sciences*, **280**, e20131865.
937
938 – and WILLS, M. A. 2016. Comparable disparity in the appendicular skeleton across the fish–
939 tetrapod transition, and the morphological gap between fish and tetrapod postcrania.
940 *Palaeontology*, **59**, 249–267.
941
942 SANSOM, R. S., GABBOTT, S. E. and PURNELL, M. A. 2010. Non-random decay of
943 chordate characters causes bias in fossil interpretation. *Nature*, **463**, 797.
944
945 SCHANK, J. C and WIMSATT, W. C. 1986. Generative Entrenchment and Evolution. 33–
946 60. In FINE, A. and MACHAMER, P. K. (eds). *Proceedings of the Biennial Meeting of the*
947 *Philosophy of Science Association* 1986, East Lansing, Michigan. 384 pp.
948
949 SCHLOSSER, G. and WAGNER, G. P. (eds.). 2004. *Modularity in Development and*
950 *Evolution*. University of Chicago Press, Chicago, 600 pp.
951
952 SIDLAUSKAS, B. 2008. Continuous and arrested morphological diversification in sister
953 clades of characiform fishes: a phylomorphospace approach. *Evolution*, **62**, 3135–3156.
954

955 SMITH, A. J., ROSARIO, M. V., EITING, T. P. and DUMONT, E. R. 2014. Joined at the
956 hip: Linked characters and the problem of missing data in studies of disparity. *Evolution*, **68**,
957 2386–2400.

958

959 SNEATH, P. H. A. and SOKAL, R. R. 1973. *Numerical Taxonomy*, W.H. Freeman & co, San
960 Francisco, 588 pp.

961

962 STAYTON, C. T. 2015. The definition, recognition, and interpretation of convergent
963 evolution, and two new measures for quantifying and assessing the significance of
964 convergence. *Evolution*, **69**, 2140–2153.

965

966 STRELIN, M. M., BENITEZ-VIEYRA, S., FORNONI, J., KLINGENBERG, C. P. and
967 COCUCCHI, A. 2018. The evolution of floral ontogenetic allometry in the Andean genus
968 *Caiophora* (Loasaceae, subfam. Loasoideae). *Evolution & development*, **20**, 29–39.

969

970 SWOFFORD, D. L. 2003. PAUP*. Phylogenetic analysis using parsimony (*and other
971 methods), Version 4. Sinauer Associates, Sunderland, MA.

972

973 THOMAS, R. D. K. and REIF, W. E. 1993. The skeleton space: a finite set of organic
974 designs. *Evolution*, **47**, 341–360.

975

976 THORNE, P. M., RUTA, M. and BENTON, M. J. 2011. Resetting the evolution of marine
977 reptiles at the Triassic-Jurassic boundary. *Proceedings of the National Academy of Sciences*,
978 **108**, 8339–8344.

979

980 WAGNER, G. P. and LYNCH, V. 2010. Evolutionary novelties. *Current Biology*, **20**, R48–
981 R52.

982

983 WAGNER, P. J. 1997. Patterns of morphologic diversification among the Rostroconchia.
984 *Paleobiology*, **23**, 115–150.

985

986 –. 2010. Paleontological perspectives on morphological evolution. 451–479. In BELL, M. A.,
987 FUTUYMA, D. J., EANES, W. F. and LEVINTON, J. S. (eds). *Evolution Since Darwin: The*
988 *First 150 Years*. Sinauer Associates, Sunderland, MA, 688 pp.

989

990 –. 2012. Modelling rate distributions using character compatibility: implications for
991 morphological evolution among fossil invertebrates. *Biology Letters*, **8**, 143–146.

992

993 WAGNER, P. J., RUTA, M. and COATES, M. I. 2006. Evolutionary patterns in early
994 tetrapods. II. Differing constraints on available character space among clades. *Proceedings of*
995 *the Royal Society of London, Series B: Biological Sciences*, **273**, 2113–2118.

996

997 WILKINSON, M. 1995. Coping with abundant missing entries in phylogenetic inference
998 using parsimony. *Systematic Biology*, **44**, 501–514.

999

1000 WILLS, M. A. 2001. Morphological disparity: a primer. 55–144. In ADRAIN, J. M.,
1001 EDGECOMBE, G. D. and LIEBERMAN B. S. (eds). *Fossils, phylogeny, and form: an*
1002 *analytical approach*. Springer, Boston, 402 pp.

1003

1004

FIGURE CAPTIONS

FIG. 1. Morphospace and ordination in reduced-space. A, the traditional depiction of morphospace, here by means of principal coordinate analysis. Taxa are represented as points in a space of continuous quantitative variables (1: *Batrachotomus*, 2: *Effigia*, 3: *Prestosuchus*, 4: *Lotosaurus*, 5: *Aetosaurus*, 6: *Riojasuchus*, 7: *Arizonasaurus*, 8: *Saurosuchus*, 9: *Postosuchus*, 10: *Gracilisuchus*, 11: *Ornithosuchus*, 12: *Revueltosaures*, 13: *Shuvosaurus*, 14: *Terrestrisuchus*, 15: *Rutiodon*, 16: *Hesperosuchus*, 17: *Desmotosuchus*, 18: *Mystrisuchus*). B, the same ordination space but the true, discrete architecture of the morphospace, a 10-hypercube, is shown by drawing the edges connecting neighbouring vertices. C, another visualization of the morphospace where only a subset of edges is represented. The subset is defined to ensure the complete connectedness of the occupied vertices. The size of points is proportional to the score on the third principal coordinate axis (orthogonal to the plane defined by the first two principal coordinate axes). The circular ellipse circumscribes ~95% of the locations of possible morphologies. D, mean variation of the density of vertices along a principal coordinate axis under 500 random orientations of the hypercube. The black line is the average of the 500 runs represented in grey.

FIG. 2. The mapping of phylogenetic tree onto morphospace. A, a simple phylogenetic hypothesis relating five taxa {A, B, C, D, E} and corresponding to the most parsimonious tree associated with the discrete character matrix shown on the right. The latter includes 3 parsimony informative characters and 5 autapomorphic characters. B, the visualization of the

tree in the ordination space when the estimates of ancestral states at internal nodes {f, g, h, i} properly account for the discrete architecture of the morphospace, a 8-hypercube (inferred ancestral states are displayed in the matrix of the first panel). C, the visualization of the tree when the ancestral states are incorrectly inferred from the continuous Euclidean coordinate system of the ordination space (squared-change parsimony). D, same as B, but the subspace of parsimony informative characters is highlighted. It is a cube and autapomorphies push the five taxa away from it and from each other in orthogonal directions. Note that the projection of the morphospace here does not correspond to a principal coordinate analyses of the matrix of pairwise distances among {A, B, C, D, E}. It has instead been defined to better visualise the discrepancy between the two modes of ancestral states reconstruction, the architecture of the parsimony informative subspace and the effect of autapomorphic characters. Such an orientation could happen for instance with the presence of other groups of taxa and shows why reconstructed ancestors can appear “outside” the convex hull of the set of taxa from which ancestors are inferred.

FIGURE 1