Macroecological patterns in coarse-grained microbial communities

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Abstract

Microbial communities are intrinsically hierarchical due to the shared evolutionary history of community members. This history is primarily captured through taxonomic assignment and phylogenetic reconstruction, sources of information that are frequently used to group microbes into higher levels of organization in experimental and natural communities. However, our understanding of how community diversity depends on one's scale of observation has yet to be systematically examined. This omission is not simply a methodological detail, as the shared history of community members captured by taxonomic and phylogenetic information provides an opportunity to investigate how patterns of diversity and abundance (i.e., macroecology) are altered across scales of organization. Here, we evaluate the extent that macroecological laws endure across taxonomic and phylogenetic scales among disparate environments using data from the Earth Microbiome Project. We found that measures of biodiversity at a given scale can be consistently predicted using predictions derived from a minimal model, the Stochastic Logistic Model of growth (SLM). Extending these within-scale results, we examine the relationship between measures of biodiversity calculated at different scales (e.g., genus vs. family), an empirical prediction known as the Diversity Begets Diversity (DBD) hypothesis. We found that the relationship between richness estimates at different scales can be quantitatively predicted assuming independence among community members. Contrastingly, only by including correlations between species abundances (e.g., as consequence of interactions) we can predict the relationship between estimates of diversity at different scales. The results of this study characterize novel microbial patterns across scales of organization and establish a sharp demarcation between recently proposed macroecological patterns that can and cannot be captured by a minimal model of biodiversity.

Introduction

An essential feature of microbial communities is their heterogeneous composition. A single environmental sample typically has a high richness, harboring hundreds to thousands of community members [1, 2]. This high level of richness reaches an astronomical quantity at the global level, as scaling relationships and models of biodiversity predict upwards of one trillion ($\sim 10^{12}$) species on Earth [3, 4]. Even experimental communities in laboratory settings with a single carbon source can harbor ≥ 40 community members, culminating in a total richness of hundreds of species among replicate communities (e.g., [5]). This richness contributes to the sheer diversity of

microbial communities, a challenge for researchers attempting to identify the general principles that govern their dynamics and composition.

While richness estimates of microbial communities are undoubtedly high, our choice of assigning a community member to a given taxon remains intrinsically arbitrary. This arbitrariness remains regardless of whether our definition of a taxon is based on physiological attributes measured in the laboratory, entire genomes (i.e., metagenomics), or single-gene amplicon-based methods (i.e., 16S rRNA annotation). Despite their methodological differences, these approaches can all be viewed as different ways to cluster individuals within a community into groups. To contend with the sheer richness of microbial communities, researchers frequently rely on annotation-based approaches, i.e., by summing the abundances of species that belong to the same group at a given taxonomic scale (e.g., genus, family, etc.). This approach pares down communities to a size that is amenable for the visualization of individual groups and allows for questions of scale-dependent community reproducibility to be addressed [5–11].

The trend of performing analyses at a given taxonomic scale raises the question of how the composition of a community at one scale relates to that at another. To address these questions, researchers have examined the relationship between biodiversity measures at different scales in order to pare down the set of plausible ecological mechanisms that govern community composition. Specifically, recent efforts have found that microbial richness/diversity within a given taxonomic group (e.g., genus) is typically positively correlated with the richness/diversity of the remaining groups (e.g., family) [8, 12], an empirical pattern that aligns with the diversity begets diversity hypothesis (DBD) [13–15]. Evidence of the DBD hypothesis has historically been attributed to the construction of novel niches within a community through member interactions [13, 16], with similar mechanisms having been proposed to explain the existence of a positive intra vs. inter-group relationship in microbial communities [12]. However, we still lack a quantitative understanding of how community composition at one scale should relate to that of another. Proceeding towards this goal requires two elements: 1) a systematic view of what it means to group community members and 2) an appropriate null model for the comparison of observations.

The operation of summing the abundance of community members that belong to an ascribed group can be viewed as a form of coarse-graining. While it is often not explicitly acknowledged as such, coarse-graining can be viewed as a core concept in the microbial life sciences [17]. By smoothing over microscopic details at a lower level of biological organization in order to make progress at a higher level, the concept of coarse-graining has contributed towards the development of effective models of physiological growth [18, 19], evolutionary dynamics [20, 21], and the dependence of ecosystem properties on the diversity of underlying communities [22]. Coarse-graining has even been used to glean insight into the question of whether "species" as a unit has meaning for microorganisms, as modeling efforts have found that the operation allows for the delimitation of community members when resource preferences are structured [23]. These theoretical and empirical efforts suggest that coarse-graining may provide an appropriate framework for investigating patterns of diversity and abundance within and between taxonomic scales of observation.

When evaluating the novelty of an empirical pattern it is useful to identify an appropriate null model for comparison [24–26]. Prior research efforts have demonstrated the novelty of the intra vs. inter-group relationship by contrasting inferences from empirical data with predictions obtained from the Unified Neutral Theory of Biodiversity (UNTB) [12, 27–29]. Specifically, predictions were obtained using a form of the UNTB that predicts that the distribution of abundances within a given site follows a zero-sum multinomial distribution [30]. These predictions generally failed to reproduce slopes inferred from empirical data [12], implying that the intra vs.

inter-group relationship represents a novel macroecological pattern that cannot be quantitatively explained by existing ecological models. Though the task of identifying an appropriate null model for comparison is not straightforward. Rather, the question of what constitutes an appropriate null model remains a persistent topic of discussion in community ecology [24, 31–34]. Here we take the view that a null model is appropriate for examining the relationship between two observables (e.g., community diversity at different scales) if it is capable of quantitatively predicting each observable (e.g., community diversity at one scale). By this standard, the UNTB is an unsuitable choice as a null as it generally fails to capture patterns of microbial diversity and abundance at a single scale [35–37]. One relevant example is that the UNTB predicts that the distribution of mean abundances of species across sites is extremely narrow (i.e., a delta distribution), whereas analyses suggest that empirical data tends to follow a broad lognormal distribution [37]. Contrastingly, recent efforts have determined that the predictions of a model of self-limiting growth with environmental noise, the Stochastic Logistic Model of growth (SLM), is capable of quantitatively capturing multiple empirical macroecological patterns in microbial communities [37–41]. The stationary solution of this model predicts that the abundance of a given community member across sites follows a gamma distribution [37], a result that provides the foundation necessary to predict macroecological patterns among and between different taxonomic and phylogenetic scales.

In this study, we evaluated macroecological patterns of microbial communities across scales of evolutionary resolution. To limit potential biases that may result due to taxonomic annotation errors and to use all available data, we investigated the macroecological consequences of coarse-graining by developing a procedure that groups community members using the underlying phylogeny in addition to relying on taxonomic assignment. Using the Earth Microbiome Project (EMP), a public catalogue of microbial community barcode data, we first assessed the extent that microbial diversity varies as the abundances of community members are coarse-grained by phylogenetic distance and taxonomic rank. The results of these analyses lead us to consider whether the predictive capacity of the gamma remains robust in the face of coarse-graining, a prediction that we quantitatively evaluated among community members and then extended to predict overall community richness and diversity. The accuracy of the gamma provided motivation to test whether the gamma was capable of predicting the intra vs. inter-group relationship between different degrees of taxonomic and phylogenetic coarse-graining. Together, these analyses present evidence of the scale invariance of macroecological patterns in microbial communities as well as the applicability of the gamma distribution as a minimal model of microbial biodiversity.

Results

The macroecological consequences of phylogenetic and taxonomic coarse-graining

While microbial communities are often coarse-grained into higher taxonomic scales, their effect on measures of biodiversity and the underlying phylogeny are rarely examined. Before proceeding with the full analysis using public 16S rRNA amplicon data from the EMP, we elected to quantify the fraction of remaining community members across coarse-graining thresholds, a reflection of the extent that coarse-graining reduces global richness and the relation between taxonomic and phylogenetic coarse-graining. We first define a coarse-grained group g as the set of OTUs that have the same label in a given taxonomic rank out of G groups (e.g., *Pseudomonas* at the genus level) or are collapsed when the phylogeny is truncated by a

given root-to-tip distance (Figs. 1, S1). The relative abundance of group g in site j is defined as $x_{g,j} = \sum_{i \in g} x_{i,j}$. We see that coarse-graining had a drastic effect on the total number of community members within an environment, reducing global richness by $\sim 90\%$ even at just the genus level (Fig. S2a). By coarse-graining over a range of phylogenetic distances, we see that a fraction of coarse-grained community members comparable to that of genus-level coarse-graining occurs at a phylogenetic distance of ~ 0.1 (Fig. S2b). This distance translates to only $\sim 3\%$ of the total distance of the tree, meaning that the majority of OTUs are coarse-grained over a minority of the tree. This pattern is likely driven by the underlying structure of microbial phylogenetic trees, where most community members have short branch lengths [42]. This result suggests that while coarse-graining communities to the genus or family level substantially reduces global richness, it does so without coarse-graining the majority of the evolutionary history that is captured by the phylogeny. Assuming that phylogenies capture ecological changes through evolutionary time, this detail implies that ecological divergence should be retained even when communities are considerably coarse-grained.

With our coarse-graining procedures established, we begin our macroecological investigation. Recent efforts have found that the distribution of abundances of a given taxon maintains a consistent statistically similar form across independent sites and time, a pattern known as the Abundance Fluctuation Distribution [37–39, 43, 44]. By coarse-graining empirical AFDs and rescaling them by their mean and variance (i.e., standard score), we see that AFDs from the human gut microbiome retain their shape across phylogenetic scales (Fig. 2a). This pattern of invariance holds across environments for both phylogenetic and taxonomic coarse-graining (Figs. S3, S4), suggesting that AFDs can likely be described by a single probability distribution.

It has been previously demonstrated that microbial AFDs are well-described by a gamma distribution

$$x_i \sim \text{Gamma}\left(\beta_i, \frac{\beta_i}{\bar{x}_i}\right) \tag{1}$$

where $\bar{x}_i$ is the mean relative abundance across sites and $\beta_i = \frac{\bar{x}_i^2}{\sigma_i^2}$ is the squared inverse of the coefficient of variation [37]. This distribution can be viewed as the stationary distribution of the SLM [37, 45] (Materials and Methods). However, we note that because we are not examining patterns of abundance over time, the gamma distribution does not depend in principle on the validity of the SLM or alternatively formulated stochastic differential equations that also predict a gamma distribution (e.g., [46]).

Using this result, we can determine whether the gamma sufficiently characterizes coarse-grained AFDs. However, we do not directly observe x_i. Rather, our ability to observe a community member is dependent on our sampling effort (i.e., total number of reads for a given site). To account for this, one can derive a form of the gamma distribution that explicitly accounts for sampling, obtaining the probability of obtaining n reads out of N total reads belonging to a community member $\Pr[n|N, \beta_i, \beta_i/\bar{x}_i]$ (Materials and Methods, [37]). Given that $n = 0$ for a species we do not observe, we can define the fraction of M sites where a species was observed (i.e., occupancy, o_i) as

$$\langle o_i \rangle = 1 - \frac{1}{M} \sum_{m=1}^{M} P(0|N_m, \bar{x}_i, \beta_i) \tag{2}$$

We can then compare this prediction to observed estimates of occupancy to assess the accuracy of the gamma distribution across coarse-grained thresholds. We see that Eq. 2 generally succeeds in predicting observed occupancy across phylogenetic and taxonomic scales for all environments (Figs. S5, S6). We can then determine whether the gamma is capable of predicting the relationship between macroecological quantities. One such relationship is that the occupancy of a species should increase with its mean

abundance, known as the abundance-occupancy relationship [47]. This pattern has been found across microbial systems [48–50] and can be quantitatively predicted using the gamma [37]. We see that this relationship is broadly captured across taxonomic and phylogenetic scales for all environments (Figs. 2b, S7 S8). This result implies that the ability to observe a given taxonomic group is primarily determined by its mean abundance across sites and the sampling effort within a site [37].

To quantitatively assess the gamma we calculated the relative error of our occupancy predictions (Eq. 9) for all coarse-graining thresholds. We found that the mean logarithm of the error only slightly increases for the initial taxonomic and phylogenetic scales, where it then exhibits a sharp decrease across environments (Fig. S9a,b). The error then only begins to decrease when the community is highly coarse-grained based on the phylogeny, harboring a global richness (union of all community members in all sites for a given environment) < 20 . This result means that, if anything, the accuracy of the gamma distribution only improves with coarse-graining.

Reconciling coarse-graining and the predictions of the gamma distribution

The consistent predictive success of the gamma distribution in the face of coarse-graining raises the question of why it remains a sufficient null model. The sum of independent gamma distributed random variables only returns a gamma if all variables have identical rate parameters ($\beta_i/\bar{x}_i = \beta/\bar{x}$), a requirement that microbial communities clearly do not meet since they typically harbor broad mean abundance distributions. Given that a gamma AFD cannot predict the distribution of correlations between AFDs [37], it is first worth examining whether the degree of dependence among AFDs shapes coarse-grained variables. We first consider the relation between the variance of the sum and the sum of variances.

$$\mathrm{Var}(\sum_{i}^{S_{\mathrm{tot}}} x_i) = \sum_{i}^{S_{\mathrm{tot}}} \mathrm{Var}(x_i) + 2\sum_{i<j} \mathrm{Cov}(x_i, x_j) \tag{3}$$

By plotting $\mathrm{Var}(\sum_i^{S_{\mathrm{tot}}} x_i)$ against $\sum_i^{S_{\mathrm{tot}}} \mathrm{Var}(x_i)$ across coarse-grained thresholds, we see that the contribution of covariance is weak, meaning that the statistical moments at higher scales can be approximated by those at lower scales (Figs. S10, S11). This result is consistent with previous efforts demonstrating that the strongest correlations between AFDs are typically concentrated among pairs of closely related community members (i.e., low phylogenetic distance) [51], implying that the effect of correlation should dissipate when communities are coarse-grained by their taxonomy or phylogeny. Given that the variance of the sum can be approximated by the sum of the variances and that, by definition, the mean of a sum is the sum of the means, it is reasonable to propose that the statistical moments of coarse-grained AFDs are sufficient to characterize the distribution.

Finally, while there is no general closed-form solution for the sum of independent gamma distributed random variables with different rate parameters (equivalent to considering the convolution of many AFDs with different carrying capacities), continued progress has been made towards obtaining suitable approximations [52–56]. This body of work includes an analysis demonstrating that a single gamma distribution can provide a suitable approximation to the distribution of the sum of many gamma random variables with different rate parameters [57]. In summary, the gamma distribution successfully captures patterns of richness under taxonomic and phylogenetic coarse-graining because the correlation between community members is typically low

and the convolution of many gamma distributions can often be approximated by a single gamma distribution.

Predicting measures of richness and diversity within a coarse-grained scale

Given that the presence or absence of a community member is used to estimate community richness, a measure previously used to make claims about patterns of microbial diversity across taxonomic scales [12], we can visualize the sufficiency of the gamma by predicting the mean richness within an environment at a given coarse-grained threshold (Eq. 10). Likewise, we can use the entirety of the distribution of read counts to predict the diversity within a site, a measure that reflects richness as well as the distribution of abundances within a community (Eq. 11), analytic predictions that we validated through simulations (Fig. S12).

Focusing on the human gut microbiome as an example, we see that we can predict the typical richness of a community across phylogenetic scales using the gamma distribution (Fig. 3a). This success is repeated when we examine the predicted diversity (Fig. 3b). By examining all nine environments, we see that despite the dissimilarity in environments we are able to predict mean richness and diversity in the face of coarse-graining (Fig. 3c,d). The results of this analysis suggest that the composition of microbial communities remains largely invariant in the face of coarse-graining and that the gamma distribution remains a suitable null model for predicting average community measures across coarse-grained scales. Identical results were obtained for taxonomic coarse-graining (Fig. S13).

Turning to higher-order moments, we examined the variance of richness and diversity across sites. Using a similar approach that was applied to the mean, we derived analytic predictions for the variance (Eq. 14). With the human gut as an example, we see that analytic predictions typically fail to capture estimates of variance obtained from empirical data for phylogenetic coarse-graining (Fig. 4a,b). This lack of predictive success was consistent across environments (Fig. 4c,d), implying that a model of independent species with gamma distributed abundances is insufficient to capture the observed variation across communities. A major assumption made in our derivation was that species are independent, an assumption that is almost certainly wrong given that the gamma distribution has been previously demonstrated to be unable to capture the distribution of correlations in the AFDs of community members [37]. However, correlations between variables are a notoriously difficult quantity to capture in predictions of mean-field models such as the SLM. To attempt to remedy this failed prediction, we again turn to the law of total variance by estimating the covariance of richness and diversity from empirical data and adding this term to each measure's respective predicted variance. We found that the addition of this empirical estimate is sufficient to predict the observed variance in the human gut (Fig. 4a,b) as well as across environments (Fig. 4e,f), implying that the underlying model is fundamentally correct but lacking the interactions necessary to explain higher statistical moments of richness and diversity. Identical results were obtained with taxonomic coarse-graining (Fig. S14).

Predicting patterns of richness and diversity between coarse-grained scales

Our predictions of the statistical moments of richness and diversity using the gamma distribution provide the foundation necessary to investigate macroecological patterns between different coarse-grained scales. One such prominent pattern is the relationship between the fine-grain richness/diversity within a given coarse-grained group vs. the

coarse-grained richness/diversity among all remaining groups (e.g., the number of classes within Firmicutes vs. the number of phyla excluding the phylum Firmicutes), a pattern that has been purported to reflect the existence of DBD in microbial systems. Before continuing, we note that the acronym DBD technically refers to the hypothesis that such a a positive relationship reflects the existence of ecological mechanisms through which coarse-grain diversity bolsters the accumulation of fine-grain diversity (e.g., niche construction [14, 58]). While we are primarily interested in the predictive power of an empirically-validated null model of biodiversity, we refer to the slope as the intra vs. inter-group relationship throughout the remainder of this manuscript.

The intra vs. inter-group relationship can be quantified as the slope of the relationship between the fine-grained richness within coarse-grained group g ($S_{g,m}$) and the richness in the remaining $G-1$ coarse-grained groups: $S_{g,m} \propto \alpha S_{G\setminus g,m}$, where $G \setminus g$ denotes the exclusion of group g and α is the slope of the relationship. Using Eq. 2, we can define each of these estimators in terms of the sampling form of the gamma while accounting for sampling

$$S_{g,m} = |g| - \sum_{i \in g} P(0|N_m, \bar{x}_i, \beta_i) \tag{4a}$$

$$S_{G\setminus g,m} = (|G| - 1) - \sum_{\substack{g' \in G \\ g' \neq g}} P(0|N_m, \bar{x}_{g'}, \beta_{g'}) \tag{4b}$$

Similarly, we can use Eq. 11 to derive predictions for intra and inter-group diversity.

$$H_{g,m} = -\sum_{i \in g} \langle x \ln [x] \, | N_m, \bar{x}_g, \beta_g \rangle \tag{5a}$$

$$H_{G\setminus g,m} = -\sum_{\substack{g' \in G \\ g' \neq g}} \langle x \ln [x] \, | N_m, \bar{x}_{g'}, \beta_{g'} \rangle \tag{5b}$$

By repeating this calculation for all M sites, we obtain vectors of coarse and fine-grain of richness estimates for group g from which we can infer the slope through ordinary least squares regression. By repeating this process for all G groups we obtain a distribution of slopes that can be directly compared to the one obtained from empirical data.

Before performing a direct comparison, we first note the features of the empirical slopes and how they pertain to the predictions we obtained. By examining the distribution of empirical slopes pooled over all coarse-graining thresholds for each environment, we see that they are rarely less than zero (Figs. 5a, S19a). The few negative slopes inferred from empirical data were extremely small, having absolute values $< 10^{-4}$ and can be treated as zeros. Furthermore, the distribution of slopes follows the same form across environments, suggesting that the intra vs. inter-group slope reflects a general feature of community sequence data rather than the ecology of specific environments. Like the empirical slopes, the gamma distribution virtually always predicts a positive slope for all environments for both taxonomic and phylogenetic coarse-graining. This paucity of negative slopes suggests that the prediction of the alternative to the DBD hypothesis, the Ecological Controls hypothesis [59], is virtually absent in empirical data and cannot be generated from an empirically validated null model of microbial biodiversity.

However, only observing positive slopes does not necessarily provide support to the DBD hypothesis. A direct comparison of slopes predicted from the gamma distribution to those inferred from empirical data is necessary to determine whether the predictions

of DBD lie outside what can be reasonably captured by a mean-field model. To evaluate the novelty of the intra vs. inter-group slopes we directly compared the values of observed slopes to those obtained from mean-field predictions. We found that the predictions of the gamma distribution closely match the observed slopes across environments for both taxonomic and phylogenetic coarse-graining (Figs. S15, S16). We can consolidate these results by taking the average slope for a given coarse-grained level, from which we see that the mean slope predicted by the gamma distribution does a reasonable job capturing empirical slopes across environments (Figs. 5b, S19b). These results indicate that we should expect to see a positive relationship between richness estimates at different scales and that the relationships we observe can be quantitatively captured by a gamma distributed AFD. It is worth noting that the intra vs. inter-group slope could be sufficiently predicted even though the gamma distribution only succeeded at predicting average richness, suggesting that higher order statistical moments, much less interactions, are unnecessary to quantitatively capture the positive relationship between fine and coarse-grained estimates of richness.

While richness is a widespread and versatile estimator that is commonly used in community ecology, it can neglect a considerable amount of information by focusing on presences and absences instead of the entirety of the distribution of species abundances. To rigorously test the predictive power of the gamma distribution it is necessary to evaluate the intra vs. inter-group relationship for diversity. We again find that disparate environments have similar distributions of slopes from empirical data (Figs. 5c, S19c), suggesting that the slope of the relationship is likely a general property of microbial communities rather than an environment-specific pattern. However, unlike richness, diversity predictions obtained from the gamma distribution generally fail to capture observed slopes, as the squared correlation between observed and predicted slopes can be less than that of richness by over an order of magnitude (Figs. 5d, S17, S18, S19d). Here we see where the predictions of a mean-field model succeed and fail to predict observed macroecological patterns.

Given that the gamma distribution failed to predict the observed diversity slope, it is worth evaluating whether additional features could be incorporated to generate successful predictions. A notable omission is that there is an absence of interactions between community members in predictions derived from mean-field models such as the SLM. However, while considerable progress has been made [10], predicting the observed distribution of correlation coefficients between community members remains a non-trivial task. Given that the gamma distribution succeeds at predicting other macroecological patterns, we elected to perform a simulation where a collection of sites is modeled as an ensemble of communities with correlated gamma-distributed AFDs with the means, variances, correlation matrix, and total depth of sampling set by estimates from empirical data (Materials and methods). By including correlations between AFDs into the simulations, the statistical outcome of ecological interactions between community members, we were able to largely capture the observed intra vs. inter-group diversity slope (Figs. 6, S20, S21, S22). These results suggest that rather than diversity at a fine-scale begetting diversity at a coarse-scale, the correlations that exist at a fine-scale do not dissipate under coarse-graining, resulting in a positive relationship between measures of diversity at different scales.

Discussion

The results of this study demonstrate that macroecological patterns remain largely invariant across taxonomic and phylogenetic scales. By focusing on the predictions of the SLM, a mean-field model of microbial growth under environmental fluctuations, we were able to evaluate the extent that measures of biodiversity can be predicted under

coarse-graining. We were largely able to predict said measures using the same model with zero free parameters (i.e., no statistical fitting) across scales, implying that certain macroecological patterns of microbial communities remain self-similar across taxonomic and phylogenetic scales. Building off of this result, we investigated the dependence of community measures between different degrees of coarse-graining, a pattern that has been formalized as the Diversity Begets Diversity hypothesis [12, 13]. While predictions derived from the sampling form of the gamma distribution quantitatively captured the observed slopes for richness, correlations between community members that are not captured by the distribution that were necessary to predict the slopes of the intra vs. inter-group relationship.

Our richness results complement past work which demonstrated that occupancy, the constituent of richness, is highly dependent on sampling depth (i.e., total read count) and the mean abundance of a community member [37]. This past work and the relationships between the mean abundance and occupancy evaluated in this manuscript demonstrate that occupancy alone is unlikely to contain ecological information that is not already captured by the distribution of abundances across hosts (i.e., the AFD). Our analyses of the relationship between intra and inter-group richness support this conclusion, as predictions derived from a gamma distribution quantitatively captured the observed slope. The successful prediction of richness slopes using a mean-field model that neglects community interactions that also failed to capture the variance of richness is an indictment of the appropriateness of estimators that rely solely on the presence of a community member. Rather, our results suggest that the slope of richness as a measure of community composition between fine and coarse-grain scales will harbor little information about the underlying ecological dynamics of a community that is not already captured by the sampling form of the gamma.

Contrastingly, the predictions of diversity from the gamma sampling distribution were unable to capture intra vs. inter-group relationships from empirical data. Given that diversity as a measure incorporates information about the richness and evenness of a community [60], the comparative deficiency of our diversity relationship predictions suggests that mean-field models cannot capture relationships at different taxonomic or phylogenetic scales that depend on the evenness of the distribution of abundances. This seeming failure illustrates the utility of applying previously empirically successful null models to novel empirical patterns. In microbial ecology, such an approach allows one to establish a sharp demarcation between macroecological patterns that can and cannot be explained by a mean-field model. In this instance, the predictions of the sampling form of the gamma considerably improved when correlations between community members were included, a non-trivial detail that can be used to extend the utility of established models.

While the gamma as a null model derived from the SLM fails to capture observed slopes without the inclusion of AFD correlations, caution is warranted before one ascribes the particular mechanisms that fall under the scope of the DBD hypothesis. This is because the SLM is ultimately a phenomenological model, a strength in that it allows one to intuitively capture core features of microbial dynamics, but a limitation in that it can be difficult to incorporate microscopic details (e.g., consumer-resource dynamics) and examine their macroecological consequences. Experimental investigations of the macroecological patterns evaluated here have found that positive slopes can be found in artificial communities maintained in a laboratory setting and simulations have confirmed that the strength of the correlation is driven by the secretion of secondary metabolites by community members [8]. This phenomenon is known as cross-feeding and it can be viewed as mechanism that is compatible with the concept of niche construction [14]. The existence of intra vs. inter-group diversity relationships in well-controlled experimental systems and their quantitative

manipulation via the details of consumer-resource models implies that the inclusion of microscopic details would likely improve the predictive capacity of the SLM.

In the interest of providing macroecological insight into the DBD hypothesis, we solely focused on coarse-graining procedures that rely on phylogenetic reconstruction and taxonomic assignment. However, it is worth noting that it is also possible to coarse-grain community members by the strength of their correlations (i.e., sum the abundances of each pair of community members with the strongest correlation in AFDs). This procedure has been named the phenomenological renormalization group method due to its ability to identify fixed points in nonlinear systems where the underlying microscopic dynamics are unknown [61, 62]. However, given that the AFD correlation of two community members is strongly related to their phylogenetic distance, such an analysis would likely be largely redundant as the first iteration of coarse-graining based on the strength of correlation would simultaneously coarse-grain the most closely related community members [51].

While we have successfully characterized and predicted empirical macroecological patterns across taxonomic and phylogenetic scales, it is necessary to investigate the limitations of this work. First, we neglected two major macroecological contributors: space and time. Throughout this study we adopted an ensemble approach, where we viewed different sites/hosts as virtual copies of a given environment. This assumption is invalid for longitudinal studies where the temporal autocorrelation of community dynamics can be sufficiently characterized. Due to this autocorrelation, we would expect stronger intra vs. inter-group diversity relationships for community samples taken closer together in time. Second, due to the lack of available observational data, we neglected to include spatial structure. Without spatial information we cannot investigate how 1) the diversity relationship we documented depends on one's spatial scale of observation or 2) how the relationship depends on the spatial distance between sites. Considering these limitations, we are able to state that several macroecological patterns remain invariant across phylogenetic and taxonomic scales (i.e., scale-free) when the necessary criteria are met for different sites to be treated as an ensemble, though we do not know the extent that space and time induce qualitative changes to macroecological patterns.

Our second limitation is that we did not examine the relationship between diversity at ecological and evolutionary scales. All our analyses were performed using 16S rRNA marker gene data with few paired metagenomic samples, meaning that the relationship between the diversity of a community and the genetic diversity of its constituents lies outside of the purview of this study. However, recent efforts have been made to characterize this relationship in the human gut microbiome, having found that community richness and diversity can be correlated with levels of standing genetic diversity and the number of strains within a species [63]. Given that the success of the gamma implies that patterns which rely on richness estimates are unlikely to contain information about ecology beyond that which is captured by mean-field models, it is reasonable to extend this conclusion to eco-evolutionary patterns that rely on richness. However, the same conclusion cannot be reached for diversity, a potential avenue for subsequent explorations of eco-evolutionary interactions. Though an arguably larger issue is that even if the necessary data were provided, the SLM and its predictions are unsuitable for investigating the relationship between ecological and evolutionary diversity in its current form due to its phenomenological nature. Instead, recent research efforts have examined this dependence through mechanistic models of community evolution that generate eco-evolutionary feedbacks which reproduce observed patterns of diversity in observational data [11], building off a previously developed model that couples the microscopic details of consumer-resource dynamics with evolution [64].

Materials and methods

Data acquisition and processing

We used amplicon sequence data from the V4 region of the 16S rRNA gene generated and curated by the Earth Microbiome Project [1]. We restricted our analysis to the quality control (QC)-filtered subset of the EMP, which was annotated using the closed-reference database SILVA [65] and consists of 96 studies culminating in 23,828 total samples with each processed sample having $\geq$ 10,000 reads. We downloaded the public Silva reference tree for OTUs with 97% similarity `97_otus.tre` from the EMP database. We identified nine heavily sampled environments in the metadata file `emp_qiime_mapping_qc_filtered.tsv` and selected 100 random samples from each environment.

We briefly note that our occupancy and richness predictions depend on the form of the gamma distribution that explicitly accounts for sampling as a multinomial process. The multinomial distribution describes the probability of sampling n reads given a relative abundance of x and total read count N with replacement, a process we can model as the Poisson limit of a binomial sampling process for individual community members. Given this choice and the past success of the gamma distribution, we deviated from past analyses by electing to not sub-sample read counts to the same depth across samples, as the process of sampling without replacement would bias the sampling distribution for rare community members [12].

Coarse-graining protocol

Taxonomic coarse graining was performed as the summation of the abundances of all OTUs within a given taxonomic group. We removed taxa with indeterminate labels to prevent potential biases due to taxonomic misassignment, (e.g., "uncultured", "ambiguous taxa", "candidatus", "unclassified", etc.). Manual inspection of EMP taxonomic annotations revealed a low number of OTUs that had been assigned the taxonomic label of their host (e.g., *Arachis hypogaea* (peanut)). These marked OTUs were removed from all downstream analyses.

Phylogenetic coarse-graining was performed using the phylogenetic tree provided by SILVA 123 `97_otus.tre` in the EMP release. Each internal node of a phylogenetic tree was collapsed if the mean branch lengths of its descendants was less than a given distance. All phylogenetic operations were performed using the Python package `ETE3` [66].

Deriving biodiversity measure predictions

While the gamma distribution as the stationary solution of the SLM and the sampling form of the gamma have been previously derived [37], we briefly outline relevant derivations here for the convenience of the reader before deriving the predicted richness and diversity of a community.

$$\frac{dx_i}{dt} = \underbrace{\frac{x_i}{\tau_i}\left(1 - \frac{x_i}{K_i}\right)}_{\text{Self-limiting growth}} + \underbrace{\sqrt{\frac{\sigma_{\tau_i}}{\tau_i}} x_i \cdot \eta(t)}_{\text{Environmental noise}} \tag{6}$$

Here τ_i, K_i, and σ_{τ_i} represent the timescale of growth, the carrying capacity, and the coefficient of variation of growth rate fluctuations, respectively. The term $\eta(t)$ represents Brownian noise $\langle \eta(t) \rangle = 0$ and $\langle \eta(t)\eta(t') \rangle = \delta(t - t')$. The product of this term and relative abundance term x_i represents multiplicative environmental (i.e., external) noise [67]. The stationary distribution of the SLM can be derived using the Itô

$\leftrightarrow$ Fokker-Planck equivalence and taking the stationary solution [37, 45], resulting in the gamma distributed AFD (Eq. 1). Through the SLM, we can define the mean relative abundance and its squared inverse coefficient of variation as $\bar{x}_i = K_i\left(1 - \frac{\sigma_{\tau_i}}{2}\right)$ and $\beta_i = \frac{2-\sigma_{\tau_i}}{\sigma_{\tau_i}}$, respectively. By using the Poisson limit of a binomial sampling process, the sampling form of the AFD can been derived by taking the convolution of the Poisson and the gamma [37]. The result allows us to calculate the probability of obtaining n reads out of a total sampling depth of N for the ith OTU as

$$P_i(n|N_m, \bar{x}_i, \beta_i) = \frac{\Gamma(\beta_i + n)}{n!\Gamma(\beta_i)} \left(\frac{\bar{x}_i N_m}{\beta_i + \bar{x}_i N_m}\right)^{n_i} \left(\frac{\beta_i}{\beta_i + \bar{x}_i N_m}\right)^{\beta_i} \tag{7}$$

Noticing that the probability of a community member's absence is the complement of its presence, we can define the expected occupancy of a community member across M sites as

$$\langle o_i \rangle = \sum_{m}^{M} (1 - P(0|N_m, \bar{x}_i, \beta_i)) \tag{8}$$

The success of our predictions was assessed using the relative error.

$$\varepsilon = \left|\frac{\text{Obs.} - \text{Pred.}}{\text{Obs.}}\right| \tag{9}$$

Using the definition of occupancy from the sampling form of the gamma, we derive the expected richness of a community as

$$\langle S \rangle = \sum_{i=1}^{S_{\text{total}}} \langle o_i \rangle \tag{10a}$$

$$= \frac{1}{M} \sum_{m=1}^{M} \sum_{i=1}^{S_{\text{obs}}} (1 - P(0|N_m, \bar{x}_i, \beta_i)) \tag{10b}$$

$$= S_{\text{total}} - \frac{1}{M} \sum_{m=1}^{M} \sum_{i=1}^{S_{\text{total}}} P(0|N_m, \bar{x}_i, \beta_i) \tag{10c}$$

Similarly, we can derive the expected diversity as

$$\langle H \rangle = -\frac{1}{M} \sum_{m=1}^{M} \sum_{i=1}^{S_{\text{obs}}} \langle x \ln[x] \, |N_m, \bar{x}_i, \beta_i \rangle \tag{11a}$$

$$= -\frac{1}{M} \sum_{m=1}^{M} \sum_{i=1}^{S_{\text{total}}} \int_0^{N_m} \frac{n'}{N_m} \ln\left[\frac{n'}{N_m}\right] \cdot P(n'|N_m, \bar{x}_i, \beta_i) dn' \tag{11b}$$

We can directly calculate Eq. 10 from the empirical data. However, there is no analytic solution for the integral inside the sum of Eq. 11. To calculate $\langle H \rangle$, we performed numerical integration on each integral for each taxon in each sample at a given coarse-grained resolution using the `quad()` function from `SciPy`.

To predict the variance of each measure we derived the expected value of the second moment, assuming independence among community members. We derive the second moments of richness and variance

$$\left\langle S^2 \right\rangle = \left\langle \left(\sum_i^{S_{\text{total}}} o_i \right)^2 \right\rangle \tag{12a}$$

$$= \frac{1}{M} \sum_m^M \left(\sum_i^{S_{\text{total}}} o_{i,m} \right)^2 \tag{12b}$$

$$= \frac{1}{M} \sum_m^M \sum_{i,j} o_{i,m} o_{j,m} \underbrace{\int dNP(N) \delta_{N,N_m}}_{=1} \tag{12c}$$

$$= \int dNP(N) \sum_{i,j} \frac{1}{M} \sum_m^M \delta_{N,N_m} o_{i,m} o_{j,m} \tag{12d}$$

$$= \sum_{i=1}^{S_{\text{total}}} \int dNP(N) \left\langle o_i^2 | N \right\rangle + \sum_{i \neq j} \int dNP(N) \left\langle o_i | N \right\rangle \left\langle o_j | N \right\rangle \tag{12e}$$

$$= \frac{1}{M} \sum_m^M \sum_{i=1}^{S_{\text{total}}} \left\langle o_i^2 | N_m \right\rangle + \frac{1}{M} \sum_m^M \sum_{i \neq j} \left\langle o_i | N_m \right\rangle \left\langle o_j | N_m \right\rangle \tag{12f}$$

where $\delta_{i,j}$ is the Kronecker delta.

By performing an analogous series of operations, we obtain the expected value of the second moment for diversity.

$$\left\langle H^2 \right\rangle = \left\langle \left(\sum_i^{S_{\text{total}}} x_i \ln [x_i] \right)^2 \right\rangle \tag{13a}$$

$$= \frac{1}{M} \sum_m^M \left(\sum_i^{S_{\text{total}}} x_i \ln [x_i] \right)^2 \tag{13b}$$

$$= \frac{1}{M} \sum_m^M \sum_{i,j} \left(x_i \ln [x_i] \right) \left(x_i \ln [x_i] \right)^2 \cdot \int dNP(N) \delta_{N,N_m} \tag{13c}$$

$$= \sum_{i=1}^{S_{\text{total}}} \int dNP(N) \left\langle \left(x \ln [x] \, | N_m, \bar{x}_i, \beta_i \right)^2 \right\rangle \tag{13d}$$

$$+ \sum_{i \neq j} \int dNP(N) \left\langle x \ln [x] \, | N_m, \bar{x}_i, \beta_i \right\rangle \left\langle x \ln [x] \, | N_m, \bar{x}_j, \beta_j \right\rangle \tag{13e}$$

$$= \frac{1}{M} \sum_m^M \sum_{i=1}^{S_{\text{total}}} \left\langle \left(x \ln [x] \, | N_m, \bar{x}_i, \beta_i \right)^2 \right\rangle \tag{13f}$$

$$+ \frac{1}{M} \sum_m^M \sum_{i \neq j} \left\langle x \ln [x] \, | N_m, \bar{x}_i, \beta_i \right\rangle \left\langle x \ln [x] \, | N_m, \bar{x}_j, \beta_j \right\rangle \tag{13g}$$

Where the expected value of the second moment of the diversity term is defined as $\left\langle (x \ln [x])^2 | N_m, \bar{x}_s, \beta_s \right\rangle = \int_0^{N_m} \left(\frac{n'}{N_m} \ln \left[\frac{n'}{N_m} \right] \right)^2 * P(n' | N_m, \bar{x}_s, \beta_s) dn'$. From which we obtain the expected value of the variance

$$\langle \mathrm{Var}(S) \rangle = \langle S^2 \rangle - \langle S \rangle^2 \tag{14a}$$

$$\langle \mathrm{Var}(H) \rangle = \langle H^2 \rangle - \langle H \rangle^2 \tag{14b}$$

Intra vs. inter-group slope inference

In order to predict the relationship between the measures within a coarse-grained group and that among all remaining groups, we calculated a vector of predicted richness or diversity estimates for all sites using Eq. 4a or Eq. 5a within a given coarse-grained group and 4b or Eq. 5b among the remaining groups. This "leave-one-out" procedure was originally implemented in Madi et al., where the authors examined the slope of intra vs. inter-group measures of diversity as a sliding window across taxonomic ranks with both the fine and coarse scales increasing with each rank (e.g., genus:family, family: order, etc.) [12]. To maintain consistency, we used the same definition for our predictions. We also extended the definition to the case of phylogenetic coarse-graining, where we compared fine and coarse scales using different phylogenetic distances while retaining the same ratio (e.g., 0.1:0.3, 0.3:0.5, etc.).

Slopes were estimated using ordinary least squares regression with `SciPy`. Throughout the manuscript the success of a prediction was evaluated by calculating its relative error as follows. We only inferred the slope if a fine-grained group had at least five members. We only examined the slopes of a given coarse-grained threshold if at least three slopes could be inferred.

Simulating communities of correlated gamma-distributed AFDs

Correlated gamma-distributed AFDs were simulated by performing inverse transform sampling. For each environment with M sites, an $M \times S_{\mathrm{obs}}$ matrix $\mathbf{Z}$ was generated from the standard Gaussian distribution using the empirical $S_{\mathrm{obs}} \times S_{\mathrm{obs}}$ correlation matrix of empirical relative abundances. The cumulative distribution $\mathbf{U} = \Phi(\mathbf{Z})_{\mathrm{Gaus.}}$ was obtained and a matrix of SADs was obtained using the point percentile function of the gamma and empirical distribution of mean relative abundances and the squared inverse coefficient of variation of abundances: $\bar{\mathbf{x}} = \bar{x}_1, \bar{x}_2, \cdots, \bar{x}_{S_{\mathrm{obs}}}$, $\boldsymbol{\beta} = \beta_1, \beta_2, \cdots, \beta_{S_{\mathrm{obs}}}$. To simulate the process of sampling, each SAD of the resulting $M \times S_{\mathrm{obs}}$ matrix of true relative abundances $\mathbf{X} = \Phi(\mathbf{U})^{-1}_{\mathrm{Gamma}}$ was sampled using a multinomial distribution with the empirical distribution of total read counts.

Data and code availability

All sequencing data used in this study was obtained from the EMP (URL: `ftp://ftp.microbio.me/emp/release1/`). Processed data are available on Zenodo, DOI: `10.5281/zenodo.7692046`. All code written for this study is available on GitHub under a GNU General Public License: `macroeco_phylo`

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Author contributions

W.R.S. and J.G. conceptualized the project, completed the derivations, and wrote the manuscript. W.R.S. performed all analyses.

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Figures

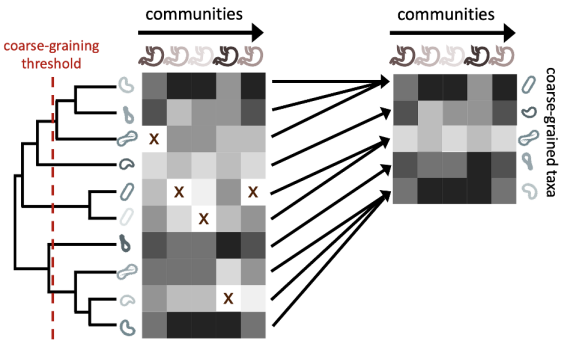

Figure 1. The process of coarse-graining abundances using the phylogeny. Taxonomic assignment in 16S rRNA amplicon sequence data provides the opportunity to investigate how properties of communities vary at different taxonomic scales. The most straightforward means of coarse-graining here is to sum the abundances of OTUs/ASVs that belong to the same taxonomic group. Amplicon data-based studies provide information about the shared evolutionary history of community members, information that can be leveraged by the construction of phylogenetic trees. A coarse-graining procedure can be defined that is analogous to one based on taxonomy, where a phylogenetic distance is chosen, and terminal nodes are collapsed if their distance to a common ancestor is less than the prescribed distance.

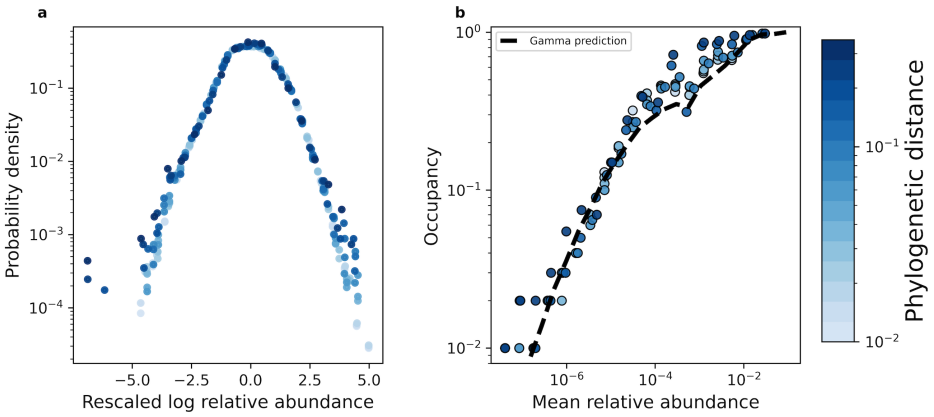

Figure 2. The AFD remains invariant under coarse-graining. We can see that despite phylogenetic coarse-graining, **a)** the general shape of the AFD for OTUs that were present in all samples (i.e., an occupancy of one) and **b)** the relationship between the mean coarse-grained abundance and occupancy across sites remains invariant. Furthermore, predictions obtained from the gamma distribution are capable of capturing the relationship between the mean and occupancy, suggesting that the gamma remains a useful quantitative null model despite coarse-graining. All data in this plot is from the human gut microbiome.

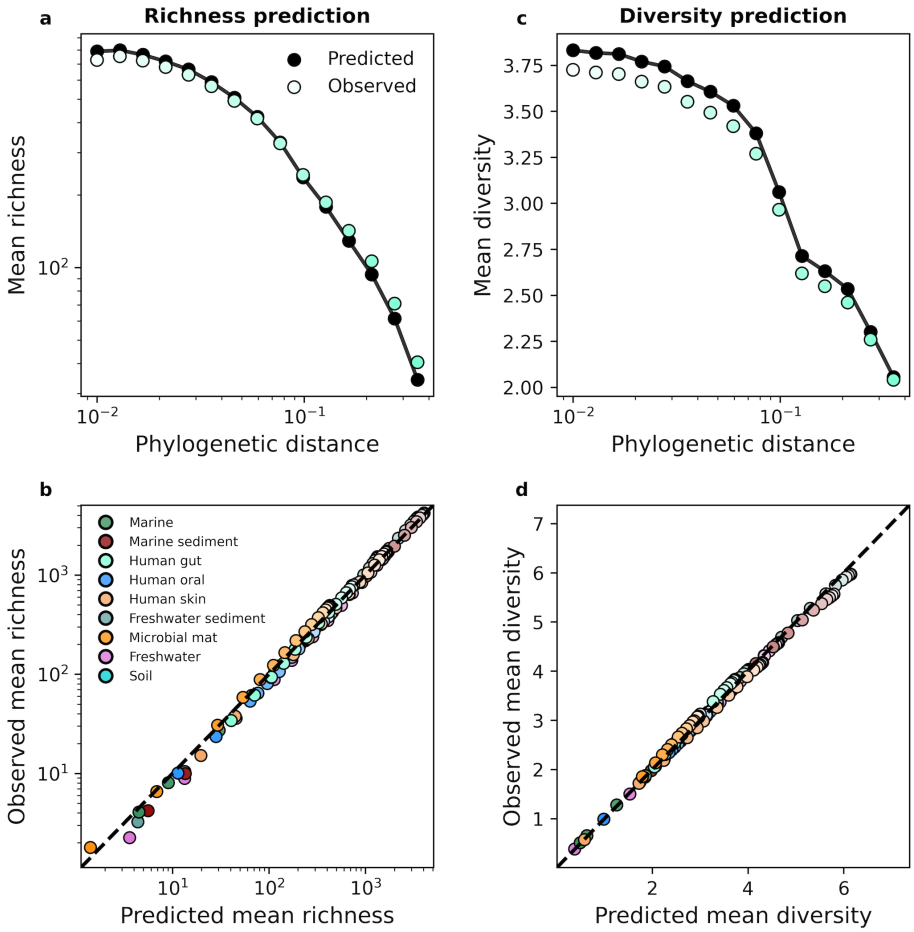

Figure 3. The gamma distribution successfully predicts mean richness and diversity under phylogenetic coarse-graining. a) The expected richness predicted by the gamma (Eq. 10) was capable of predicting richness across phylogenetic coarse-graining scales, as illustrated by data from the human gut. **b)** Predictions remained successful across all environments. **c,d)** Similarly, predictions of expected diversity (11) succeeded across coarse-graining scales among all environments.

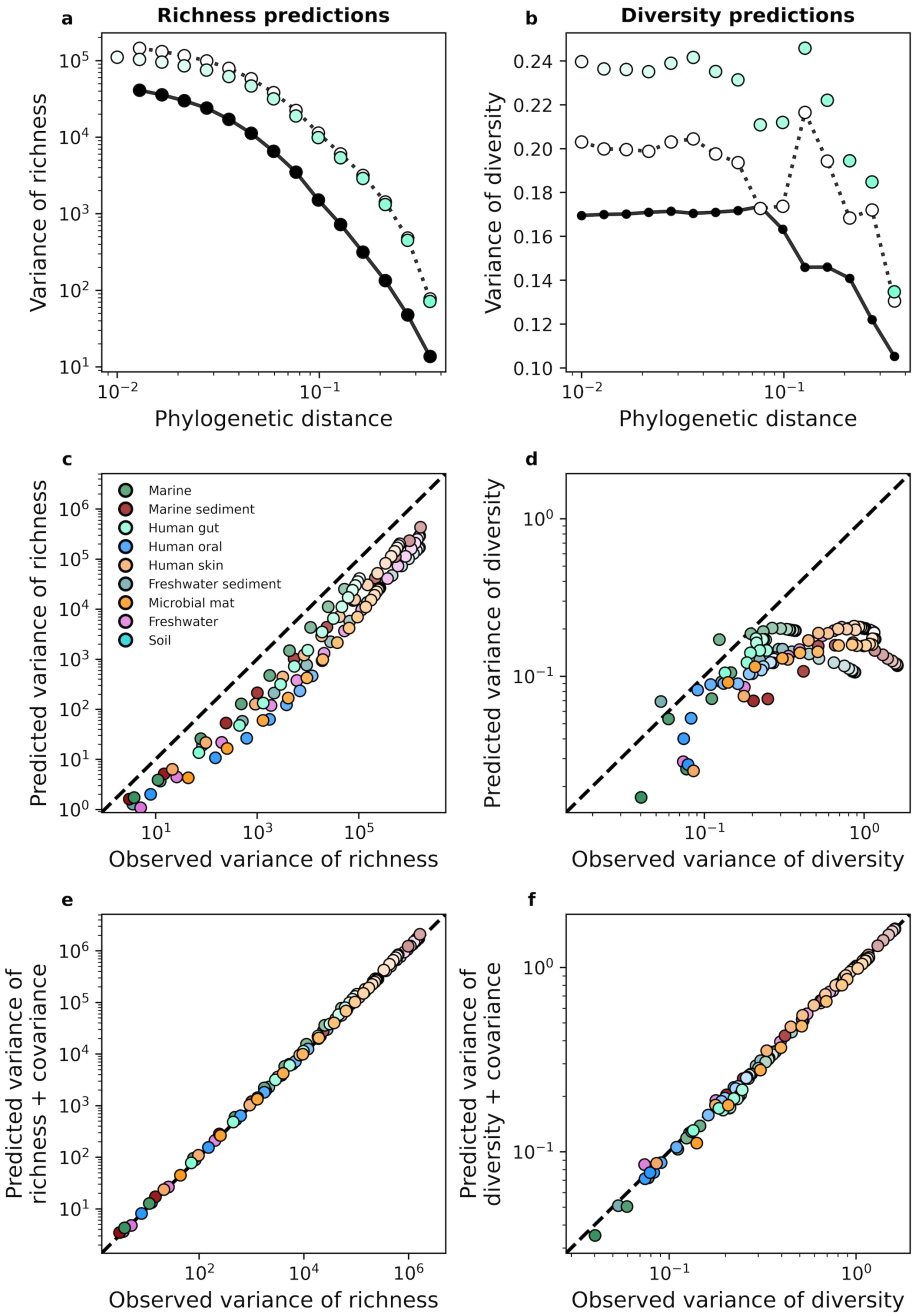

Figure 4. The gamma can only predict the variance of richness and diversity under phylogenetic coarse-graining when covariance is included. a,b) In contrast with the mean, the variance of richness and diversity estimates predicted by the gamma (Eq. 14) assuming independence among species fails to capture empirical estimates from the human gut. Predictions are only comparable when empirical estimates of covariance are included in the predictions of the gamma distribution. **c,d)** This lack of predictive success is constant across environments, **e,f)** though the addition of covariance consistently improves our analytic predictions.

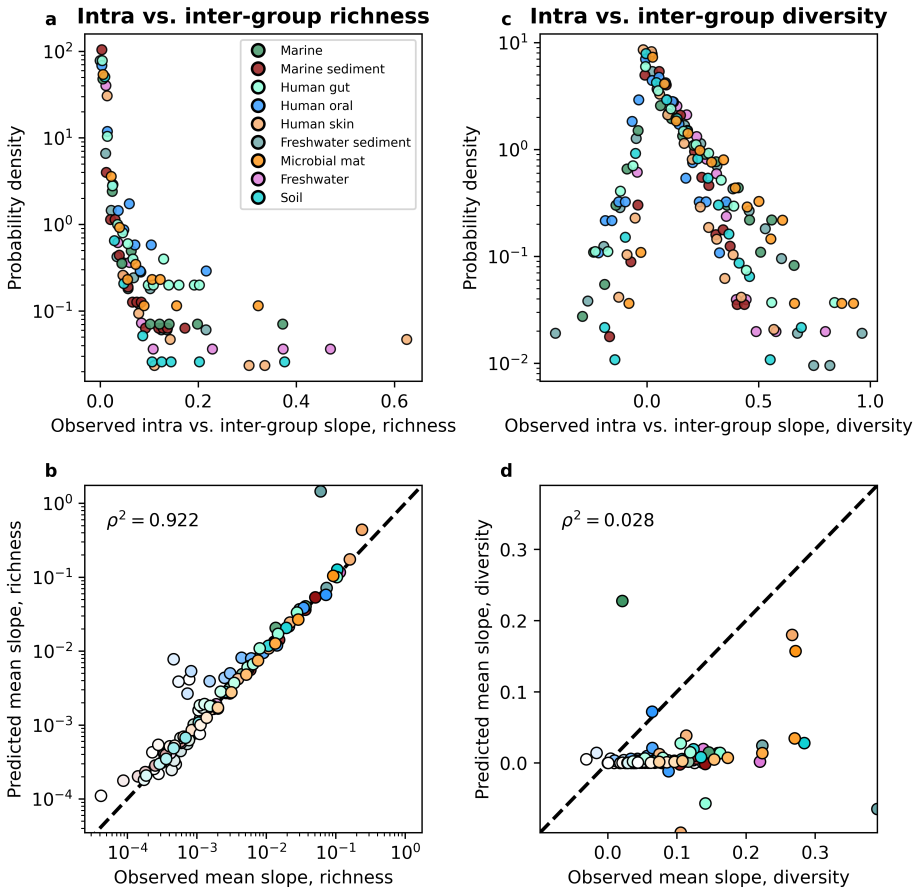

Figure 5. The gamma distribution as a tool for investigating the novelty of intra vs. inter-group slopes. a,b) The predictions of the gamma distribution (Eq. 4) successfully reproduce observed intra vs. inter-group richness slopes across scales of phylogenetic coarse-graining. **c,d)** In contrast, the predictions of the gamma distribution fail to capture diversity slopes (Eq. 5).

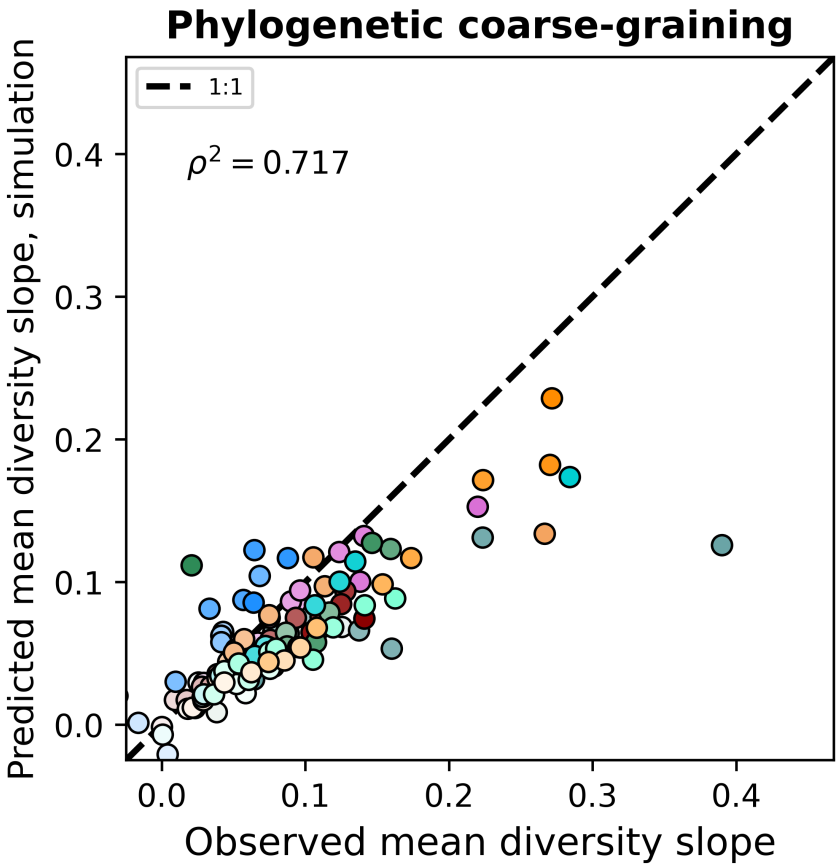

Figure 6. Gamma distribution simulations with correlations capture observed diversity slopes. Observed intra vs. inter-group diversity slopes can be quantitatively reproduced under phylogenetic coarse-graining by simulating correlated gamma distributed AFDs at the OTU-level.