PALEOBIOLOGY
A PUBLICATION OF THE
Paleontological
SOCIETY

Article

Spatial scaling of beta diversity in the shallow-marine fossil record

Tom M. Womack , *James S. Crampton* , *and Michael J. Hannah*

Abstract.—Beta diversity quantifies the spatial structuring of ecological communities and is a fundamental partition of biodiversity, central to understanding many macroecological phenomena in modern biology and paleobiology. Despite its common application in ecology, studies of beta diversity in the fossil record are relatively limited at regional spatial scales that are important for understanding macroevolutionary processes. The spatial scaling of beta diversity in the fossil record is poorly understood, but has significant implications due to temporal variation in the spatial distribution of fossil collections and the large spatio-temporal scales typically employed. Here we test the spatial scaling of several common measures of beta diversity using the Cenozoic shallow-marine molluscan fossil record of New Zealand and derive a spatially standardized time series of beta diversity. To measure spatial scaling, we use and compare grid-cell occupancy based on an equal-area grid and summed minimum spanning tree length, both based on reconstructed paleocoordinates of fossil collections. We find that beta diversity is spatially dependent at local to regional scales, regardless of the metric or spatial scaling utilized, and that spatial standardization significantly changes apparent temporal trends of beta diversity and, therefore, inferences about processes driving diversity change.

Tom M. Womack, James S. Crampton, and Michael J. Hannah. School of Geography, Environment and Earth Sciences, Victoria University of Wellington, Post Office Box 600, Wellington, New Zealand. E-mail: tom. womack@vuw.ac.nz, james.crampton@vuw.ac.nz, michael.hannah@vuw.ac.nz

Introduction

The correct interpretation of past patterns of biodiversity is fundamental to our understanding of how life responds to environmental change and provides a valuable context for the current biodiversity crisis (Urban 2015; Blowes et al. 2019). Biodiversity can be subdivided broadly into three main partitions: alpha, beta, and gamma diversity (Whittaker 1960). Alpha is diversity at the finest scale—the point sample—and gamma is diversity at the largest scale of observation (Patzkowsky and Holland 2012). Beta diversity represents spatial variation of species among sites at the scale of observation, and in a sense it links alpha and gamma diversities (Anderson et al. 2011). The spatial scale of observation is contextual, and gamma diversity may reflect diversity at relatively small to global scales. Alpha and gamma diversity are, in theory, directly measurable in ecology, that is, through exhaustive investigation, whereas beta diversity reflects a derived quantity. Beta diversity is a fundamental partition of biodiversity and

is central to many macroecological phenomena (Lennon et al. 2001). It has been shown to be a significant contributor to gamma diversity in ecological (Lennon et al. 2001; McKnight et al. 2007; Veech and Crist 2007) and paleoecological studies (Holland 2010; Na and Kiessling 2015) and an important factor in understanding the drivers of biodiversity (Aberhan and Kiessling 2012; Patzkowsky and Holland 2012; Hofmann et al. 2019). Previous studies within the fossil record have highlighted that there is a need for analyses at finer spatial and geographic scales (Aberhan and Kiessling 2012; Patzkowsky and Holland 2012), particularly at the regional scale, which has been identified as a biogeographically important scale for understanding macroevolutionary patterns (Vermeij and Leighton 2003). Studies of beta diversity at the regional scale are relatively limited, and even scarcer are studies on the spatial dependence of beta diversity (Barton et al. 2013). This is particularly important in the fossil record, where temporal variation in spatial distribution of fossil localities is a known and

CrossMark

pervasive bias (Vilhena and Smith 2013; Close et al. 2017, 2020a,b).

Previous studies of beta diversity in the fossil record at large spatiotemporal scales have allowed for spatial variability in sampling by combining collections based on either a grid system (Crampton et al. 2011; Brocklehurst et al. 2018; Penny and Kröger 2019) or a specified distance (He et al. 2018). However, these approaches do not necessarily account for temporal variation in spatial distribution or area, and time series of beta diversity may be affected by this. Broadly speaking, beta diversity is commonly measured by the direct relationship between alpha and gamma components, true beta diversity sensu stricto (see Tuomisto 2010a,b), or by measuring compositional dissimilarity between point samples (Anderson et al. 2011). Conceptually and in ecological terms, assuming a fixed grain size (the spatial scale of individual units of observation) and variable extent (the spatial scale encompassing all units of observation), we would expect beta diversity, measured from the direct relationship of alpha and gamma, to increase with increasing area (Barton et al. 2013). The rate of increase is expected to decline from local to regional scales as fewer new species are encountered and one approaches total regional (gamma) diversity, in the manner shown by the triphasic species–area relationship (Rosenzweig 1995). Intuitively, this would be applicable to the fossil record, as we anticipate the same relationship (Sclafani and Holland 2013). The relationship between spatial scale and compositional dissimilarity is, however, more complex and dependent on taxa and grain and extent size (Barton et al. 2013) and is still debated in current ecological research (Barton et al. 2013; Antão et al. 2019).

Quantifying spatial scales in the fossil record is further complicated by uneven sampling and uncertainties in paleogeographic configuration. Thus, spatial distribution of the sampled fossil record may be a result of uneven sampling—patchy preservation of the rock record and sampling of that record, for instance—or true changes in the spatial structuring of environments, such as increase, decrease, or changing location of continental shelf area or landmass. To complicate matters, the confounding effects of sampling and the quality of the fossil record may have been simultaneously affected by latent common-cause factors (Smith 2001; Crampton et al. 2011; Peters and Heim 2011). Understanding the spatial variation in beta diversity provides a unique perspective on this problem.

To our knowledge, no studies have previously focused on or corrected for spatial scaling of beta diversity in the fossil record. However, recent studies on the species–area effect in the fossil record have shown that there is a conspicuous difference in measures of global richness once standardization to spatial regions of equal size is used (Close et al. 2017, 2020a,b). These studies employ spatial standardization based on the summed minimum spanning tree (MST) length, defined as the shortest possible total distance of segments that connect a set of fossil localities (Close et al. 2017). Here we focus primarily on testing the spatial dependence of different measures of beta diversity at the regional scale and species level using the exemplary, well-studied, and relatively complete fossil record of Cenozoic mollusks from New Zealand (Crampton et al. 2006a,b, 2011). In addition, we provide a spatially standardized time series of beta diversity using the same data.

Material and Methods

Material.—This study focuses on New Zealand's rich record of Cenozoic marine mollusks (bivalves, gastropods, and scaphopods), using occurrence data derived from the Fossil Record Electronic Database (FRED). FRED is a collection-based compilation of fossil occurrences within New Zealand, and it is well described elsewhere (Clowes et al. 2020). Data relating to Cenozoic Mollusca were downloaded from FRED in September 2018 and subsequently revised with a newly updated version of the synonymy list (employed by Crampton et al. 2006b, 2011; Womack et al. 2020), modified to take account of relevant recent literature (Beu et al. 2004; Beu 2006, 2011, 2012; Beu and Raine 2009). Analyses within this study are reported at the species level, excluding subspecies. Ambiguous identifications were removed from the dataset (including removal of taxa with the prefixes "cf." and "aff."). An additional cleaning protocol was employed to remove fossil

occurrences recorded outside their known biostratigraphic ranges as documented in the synoptic dataset (Beu and Maxwell 1990; Crampton et al. 2003, 2006a; Cooper et al. 2006; Beu and Raine 2009). The synoptic dataset is separate from FRED and comprises expert interpretations of the biostratigraphic ranges of mollusk species; it is taxonomically highly vetted, having been synthesized from the known fossil record by just two paleontologists (A. G. Beu and P. A. Maxwell) over many years. In contrast, the FRED dataset, although also vetted here, may still contain spurious or erroneous identifications that could bias measures of beta diversity based on dissimilarity.

We restrict our analysis to level-bottom shelf-dwelling taxa to allow for the disproportionately low representation of non-shelfal taxa and environments in the New Zealand Cenozoic stratigraphic record (Beu and Maxwell 1990). Shelfal taxa are defined here as those inferred to have been confined to, or to have ranged into, shelf water depths (< ~200 m water depth) (Crampton et al. 2006b). We exclude data from the Chatham Islands due to their large distance from New Zealand's mainland for most of the Cenozoic (> ~700 km). Geological ages are given in terms of New Zealand Cenozoic Stages (Fig. 1), and time bins used within this study are based on individual and combined stages, yielding 13 time bins (Fig. 1, Supplementary Table 1) with average duration of 3.5 Myr. Our analyses are restricted to occurrences from collections restricted in age to a single time bin. The final dataset analyzed here comprises 26,873 occurrences of 1713 species from 4173 collections.

Paleocoordinates.—To derive measures of beta diversity that reflect true spatial and temporal variation in biodiversity, we calculated paleocoordinates for individual collections based on their modern latitudes and longitudes. This is particularly important for New Zealand, as it straddles the obliquely convergent boundary between the Pacific and Australian plates, with reconstructions suggesting up to ~800 km of relative plate motion since ~43 Ma and 80°–90° clockwise rotation on the still-active subduction zone on the east coast of New Zealand's North Island since ~20 Ma (Lamb 2011). Paleocoordinates were reconstructed using the software GPlates (Müller et al. 2018). Reconstructions were based on a rigid-block model of New Zealand using relative finite rotations, continental polygons, and coastlines (Matthews et al. 2016) placed in the global paleomagnetic reference frame (Torsvik et al. 2012). The use of a paleomagnetic
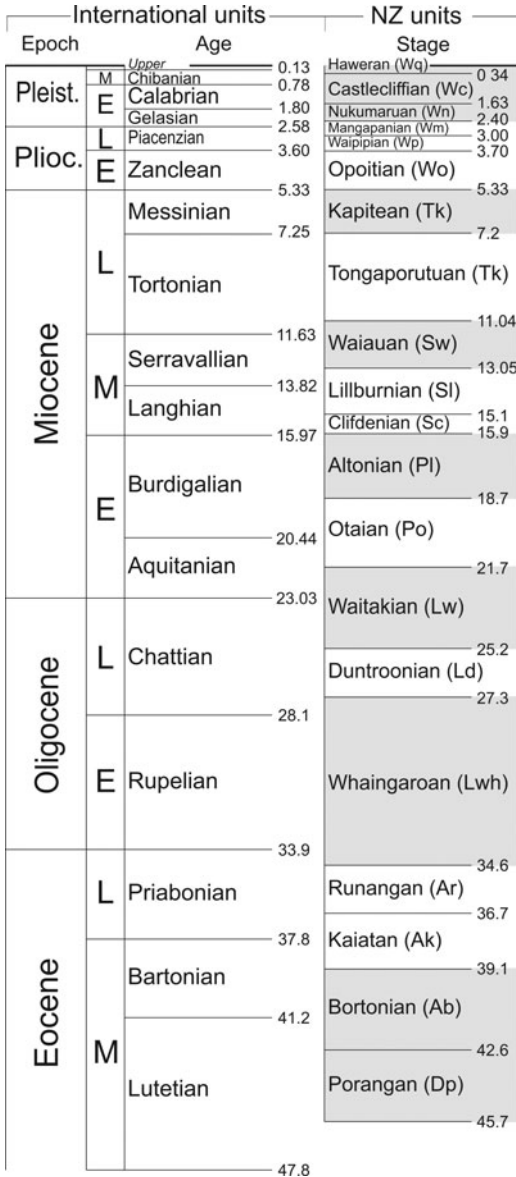

FIGURE 1. New Zealand Cenozoic timescale (after Raine et al. 2015), with units in Ma. Most analyses are undertaken at the resolution of the highlighted time bins shown here (shaded and unshaded blocks in the right-hand column); a few analyses for the past 5 Myr are undertaken at the resolution of individual New Zealand Plio-Pleistocene stages.
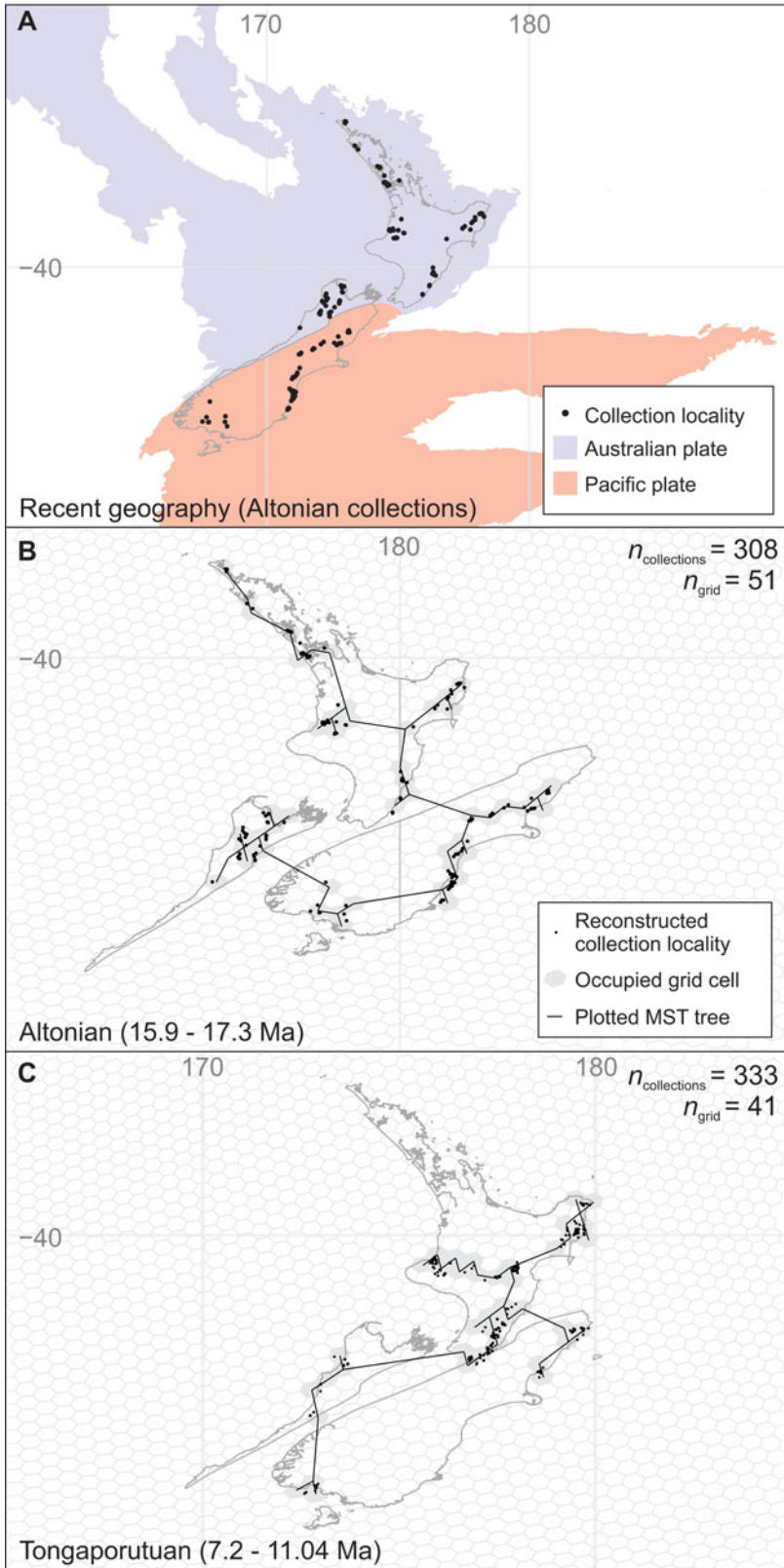
reference frame for New Zealand has been shown to place strong constraints on both the tectonic evolution of the plate-boundary zone and the dynamical controls of crustal evolution (Lamb 2011). See Figure 2 for examples of modern-day and reconstructed paleocoordinates for the Altonian Stage (18.7–15.9 Ma), and paleocoordinates for the Tongaporutuan Stage (11.04–7.2 Ma); Supplementary Figure 1 shows reconstructed paleocoordinates for all time bins.

Measuring Spatial Variation.—Quantifying spatial variation in beta diversity requires some measure of distance, area, or geographic dispersion. This poses a problem, as different methods emphasize different aspects of the distribution of fossil localities (Close et al. 2017). Principally, we are concerned with variation in area. Previous studies have focused on measuring spatial variation using the area of the convex-hull, great-circle distances, summed MST length (Alroy 2010; Close et al. 2017, 2020a,b), or a grid-based system (Crampton et al. 2011; Penny and Kröger 2019). Our data represent shelfal fossil communities; ideally, estimates of spatial area should represent shelfal area. Estimating shelfal area for New Zealand is difficult, as there are no spatially or temporally well-resolved, palinspastic paleogeographic maps for New Zealand. Based on the assumption that paleocoordinates for New Zealand shelfal fossil collections approximately fringe the paleocoastline, particularly at larger spatial scales, the area of the convex hull would be biased substantially by the area formerly occupied by land. In addition, the convex hull has been shown to be highly sensitive to sampling size and to consistently overestimate species geographic ranges (Burgman and Fox 2003). We therefore adopt a grid system as a proxy for spatial area, based on an equal-area penta-hexagonal grid generated using the R (R Development Core Team 2020) package icosa (Kocsis 2020). Studies of beta diversity in the fossil record at the global scale have opted for a grid of side 111 km (Penny and Kröger 2019). We adopt a smaller grid of side 23 km, because our data are at the regional scale. The grid system provides a measure of area occupied by collections, but does not capture any information regarding the geographic dispersion of the data—10 grid cells could be contiguous or widely dispersed across a continent. Therefore, we also consider the summed MST length as a measure of paleogeographic dispersion, calculated using the R functions of Close et al. (2017). Our calculations of summed MST length are based on the central coordinates of the individual grid cells, reducing biases related to clustering of collections in well-sampled areas. Whereas summed MST length may still be partially biased by landmass, it has been shown to correlate well with grid-cell occupation in the fossil record, can approximate complex distribution shapes (e.g., surrounding a landmass), and provides a good compromise in summarizing the spatial distribution of fossil localities based on their coordinates (Alroy 2010; Close et al. 2017).

Measuring Beta Diversity.—Measuring beta diversity is a controversial topic, and there exist a plethora of metrics (Koleff et al. 2003) with no overall consensus on which metrics should be used for addressing particular ecological questions (Anderson et al. 2011) or what actually constitutes true beta diversity (Tuomisto 2010a,b; Anderson et al. 2011). Conceptually, the spatial relationship between alpha and gamma diversity is well documented in ecology (Rosenzweig 1995; MacArthur and Wilson 2001; Scheiner 2003; Drakare et al. 2006) and paleontology (Sepkoski 1976; Barnosky et al. 2005; Sclafani and Holland 2013; Close et al. 2017). Conversely, the spatial dependence of beta diversity is relatively unknown (Barton et al. 2013). The problem is compounded when applying beta diversity to the fossil record due to confounding effects of uneven preservation and sampling of the rock and fossil records through time. A full review of beta diversity is out of the scope of this paper, and we follow Anderson et al. (2011) in their broader definition of beta diversity, discussed in the following paragraph.

Beta diversity can be separated into two types, turnover and variation (Vellend 2001; Anderson et al. 2011). "Turnover" measures the change in community composition and structure from one sampling unit to another, spatially, temporally, or over an environmental gradient; whereas "variation" is measured among all possible pairs of units, without reference to any particular gradient or direction (Anderson et al. 2011). Turnover is often

A

Recent geography (Altonian collections)

- Collection locality
- Australian plate
- Pacific plate

B

$n_{collections} = 308$
$n_{grid} = 51$

Altonian (15.9 - 17.3 Ma)

- Reconstructed collection locality
- Occupied grid cell
- Plotted MST tree

C

$n_{collections} = 333$
$n_{grid} = 41$

Tongaporutuan (7.2 - 11.04 Ma)

measured as similarity, but is also commonly expressed as dissimilarity (simply 1-similarity or by rearranging the formula; see Koleff et al. 2003). In addition, turnover can be subdivided into species replacement (commonly termed "spatial turnover") and nestedness of assemblages (species loss) (Baselga 2010). For example, take two sites of varying species richness. The first site has a higher species richness and the second site is compositionally a subset of the first site's species. The variation in species composition between the two sites is due to differences in species richness, not species replacement, and forms the core concept of nestedness (Ulrich and Almeida-Neto 2012). Subdividing turnover into species replacement and nestedness components can help reveal underlying drivers of assemblage difference that may be obscured when they are combined (Wright et al. 1997; Penny and Kröger 2019). We are interested in both the overall variation in beta diversity and the turnover across all shelfal gradients, and therefore both concepts are useful and applicable.

Fossil collection data contained in FRED are generally binary (presence–absence) and are treated as incidence data, and therefore we only discuss methods relevant to this data type. On this basis, we consider three main classes of measures of beta diversity for incidence data and their spatial scaling (see Supplementary Table 2).

1. Classical metrics, which are derived directly from the relationship between alpha and gamma diversity and are more suited to measuring overall variation. We adopt the original multiplicative (β_{Whit}) (Whittaker 1960) and additive (β_{Add}) (Lande 1996) definitions of beta diversity as measures. Both additive and multiplicative measures of beta diversity have been shown to be effective in the fossil record (Holland 2010; Aberhan and Kiessling 2012).

2. Pairwise measures, which are based on similarity indices between a pair of sites or an average of all pairs, and quantify turnover (Anderson et al. 2011). We adopt pairwise measures of the Sørensen (β_{Sor}) and Simpson (β_{Sim}) dissimilarity as expressed by Koleff et al. (2003).

3. Multiple-site measures, which are derived from multiple-site equivalents of the matching components used in certain pairwise measures and also quantify turnover (Anderson et al. 2011). We adopt multisite implementations of the Sørensen (β_{MSor}) and Simpson (β_{MSim}) pairwise dissimilarity measures (Baselga 2010; Baselga and Leprieur 2015).

Sørensen dissimilarity measures compositional differences arising from species replacement and species loss, whereas Simpson dissimilarity measures only species replacement. The nested component of turnover can be calculated simply by subtracting the Simpson dissimilarity measure from the Sørensen dissimilarity measure (β_{Nest} for pairwise and β_{MNest} for multisite) (Baselga 2010). Pairwise measures are calculated in R using the package vegan (Oksanen et al. 2007) and multisite measures using betapart (Baselga and Orme 2012). To accommodate for local variation in preservation and sampling of collections and facilitate calculation of area and distribution, we assign collections in each time bin to their corresponding grid cell based on their paleocoordinates. Collections in each grid cell are aggregated and reduced to binary incidence data and treated as a single sample; this protocol reduces the impact of local clustering of data around richly sampled localities.

We run our analyses with all available collections and a resampling procedure to reduce the impact of uneven numbers of collections per time bin. This resampling procedure is based

---

FIGURE 2.   Recent and example paleogeographic maps of New Zealand showing fossil collection localities. A, Recent geography of New Zealand showing the position of continental fragments lying on the Australian and Pacific plates and Altonian (Pl) (18.7–15.9 Ma) fossil collection localities. B, C, Reconstructed paleocoordinates with the rotated fragments of the modern New Zealand coastline outline for reference and Altonian (Pl) (18.7–15.9 Ma) (B) and Tongaporutuan (Tt) (11.04–7.2 Ma) (C) fossil collection localities. Maps (B, C) show the equal-area penta-hexagonal grid with occupied grid cells shaded and minimum spanning tree (MST). The example MSTs are based on the central coordinates of all occupied grid cells.

on 40 collections resampled 1000 times, without replacement. The number of collections per trial is based on the minimum number of collections in the most poorly sampled time bin (40 collections in the Whaingaroan Stage [Lwh]: 34.6–27.3 Ma) (see Fig. 3 for a diagram that explains the workflow). No spatial constraints are applied to the resampling procedure, allowing for spatial standardization to be calculated afterward at any chosen level. For each trial, we assign the collections to their grid cells, as described earlier, forming the sampling units. We select one of these grid cells as the focal sample and calculate the geodesic distance to all other sites, and then repeat the process, treating each occupied grid cell as the focal sample in turn. During each iteration, we calculate measures of beta diversity and measures of spatial variation incrementally, moving outward from the focal sample, adding one sample at a time until the most distant of the 40 samples is included. This allows beta diversity to be calculated in reference to a spatial gradient, rather than randomly, thereby avoiding measuring beta diversity for samples where geographic distance and calculated spatial area are essentially decoupled. For each increment, alpha diversity is calculated as the average raw species richness per sample, and gamma diversity as the raw species richness for all samples. Coverage-based subsampling is not applied to alpha and gamma diversity, because we have standardized the number of collections to 40, but could be implemented if spatially standardizing to a fixed spatial scale. Data are reported as the mean and standard error of successful trials out of 1000, based on either number of grid cells or binned summed MST lengths. Successful trials are defined as those that reach the predetermined threshold of grid cells or binned summed MST lengths. Unsuccessful trials occur because larger spatial scales will not be encountered in every resampling trial. Following the resampling procedure, spatial standardization can be achieved by taking the average measures of beta diversity for successful trials within a singular time bin at a fixed number of cells or range of summed MST lengths.

From these calculations we generate spatially and sampling standardized beta-diversity time series. We estimate measures of beta diversity at a fixed number of cells (13) and summed MST range (1000–1100 km). The level of spatial standardization is based on the minimum number of grid cells and minimum summed MST observed across all time bins after standardizing to 40 collections. For comparison, we also calculate unstandardized measures of beta diversity based on all collections and combined collections based on the penta-hexagonal grid system.

Results

Measures of variation (β_{Add} and β_{Whit}) generally conform to the a priori expectation that beta diversity increases with increasing spatial scale and that this rate of increase declines at regional spatial scales (Fig. 4, Supplementary Figs. 2, 3). This relationship is also seen in both pairwise (see Supplementary Fig. 4) and multisite measures of average Sørensen dissimilarity (Fig. 4A–C, Supplementary Figs. 5, 6). There is a large disparity between the sampling standardized measures of β_{Whit} and β_{Add} beta diversity and their counterparts based on all available data, highlighting the importance of sampling and spatial standardization for these metrics (Fig. 4D,E). Overall, we find that the multisite measures of beta diversity (β_{MSor}, β_{MSim} and β_{MNest}) are more stable across spatial scales and are less affected by sample size in comparison to other measures of beta diversity (Supplementary Figs. 2–6). Our results and interpretations are therefore based primarily on the multisite measures of beta-diversity turnover and their derived components. Henceforth, we use the following labels for the different data treatments: "collection-based" for unstandardized data taken at face value; "grid-based" for unstandardized data with collections aggregated by grid cells; and "standardized" for the sampling and spatially standardized data, where spatial standardization is achieved using either a fixed quota of cells or a fixed summed MST distance.

We find that standardized measures of β_{MSor} and β_{MSim} are slightly elevated at smaller spatial scales, and β_{MNest} is slightly smaller compared with grid-based measurements (Fig. 4).
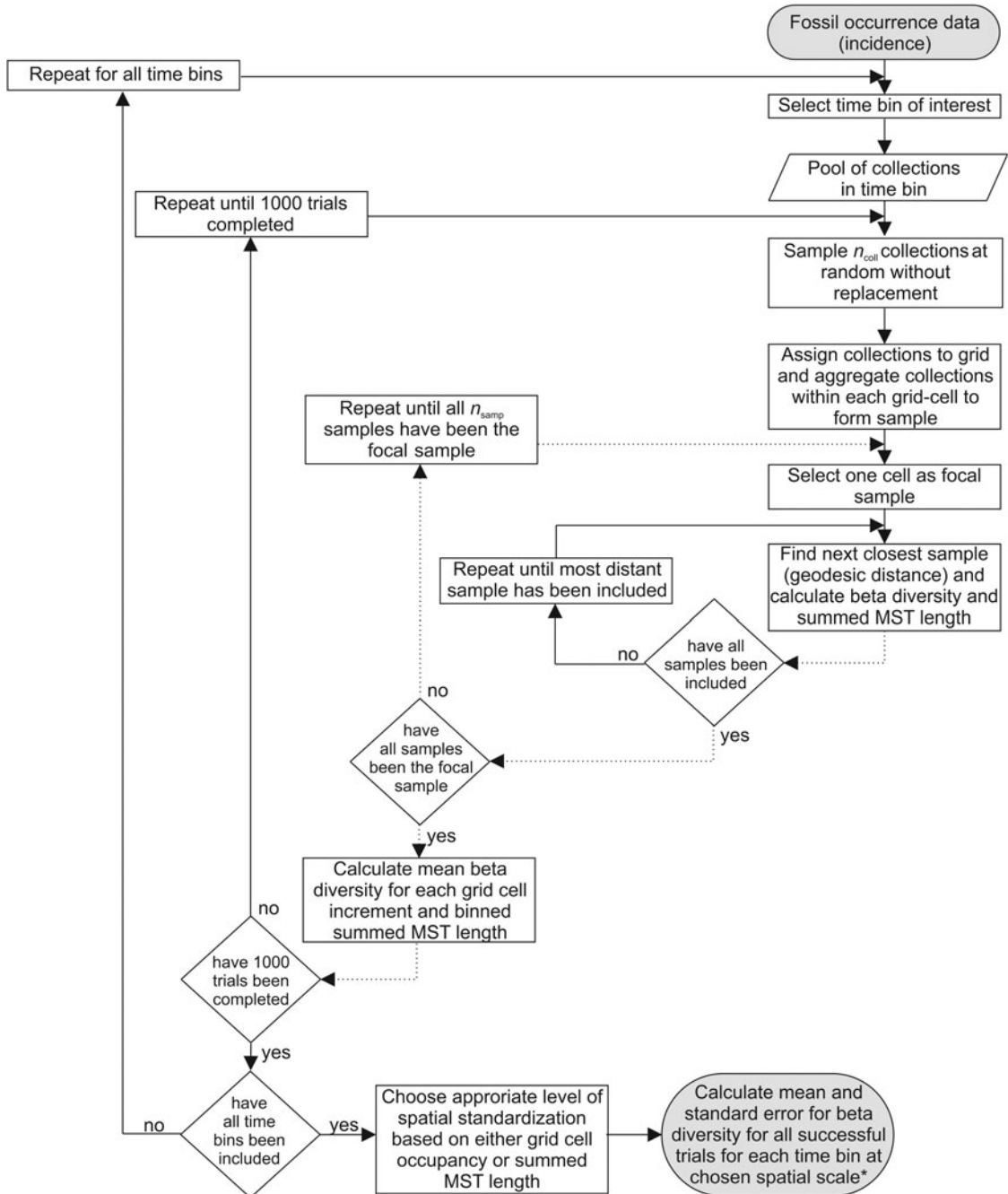
FIGURE 3.   Flowchart highlighting the methodical resampling protocol to produce measures of beta diversity for each time bin at increasing spatial scales. For this study n_{coll} is set at 40. Dashed arrow lines indicate the loop relating to what is in the text referred to as a single trial. *Mean and standard errors are based on the number of successful trials for the spatial scale of interest, that is, larger spatial scales will not be encountered in every resampling trial.

This disparity is more pronounced when measuring spatial scales using grid-cell occupancy (cf. Supplementary Figs. 5, 6). Regardless of whether standardization is implemented, both β_{MSor} and β_{MSim} increase with spatial scale, and β_{MNest} decreases (Fig. 4), with the exception
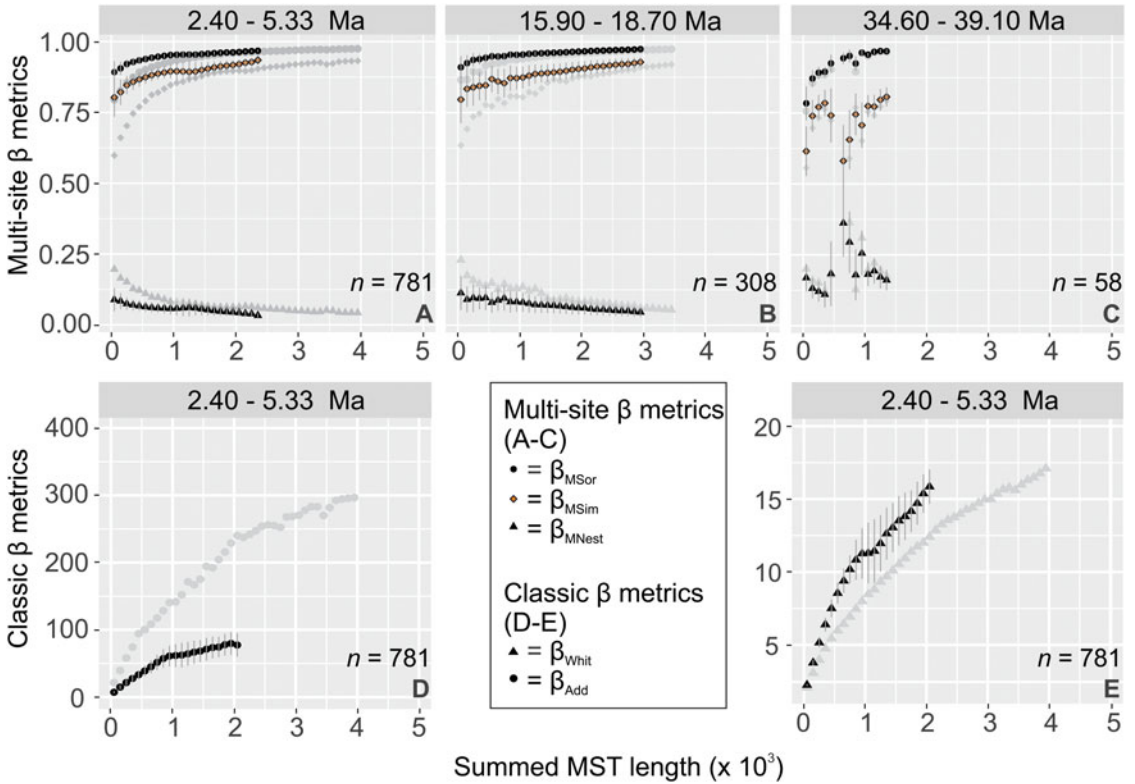
FIGURE 4. Measures of beta diversity plotted against summed minimum spanning tree (MST) length, for a representative selection of time bins. Unstandardized results are shown in gray, based on all collections (aggregated by grid cells). Error bars are presented for sampling standardized results only and are based on the standard error of successful trials (maximum 1000) aggregated by summed MST length bins used to calculate average beta diversity (where summed MST was aggregated into 100 km bins). See Fig. 3 for detailed method of resampling protocol. A–C, Multisite measures of beta diversity (β_{MSor}, β_{MSim}, and β_{MNest}) for three time bins: A, Mangapanian–Opoitian (Wm-Wo) (5.33–2.4 Ma); B, Altonian (Pl) (18.7–15.9 Ma); and C, Runangan–Kaiatan (Ar-Ak) (39.1–34.6 Ma). Graphs (A, B) highlight time bins with well-ordered data, contrasting with C, where β_{MSim} and β_{MSor} do not conform to a simple logarithmic trend. This is likely a result, at least in part, of geographic clustering of grid cells within this time bin into two confined groups (see Supplementary Fig. 1). D, E, Classic measures of beta diversity: additive (β_{Add}) (D) and multiplicative (β_{Whit}) (E) plotted against summed MST length for Mangapanian–Opoitian (Wm-Wo) (5.33–2.4 Ma). The number of collections per time bin is denoted by n.

of the combined Runangan and Kaiatan (Ak-Ar) time bin (39.1–34.6 Ma), which shows a variable pattern of β_{MSim} and β_{MNest}. Collections in this time bin are split into two distinct geographic clusters (see Supplementary Fig. 1), which are likely to affect the derived spatial measures and components of turnover. The general pattern of decrease in β_{MNest} with increased spatial scale suggests that nestedness is decreasingly important from local to regional spatial scales, and at the regional scale, species replacement (β_{MSim}) is the primary component of compositional dissimilarity.

We experiment with several regression trendlines (linear, power, logarithmic, and general

additive model) to interpolate a spatially standardized measure of multi-site beta diversity. A logarithmic trendline shows the best fit for summed MST length and grid-cell occupancy versus average values of β_{MSor} and, to a lesser extent β_{MSim} and β_{MNest} (see Supplementary Figs. 5, 6), based on both fit to the data and visual assessment of the plausibility of the extrapolation. However, this relationship diminishes in older time bins, and given the close match between the logarithmic fits and measured average values of beta diversity in younger time bins at our chosen standardization quotas, we avoid this additional computational step and use the measured values of beta diversity to derive

our time series of Cenozoic beta diversity. Likewise, we avoid extrapolation using logarithmic regression, because in some cases, the trendlines yield values of β_{MSor} greater than 1.0, particularly for time bins with low spatial measures and when using grid-cell occupancy as the spatial unit (see Supplementary Fig. 6).

Standardized measures of β_{MSor}, β_{MSim}, and β_{MNest} show substantially greater proportional volatility through the Cenozoic than unstandardized collection-based and grid-based measures (Fig. 5, Supplementary Fig. 7). Collection-based measures suggest beta diversity (β_{MSor}) increases steadily through the Cenozoic, with a similar steady increase in species replacement (β_{MSim}) and decrease in nestedness (β_{MNest}). Conversely, standardized measures suggest a declining trend in beta diversity (β_{MSor}) in the early Miocene and a large increase in β_{MNest} in the Waitakian (Lw) (25.2–21.7 Ma), coinciding with a large decrease in β_{MSor} and β_{MSim}. When spatial and sampling standardization is employed for ungrouped Plio-Pleistocene stages (see Fig. 1), the same downward trend is observed (Fig. 6, Supplementary Fig. 8). Grid-based measures produce results that are more similar to standardized measures than collection-based measures, although there are still notable differences in amplitude in peaks and overall trend. Similar disparities are observed between unstandardized and standardized time series of beta-diversity variation (β_{Add} and β_{Whit}) (Supplementary Fig. 9).

To assess the effect of spatial standardization, we calculate the correlation between time series of multisite beta-diversity turnover and total per–time bin measurements of summed MST length and grid-cell occupancy. Correlations are calculated for three levels of standardization: (1) unstandardized based on raw collections; (2) unstandardized based on collections aggregated by grid cell; and (3) sampling and spatially standardized. We employ Spearman's rank-order correlation coefficient (r_s) based on first differences (denoted by the symbol Δ). We find that correlation coefficients are strong and significant for β_{MSor} and moderately strong and significant for β_{MSim} (marginal in the case of grid-cell occupancy) when unstandardized based on collections for both summed MST length and grid-cell occupancy (Table 1). Effect size decreases when collections are aggregated by grid cell, but are still moderately strong and significant for β_{MSor} and moderate for β_{MSim} versus for grid-cell occupancy. When sampling and spatial standardization are employed, effect size is negligible for summed MST length, but still slightly elevated for grid-cell occupancy. This suggests that both methods are suitable for spatial standardization and summed MST length may be more effective.

It is also possible that beta diversity is dependent, in part, on time-bin duration. Collections in long time bins may be more separated in time compared with those in short time bins, and this might bias measures of dissimilarity. To test this, we calculate the correlation between time series of standardized measures of multisite beta-diversity turnover and time-bin duration, using Spearman's rank-order correlation coefficient based on first differences. We find that all values are nonsignificant and correlation coefficients for β_{MNest} are low and moderate to moderately low for β_{MSor} and β_{MNest}, respectively (Table 2). Whereas correlation coefficients for β_{MSor} and β_{MNest} are slightly elevated, they are nonsignificant and, importantly, show the opposite trend that would be anticipated if time-bin duration biased beta. Therefore, the elevated correlation coefficients are likely a result of spurious correlation. This suggests volatility in beta diversity is not strongly influenced by time-bin duration.

Discussion and Summary

All measures of beta diversity (with the exception of β_{MNest}) increase with spatial scale and show declining rates of increase at regional spatial scales. For the New Zealand Cenozoic mollusk data, multisite measures of turnover and their components (β_{MSor}, β_{MSim}, and β_{MNest}) show an approximately logarithmic relationship with summed MST length and grid-cell occupancy, particularly in younger time bins (27.3–0 Ma) (Supplementary Figs. 5, 6). The relationship between spatial scale and beta diversity measured as compositional turnover is complex and dependent on a number of factors, including taxa and grain and extent size, and the metric itself. It is possible that the logarithmic relationship observed may, in part, be related to the species–area relationship, where
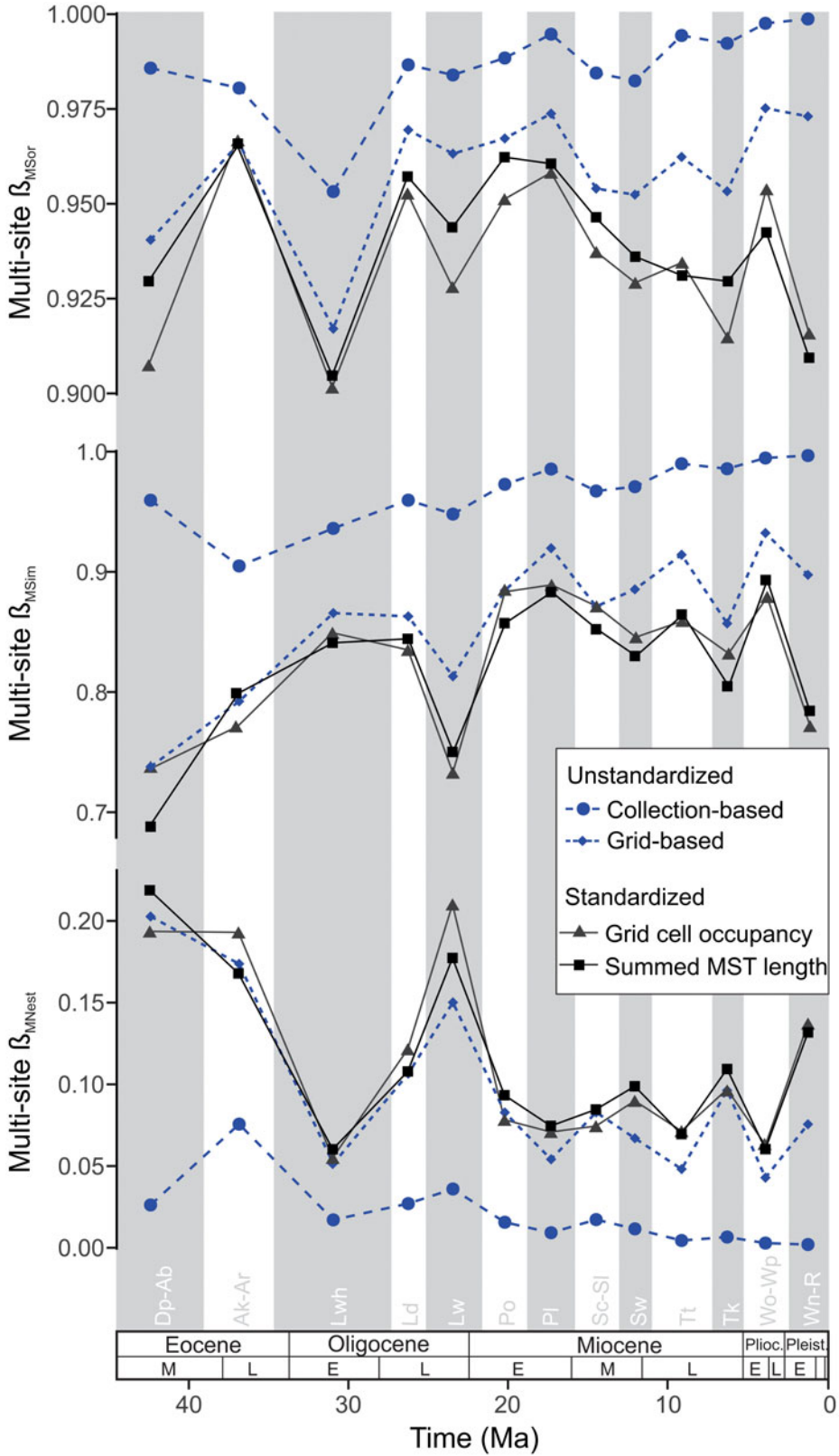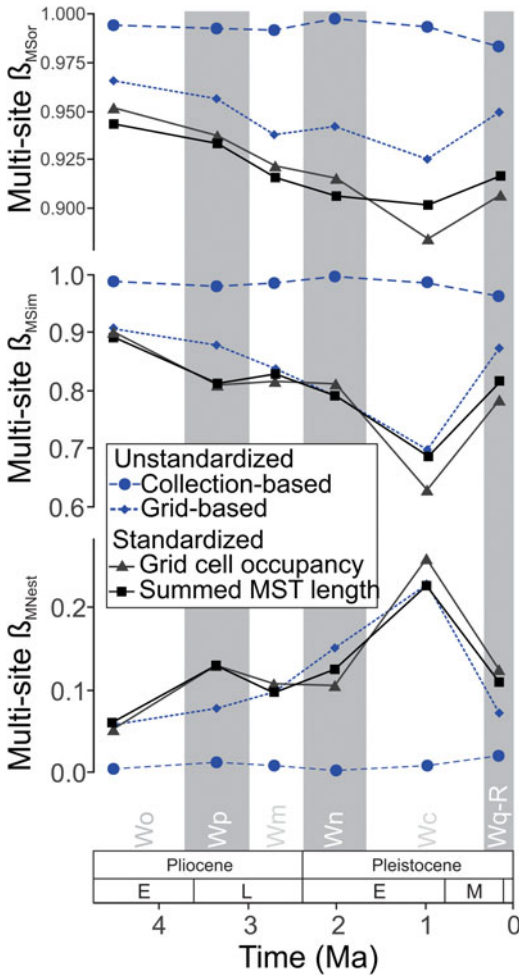
FIGURE 6. Plio-Pleistocene time series of multisite beta diversity (β_{MSor}, β_{MSim}, and β_{MNest}). We present two unstandardized measures: collection-based and grid-based (collections aggregated by grid cell) (dashed lines); and two spatially and sampling standardized time using grid-cell occupancy and summed minimum spanning tree (MST) length (solid lines). Analyses are undertaken at the resolution of the Plio-Pleistocene New Zealand Stages shown here (see abbreviated stage labels and Fig. 1 for reference), and points are plotted at time-bin midpoints (see Fig. 1, Supplementary Table 1). For clarity, standard error bars are omitted; see Supplementary Fig. 8 for plots with error bars.

Time series derived by standardizing on summed MST length and grid-cell occupancy reveal similar patterns, but summed MST length is considered to be the superior approach, because it captures the geographic dispersal of the data. For example, in the Altonian (Pl) (17.3–15.9 Ma), collection locations are spread relatively evenly in paleogeographic coordinates, whereas Tongaporutuan (Tt) (11.04–7.2 Ma) collections are clumped predominately in the north (Fig. 2). Both time bins have similar numbers of collections, and the Altonian (Pl) has 19% more occupied grid cells relative to the Tongaporutuan (Tt) (Fig. 2). Based on the average summed MST length and grid-cell occupancy for 40 collections (for all 1000 trials), grid-cell occupancy increases by 17% from the Tongaporutuan (Tt) to the Altonian (Pl), whereas mean summed MST length increases by 28%, a value that captures the observable increase in geographic dispersal. These relative differences in measures of geographic extent explain, in part at least, the differences we see in time series based on the two methods, in particular using β_{Whit} (Supplementary Fig. 9). Studies at larger spatial scales or with less evenly spaced data should consider this potential bias for spatial standardization.

Partitioning turnover (β_{MSor}) into nestedness (β_{MNest}) and species replacement (β_{MSim}) facilitates a greater understanding of patterns in beta diversity. Species replacement (β_{MSim}) is the dominant component of compositional dissimilarity and increases with spatial scale, whereas nestedness (β_{MNest}) decreases. These patterns are logical consequences, in part at least, of environmental and ecological factors that operate at different spatial scales. Hence, as spatial scale increases, climate and environmental contrasts related to latitude will also increase and dispersal limitation of species will become more significant, both factors that are likely to increase species replacement and decrease nestedness.

the decreasing number of new species encountered at increasingly larger spatial scales may limit compositional dissimilarity.

FIGURE 5. Cenozoic time series of multisite beta diversity (β_{MSor}, β_{MSim}, and β_{MNest}). We present two unstandardized measures: collection-based and grid-based (collections aggregated by grid cell) (dashed lines); and two spatially and sampling standardized time series using grid-cell occupancy and summed minimum spanning tree (MST) length (solid lines). Analyses are undertaken at the resolution of the highlighted time bins shown here (see abbreviated stage labels and Fig. 1 for reference), and points are plotted at time-bin midpoints (see Fig. 1, Supplementary Table 1). For clarity, standard error bars are omitted; see Supplementary Fig. 7 for plots with error bars.

TABLE 1. Correlations between multisite beta diversity versus summed minimum spanning tree (MST) length and grid-cell occupancy. Three standardization methods are considered: (1) unstandardized, based on fossil collection localities and (2) aggregated by grid cell; and (3) sampling and spatially standardized. Correlations are based on first differences denoted by Δ.

Beta-diversity component	Standardization method	Δ Summed MST length		Δ Grid-cell occupancy	
		r_s	p	r_s	p
Δ β_{MSor}	1. Unstandardized	0.692	0.016	0.830	<0.001
Δ β_{MSim}	(based on collections)	0.664	0.022	0.574	0.051
Δ β_{MNest}		−0.350	0.266	−0.385	0.216
Δ β_{MSor}	2. Unstandardized	0.371	0.193	0.627	0.029
Δ β_{MSim}	(aggregated by grid cell)	0.406	0.193	0.536	0.073
Δ β_{MNest}		−0.112	0.733	−0.252	0.429
Δ β_{MSor}	3. Sampling and spatially	0.182	0.573	0.396	0.203
Δ β_{MSim}	standardized	0.098	0.766	0.301	0.341
Δ β_{MNest}		0.028	0.939	−0.112	0.729

Patterns of beta diversity should be considered in relation to other standardized components of diversity (alpha and gamma) and measures of environmental heterogeneity (e.g., see Crampton et al. 2011), and detailed interrogation of these New Zealand Cenozoic mollusk data will be the subject of a separate paper. Importantly, for the New Zealand Cenozoic mollusk data, time series of beta diversity that employ spatial and sampling standardization reveal different temporal trends and much greater proportional volatility than those based on unstandardized measurements, displaying contrasting results to previous estimates (Crampton et al. 2006b, 2011). These standardizations are neglected in many studies of beta diversity, but clearly may have a significant impact on paleobiological interpretations, as illustrated in the following two examples from our data.

Standardized β_{MSor} shows a decline from ~20 Ma, whereas unstandardized measures (particularly collection-based) display an increase (Fig. 5). Given that this period spans the development of the modern plate boundary through New Zealand and also global cooling, one could draw very different conclusions about one or both these factors in driving patterns of beta diversity in standardized versus unstandardized measurements.

Standardized β_{MSor} and β_{MSim} both display a prominent downward excursion in the Waitakian Stage (Lw) (25.2–21.7 Ma) that is not observed in unstandardized measures (Fig. 5). The Oligocene marks the maximum flooding of the Zealandia continent, peaking in the late Oligocene (Waitakian) (Fleming 1975; Cooper and Cooper 1995; King et al. 1999; King 2000). The relationships between sea level, environmental heterogeneity, and beta diversity are of significant interest, and interpretations based on unstandardized measures are likely to be misleading.

We show that beta diversity is spatially dependent at local to regional spatial scales in the Cenozoic shallow-marine molluscan fossil record of New Zealand and that uneven spatial sampling can influence recovered temporal trends in beta diversity. Our results suggest that multisite beta-diversity turnover and components (β_{MSor}, β_{MSim}, and β_{MNest}), standardized spatially using summed MST length, are the most suitable for elucidating patterns of beta diversity in the fossil record.

Acknowledgments

TABLE 2. Correlations between standardized multisite beta-diversity and time-bin duration. Correlations are based on first differences denoted by Δ.

	r_s	p
Δ β_{MSor} vs. Δ time-bin duration	−0.503	0.099
Δ β_{MSim} vs. Δ time-bin duration	0.070	0.834
Δ β_{MNest} vs. Δ time-bin duration	−0.343	0.276

Scholarship. We acknowledge use of the data in the New Zealand Fossil Record File, administered by the Geological Society of New Zealand and GNS Sciences (http://www.fred.org.nz). H. Seebeck (GNS Science) assisted with the generation of paleocoordinates, and we acknowledge discussions with A. G. Beu (GNS Science) and K. S. Collins (Natural History Museum, London).

Literature Cited

Aberhan, M., and W. Kiessling. 2012. Phanerozoic marine biodiversity: a fresh look at data, methods, patterns and processes. Pp. 3–22 *in* J. A. Talent, ed. Earth and life: global biodiversity, extinction intervals and biogeographic perturbations through time. Springer, Dordrecht, Netherlands.

Alroy, J. 2010. Geographical, environmental and intrinsic biotic controls on Phanerozoic marine diversification. Palaeontology 53:1211–1235.

Anderson, M. J., T. O. Crist, J. M. Chase, M. Vellend, B. D. Inouye, A. L. Freestone, N. J. Sanders, H. V. Cornell, L. S. Comita, and K. F. Davies. 2011. Navigating the multiple meanings of β diversity: a roadmap for the practicing ecologist. Ecology Letters 14:19–28.

Antão, L. H., B. McGill, A. E. Magurran, A. M. Soares, and M. Dornelas. 2019. β-diversity scaling patterns are consistent across metrics and taxa. Ecography 42:1012–1023.

Barnosky, A. D., M. A. Carrasco, and E. B. Davis. 2005. The impact of the species–area relationship on estimates of paleodiversity. PLoS Biology 3(8):e266.

Barton, P. S., S. A. Cunningham, A. D. Manning, H. Gibb, D. B. Lindenmayer, and R. K. Didham. 2013. The spatial scaling of beta diversity. Global Ecology and Biogeography 22:639–647.

Baselga, A. 2010. Partitioning the turnover and nestedness components of beta diversity. Global Ecology and Biogeography 19:134–143.

Baselga, A., and F. Leprieur. 2015. Comparing methods to separate components of beta diversity. Methods in Ecology and Evolution 6:1069–1079.

Baselga, A., and C. D. L. Orme. 2012. betapart: an R package for the study of beta diversity. Methods in Ecology and Evolution 3:808–812.

Beu, A. 2006. Marine Mollusca of oxygen isotope stages of the last 2 million years in New Zealand. Part 2. Biostratigraphically useful and new Pliocene to Recent bivalves. Journal of the Royal Society of New Zealand 36:151–338.

Beu, A. 2011. Marine Mollusca of isotope stages of the last 2 million years in New Zealand. Part 4. Gastropoda (Ptenoglossa, Neogastropoda, Heterobranchia). Journal of the Royal Society of New Zealand 41:1–153.

Beu, A. 2012. Marine Mollusca of the last 2 million years in New Zealand. Part 5. Summary. Journal of the Royal Society of New Zealand 42:1–47.

Beu, A., and P. A. Maxwell. 1990. Cenozoic Mollusca of New Zealand. New Zealand Geological Survey Paleontological Bulletin 58.

Beu, A. G., and J. Raine. 2009. Revised descriptions of New Zealand Cenozoic Mollusca from Beu and Maxwell (1990). GNS Science Miscellaneous Series 27. GNS Science, Lower Hutt, New Zealand.

Beu, A., B. Alloway, B. Pillans, T. Naish, and J. Westgate. 2004. Marine Mollusca of oxygen isotope stages of the last 2 million years in New Zealand. Part 1: Revised generic positions and recognition

of warm-water and cool-water migrants. Journal of the Royal Society of New Zealand 34:111–265.

Blowes, S. A., S. R. Supp, L. H. Antão, A. Bates, H. Bruelheide, J. M. Chase, F. Moyes, A. Magurran, B. McGill, and I. H. Myers-Smith. 2019. The geography of biodiversity change in marine and terrestrial assemblages. Science 366:339–345.

Brocklehurst, N., M. O. Day, and J. Fröbisch. 2018. Accounting for differences in species frequency distributions when calculating beta diversity in the fossil record. Methods in Ecology and Evolution 9:1409–1420.

Burgman, M. A., and J. C. Fox. 2003. Bias in species range estimates from minimum convex polygons: implications for conservation and options for improved planning. Animal Conservation Forum 6:19–28.

Close, R., R. Benson, E. Saupe, M. Clapham, and R. Butler. 2020a. The spatial structure of Phanerozoic marine animal diversity. Science 368:420–424.

Close, R. A., R. B. Benson, P. Upchurch, and R. J. Butler. 2017. Controlling for the species-area effect supports constrained long-term Mesozoic terrestrial vertebrate diversification. Nature Communications 8:1–11.

Close, R. A., R. B. Benson, J. Alroy, M. T. Carrano, T. J. Cleary, E. M. Dunne, P. D. Mannion, M. D. Uhen, and R. J. Butler. 2020b. The apparent exponential radiation of Phanerozoic land vertebrates is an artefact of spatial sampling biases. Proceedings of the Royal Society of London B 287:20200372.

Clowes C. D, J. S. Crampton, K. J., Bland, K. S. Collins, J. G. Prebble, I. J, Raine, D. P. Strogen, M. G. Marianna. 2020. The New Zealand Fossil Record File: a unique database of biological history. New Zealand Journal of Geology and Geophysics. doi: 10.1080/00288306.2020.1799827.

Cooper, A., and R. A. Cooper. 1995. The Oligocene bottleneck and New Zealand biota: genetic record of a past environmental crisis. Proceedings of the Royal Society of London B 261:293–302.

Cooper, R. A., P. A. Maxwell, J. S. Crampton, A. G. Beu, C. M. Jones, and B. A. Marshall. 2006. Completeness of the fossil record: estimating losses due to small body size. Geology 34:241–244.

Crampton, J. S., A. G. Beu, R. A. Cooper, C. M. Jones, B. Marshall, and P. A. Maxwell. 2003. Estimating the rock volume bias in paleobiodiversity studies. Science 301:358–360.

Crampton, J. S., M. Foote, A. G. Beu, R. A. Cooper, I. Matcham, C. M. Jones, P. A. Maxwell, and B. A. Marshall. 2006a. Second-order sequence stratigraphic controls on the quality of the fossil record at an active margin: New Zealand Eocene to Recent shelf molluscs. Palaios 21:86–105.

Crampton, J. S., M. Foote, A. G. Beu, P. A. Maxwell, R. A. Cooper, I. Matcham, B. A. Marshall, and C. M. Jones. 2006b. The ark was full! Constant to declining Cenozoic shallow marine biodiversity on an isolated midlatitude continent. Paleobiology 32:509–532.

Crampton, J. S., M. Foote, R. A. Cooper, A. G. Beu, and S. E. Peters. 2011. The fossil record and spatial structuring of environments and biodiversity in the Cenozoic of New Zealand. Geological Society of London Special Publication 358:105–122.

Drakare, S., J. J. Lennon, and H. Hillebrand. 2006. The imprint of the geographical, evolutionary and ecological context on species–area relationships. Ecology Letters 9:215–227.

Fleming, C. A. 1975. The geological history of New Zealand and its biota. Pp. 1–86 *in* G. Kuschel, ed. Biogeography and ecology in New Zealand. Monographiae Biologicae 27. Springer, Dordrecht, Netherlands.

He, J., H. Kreft, S. Lin, Y. Xu, and H. Jiang. 2018. Cenozoic evolution of beta diversity and a Pleistocene emergence for modern mammal faunas in China. Global Ecology and Biogeography 27:1326–1338.

Hofmann, R., M. Tietje, and M. Aberhan. 2019. Diversity partitioning in Phanerozoic benthic marine communities. Proceedings of the National Academy of Sciences USA 116:79–83.

Holland, S. M. 2010. Additive diversity partitioning in palaeobiology: revisiting Sepkoski’s question. Palaeontology 53:1237–1254.

King, P. R. 2000. New Zealand's changing configuration in the last 100 million year: plate tectonics, basin development, and depositional setting. Pp. 131–145 in New Zealand Petroleum Conference proceedings. Ministry of Economic Development, Wellington.

King, P. R., T. R. Naish, G. H. Brown, B. D. Field, and S. W. Erdbrooke. 1999. Cretaceous to recent sedimentary patterns in New Zealand. Lower Hutt, New Zealand: Institue of Geological & Nuclear Sciences Limited.

Kocsis, Á. T. 2020. icosa: global triangular and penta-hexagonal grids based on tessellated icosahedra, R package version 0.10.0. https://CRAN.R-project.org/package=icosa.

Koleff, P., K. J. Gaston, and J. J. Lennon. 2003. Measuring beta diversity for presence–absence data. Journal of Animal Ecology 72:367–382.

Lamb, S. 2011. Cenozoic tectonic evolution of the New Zealand plate-boundary zone: a paleomagnetic perspective. Tectonophysics 509:135–164.

Lande, R. 1996. Statistics and partitioning of species diversity, and similarity among multiple communities. Oikos 76:5–13.

Lennon, J. J., P. Koleff, J. J. GreenwooD, and K. J. Gaston. 2001. The geographical structure of British bird distributions: diversity, spatial turnover and scale. Journal of Animal Ecology 70:966–979.

MacArthur, R. H., and E. O. Wilson. 2001. The theory of island biogeography. Princeton University Press, Princeton, N.J.

Matthews, K. J., K. T. Maloney, S. Zahirovic, S. E. Williams, M. Seton, and R. D. Mueller. 2016. Global plate boundary evolution and kinematics since the late Paleozoic. Global and Planetary Change 146:226–250.

McKnight, M. W., P. S. White, R. I. McDonald, J. F. Lamoreux, W. Sechrest, R. S. Ridgely, and S. N. Stuart. 2007. Putting beta-diversity on the map: broad-scale congruence and coincidence in the extremes. PLoS Biology 5(10):e272.

Müller, R. D., J. Cannon, X. Qin, R. J. Watson, M. Gurnis, S. Williams, T. Pfaffelmoser, M. Seton, S. H. Russell, and S. Zahirovic. 2018. GPlates: building a virtual Earth through deep time. Geochemistry, Geophysics, Geosystems 19:2243–2261.

Na, L., and W. Kiessling. 2015. Diversity partitioning during the Cambrian radiation. Proceedings of the National Academy of Sciences USA 112:4702–4706.

Oksanen, J., F. J. Blanchet, M. Friendly, R. Kindt, P. Legendre, P. McGlinn, P. R. Minchin, R. B. O’Hara, G. L. Simpson, P. Solymos, M. H. Stevens, E. Szoecs, and H. R. Wagner. 2007. vegan: community ecology package, R package version 2.5-6. https://CRAN.R-project.org/package=vegan.

Patzkowsky, M. E., and S. M. Holland. 2012. Stratigraphic paleobiology: understanding the distribution of fossil taxa in time and space. University of Chicago Press, Chicago.

Penny, A., and B. Kröger. 2019. Impacts of spatial and environmental differentiation on early Palaeozoic marine biodiversity. Nature Ecology and Evolution 3:1655–1660.

Peters, S. E., and N. A. Heim. 2011. Macrostratigraphy and macroevolution in marine environments: testing the common-cause hypothesis. Geological Society of London Special Publication 358:95–104.

Raine, J., A. Beu, A. Boyes, H. Campbell, R. Cooper, J. Crampton, M. Crundwell, C. Hollis, H. Morgans, and N. Mortimer. 2015. New Zealand geological timescale NZGT 2015/1. New Zealand Journal of Geology and Geophysics 58:398–403.

R Development Core Team. 2020. R: a language and environment for statistical computing. R Foundation for Statistical Computing, Vienna, Austria.

Rosenzweig, M. L. 1995. Species diversity in space and time. Cambridge University Press, Cambridge.

Scheiner, S. M. 2003. Six types of species-area curves. Global Ecology and Biogeography 12:441–447.

Sclafani, J. A., and S. M. Holland. 2013. The species-area relationship in the Late Ordovician: a test using neutral theory. Diversity 5:240–262.

Sepkoski, J. J. 1976. Species diversity in the Phanerozoic: species-area effects. Paleobiology 2:298–303.

Smith, A. B. 2001. Large–scale heterogeneity of the fossil record: implications for Phanerozoic biodiversity studies. Philosophical Transactions of the Royal Society of London B 356:351–367.

Torsvik, T. H., R. Van der Voo, U. Preeden, C. Mac Niocaill, B. Steinberger, P. V. Doubrovine, D. J. Van Hinsbergen, M. Domeier, C. Gaina, and E. Tohver. 2012. Phanerozoic polar wander, palaeogeography and dynamics. Earth-Science Reviews 114:325–368.

Tuomisto, H. 2010a. A diversity of beta diversities: straightening up a concept gone awry. Part 1. Defining beta diversity as a function of alpha and gamma diversity. Ecography 33:2–22.

Tuomisto, H. 2010b. A diversity of beta diversities: straightening up a concept gone awry. Part 2. Quantifying beta diversity and related phenomena. Ecography 33:23–45.

Ulrich, W., and M. Almeida-Neto. 2012. On the meanings of nestedness: back to the basics. Ecography 35:865–871.

Urban, M. C. 2015. Accelerating extinction risk from climate change. Science 348:571–573.

Veech, J. A., and T. O. Crist. 2007. Habitat and climate heterogeneity maintain beta-diversity of birds among landscapes within ecoregions. Global Ecology and Biogeography 16:650–656.

Vellend, M. 2001. Do commonly used indices of β-diversity measure species turnover? Journal of Vegetation Science 12:545–552.

Vermeij, G. J., and L. R. Leighton. 2003. Does global diversity mean anything? Paleobiology 29:3–7.

Vilhena, D. A., and A. B. Smith. 2013. Spatial bias in the marine fossil record. PLoS ONE 8(10):e74470.

Whittaker, R. H. 1960. Vegetation of the Siskiyou Mountains, Oregon and California. Ecological Monographs 30:279–338.

Womack, T. M., J. S. Crampton, M. J. Hannah. 2020. The Pull of the Recent revisited: negligible species level effect in a regional marine fossil record. Paleobiology. doi: 10.1017/pab.2020.32.

Wright, D. H., B. D. Patterson, G. M. Mikkelson, A. Cutler, and W. Atmar. 1997. A comparative analysis of nested subset patterns of species composition. Oecologia 113:1–20.