1 Understandable Multifunctionality Measures Using Hill Numbers

2 Keywords: multifunctionality, ecosystem function, Hill numbers, diversity

Abstract

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In ecology, multifunctionality measures the simultaneous provision of multiple ecosystem functions. If species diversity describes the variety of species that together build the ecosystem, multifunctionality attempts to describe the variety of functions these species perform. A range of methods have been proposed to quantify multifunctionality, successively attempting to alleviate problems that have been identified with the previous methods. This has led to a proliferation of more-or-less closely related metrics which, however, lack an overarching theoretical framework. Here we borrow from the comprehensive framework of species diversity to derive a new metric of multifunctionality. Analogously to the effective number of species used to quantify species diversity, the metric we propose is influenced both by the number of functions as well as, crucially, the evenness of performance levels across functions. In addition, the effective multifunctionality also considers the average level at which the functions are performed. The result is a measure of the cumulative performance of the system were all functions provided equally. The framework allows for the inclusion of the correlation structure among functions, thus allowing to account for non-independence between functions. We show that the average metric is a special case of the newly proposed metric when all functions are uncorrelated and performed at equal levels. We hope that by providing a new metric of multifunctionality anchored in the rigorous framework of species diversity based on effective numbers, we will overcome the considerable skepticism that the larger community of ecologists has built against indices of multifunctionality. We thereby hope to help popularize this important concept which, as biological diversity, describes a fundamental property of ecosystems and thus lies at the heart of ecology.

Introduction

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The past decade has witnessed the growth of the concept of ecosystem *multifunctionality*, where multifunctionality is defined as a measure of the simultaneous performance of multiple functions. It has moved from a concept in the biodiversity ecosystem function literature to community ecology writ large (Angelini et al. 2015), invasion biology (Ramus et al. 2017), land management (Nelson et al. 2009, Brandt et al. 2014, Binder et al. 2018), and more. The concept of multifunctionality is broad and can even be applied outside of community and ecosystem ecology - or even outside of ecology altogether. Its adoption as a unifying concept, however, has been slow - and for good reason. Despite the popularity that the concept gained since it was first explicitly proposed over a decade ago (Hector and Bagchi 2007, Gamfeldt et al. 2008), there is still no consensus on how multifunctionality should be quantified. A range of methods have been proposed where each subsequent method attempted to alleviate problems the authors had identified with the previous method, leading to a proliferation of metrics which cannot easily be compared and can lead to inconsistent interpretations of the results (Byrnes et al. 2014a, Gamfeldt and Roger 2017). We do note that this is a difficult problem. Throwing many different ecologists against this problem in a stimulating working group over multiple years (we are thankful for NCEAS for providing this venue) has likely resulted in more ink impregnated on foreheads hitting whiteboards than should be typical, to say nothing of others who have attempted to cut this Gordian knot before and since (Hector and Bagchi 2007, Brandt et al. 2014, Dooley et al. 2015, Rodríguez-Loinaz et al. 2015, Stürck and Verburg 2017, Manning et al. 2018, Meyer et al. 2018, Hölting et al. 2019). In part, this problem is due to the lack of an underpinning body of theory describing how and where multifunctionality should arise. Regardless, this plurality of concepts has hampered a general understanding of multifunctionality and possibly its adoption outside of the subfield of Biodiversity and Ecosystem Function.

Species diversity, for a long time, suffered the same problems that multifunctionality suffers today: there are an uncountable number of metrics to estimate alpha diversity, reaching from the simple count of observed species without regard to their abundance (Richness), wide array of metrics incorporating the relative abundance (Shannon entropy, Simpson index or the Berger-Parker Dominance index to name some of the most common ones), to metrics based on the histograms of the abundance distribution (e.g. Fisher's alpha) (Magurran and McGill 2010). Yet, starting with MacArthur (1965), then Hill (1973), followed by Jost (2006), and most recently Chao et al. (2014a, 2019), a common framework for species diversity has been developed based on information theory. This framework, the effective number of species, encompasses the vast majority of previous metrics and is able to handle a wide variety of different issues in diversity estimation. We propose it can do the same for multifunctionality.

The current state of multifunctional affairs

The definition of multifunctionality presents a challenge. How do we define a metric that captures both the level of performance of a broad suite of functions as well as the distribution of differences in performance among functions? Researchers have sought to capture this question in four ways, after standardizing functions to similar levels in order to prevent apples-to-oranges comparisons. First, many have opted for simplicity and taking the average of all functions (e.g., Maestre et al. 2012). This approach is, at first glance, appealing, particularly as it provides a metric that can be put on a y-axis while a predictor is on the x-axis. However, it sacrifices crucial information about the system. An arithmetic mean tells us what level of functioning we would expect were we to sample any one function at random. Consider two plots - one where all functions are similar and performing at half their value and one where half of the functions are at their maximum while half are absent. The averaging approach says that they are identical. Geometric averaging (e.g., Hensel and Silliman 2013) appears to get around this problem to some degree, as the geometric mean is less than the arithmetic mean by a function of the variance of the observations (the two means are the same when all observations are the identical).

72 However, given its formulation, one critically low function can dominate the measurement - e.g., if even 73 one function is 0, the geometric mean will be 0. 74 Second, we have metrics of the Multivariate Diversity Interactions framework (Dooley et al. 2015). This 75 elegant framework allows us to tease apart the importance of correlations between functions and the 76 contribution of different drivers to simultaneous change in those functions. It does not, however, provide 77 a holistic metric of multifunctionality per se, much like the overlap approach before it (Hector and Bagchi 78 2007). This approach from Hector and Bagchi is a generalization of Sørenson-Dice overlap (Dice 1945, 79 Sørensen 1948). It provides key information on redundancy versus unique contributions of species. While 80 it gives us rich information about a system, it lacks holistic interpretability. 81 Last, we have the threshold approach (Gamfeldt et al. 2008). This approach defines the "presence" of a 82 function if it meets a given threshold of performance, and then sums up the number of functions 83 performing at that threshold. There are clear issues with the arbitrariness of thresholds in the absence of 84 relevant theory or management goals. To remedy this, the multiple threshold approach (Byrnes et al. 85 2014a) seeks to balance the goals of measuring the simultaneous performance of multiple ecosystem 86 functions with the arbitrariness of choosing a threshold of relevance for those functions. The results, 87 however, can be difficult to interpret. Looking at multiple relationships between diversity and threshold-88 based multifunctionality does not provide a metric per se. While there are key metrics that can be 89 extracted from looking at change in slope over different thresholds, the meaning of these quantities are 90 non-obvious in their links to the concept of multifunctionality. The values can vary dramatically 91 depending on the exact threshold chosen and on the method used to standardize the functions, even for 92 simulated communities where all functions perform identically (Gamfeldt and Roger 2017). In the 93 absence of suitable null-models, and even if the approach yields rich information about multifunctionality 94 sensu stricto, it is unwieldy for most if not all who choose to use it, and we have noticed that those who 95 do often report a single threshold in their main text anyway. Related, more recent efforts have sought to

use dimensionality-reducing techniques which have yielded metrics that, while useful, similarly lack easily interpretable meaning (Meyer et al. 2018).

Hill numbers and effective diversity

Over the last 70 years, ecologists studying how to measure species diversity have shown that the vast majority of previous diversity metrics can be organized into a common framework (Macarthur 1965, Hill 1973, Jost 2006, Chao et al. 2014a, 2019). This is true for indices such as Shannon entropy, all Simpson measures, all Renyi entropies, all HCDT or "Tsallis" entropies and species richness (Jost, 2006) and more. All can be expressed as generalized entropies that can be converted to an effective number of species of "order" q which specifies the weighting of proportional abundances. The general formula for the diversity of order q for S species is the following:

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$${}^{q}D = \left(\sum_{i=1}^{S} p_i^{q}\right)^{1/(1-q)} (1)$$

Here, pi is the relative abundance of the ith species and q is the weight given to the species' relative abundances. Species richness, the effective number of species based on Shannon entropy, the effective number of species based on the Simpson index, and the Berger-Parker dominance index are all effective numbers of species of order q = 0, 1, 2 and ∞ , respectively. (Note that the formula is undefined for q = 1, but its limit $q \to 1$ is $\exp(-\Sigma p_i \log p_i)$. The effective number of species of order q is also often referred to as Hill numbers.

We propose leveraging this framework for a more meaningful and less *ad hoc* metric of multifunctionality composed of two parts: (1) the effective *number* of functions that are performed and (2) the *arithmetic mean performance* of the functions that are measured. Our proposed multifunctionality index is then the product of both terms. This approach draws on ideas already swirling in the multifunctionality literature (Brandt et al. 2014, Rodríguez-Loinaz et al. 2015, Stürck and Verburg 2017,

Hölting et al. 2019). With this approach, we aim to provide a unifying framework for the measurement of multifunctionality.

Multifunctionality as the product of effective number of functions and average

level of functions

To define the effective number of functions, we begin with a set of measurements on *k* functions that have been standardized to a common scale (i.e., between 0 and 1 where 0 means no function and 1 means maximum level of function). Let *F_i*, *i* ∈ 1, 2, ... *K* show the level of function for function *i*. The relative proportion a function contributes to the whole is defined as

$$p_i = \frac{F_i}{\sum F_i} \quad (2)$$

We can now substitute the relative proportion into the formula for the effective number of types given in

Eq 1

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$${}^{q}N = \left(\sum_{i=1}^{K} p_i^{q}\right)^{1/(1-q)}$$
 (3)

where qN is the **effective number of functions** for some order q. *The effective number of functions here* translates to the equivalent number of functions were all functions provided at the same level. Adapting from Jost (2006), if q = 0, this is the total number of functions K, which is unimportant as it is just the number of functions measured. For q = 1, the approximation of this function is equivalent to results from Shannon diversity for species shown earlier - which we note has been used as a multifunctionality metric previously (Stürck and Verburg 2017). For q>1, functions performing at higher levels are given greater weight. At q = 2, we get results that are equivalent to the number of functions calculated from Simpson's diversity (inverse Simpson index). If one of our goals is to up-weight high performing functions, q=2 is a reasonable choice, while q=1 is sufficient as it accommodates information about unequal levels of

functioning proportional to the relative functional performance. Lower values would upweight low-performing functions - which might be desirable in certain contexts. The ability to modulate the sensitivity of the metric to high or low performing functions thus provides a strong tool for both ecologists and managers. In the absence of a justification for a particular value of q, exploring the robustness of results to different choices of q could prove fruitful as it has in biodiversity research. Further exploration of how q relates to management goals or ecological theory of multifunctionality would be a fruitful avenue for future research.

Effective number of functions does not accommodate knowledge about the absolute level of functioning in a system - a true metric of multifunctionality. As long as the distribution of p_i is the same, a system with high average function and low average function will look the same. To achieve this translation, we need to take into account the level at which the functions are performed: the arithmetic mean of the function values standardized to a common scale, which we define as A. As we are using standardized values as before, A will range from 0 to 1.

We can then calculate **effective multifunctionality** of order q as the product of both terms. This metric represents the cumulative performance of the system were it composed of functions all performing at equal levels

$${}^qM_ef = {}^qNA \quad (4)$$

This metric will have a maximum value of K, the total number of functions measured in the system, as maximum performance is all functions performing at a standardized level of 1. Alternatively, we can standardize by the total number of functions to calculate the fraction of performance achieved by the whole system, of **standardized effective multifunctionality**, which could facilitate future comparisons among studies.

$${}^{q}M = {}^{q}NA/K \quad (5)$$

However, care has to be taken when comparing multifunctionality values across systems that measure different sets of functions and the value of such comparisons is a topic that eludes consensus even among authors of this article.

Why must we consider the level of function and effective number of functions together in one metric? First, when A is less than one, multiple values of qN are possible depending on the distribution of performance of functions. Second, the average functioning and the effective number of functions are not independent of each other. The upper limit of qN is K by definition. qN is K when all functions are performing at the same level, i.e. $E[A] = F_1$, F_2 , F_3 ... F_K . This can be achieved for any value of A, low or high. Thus, qN has no information about the level of function achieved. The lower limit of qN (as long as q is not 0) occurs at the maximum level of unevenness of F across all functions. This lower limit will vary by different levels of A. For example, qN will always be K when A is 1. Similarly, if all functions but one have a value of 0, then qN will be 1, as p_i for the non-zero function will be 1. If more than 1 function is not 0, then the lower limit is set by a combination of A and the number of dominant functions, i.e., the functions performing at $F_i = 1$ (Figure 1). See Appendix 1 for derivation.

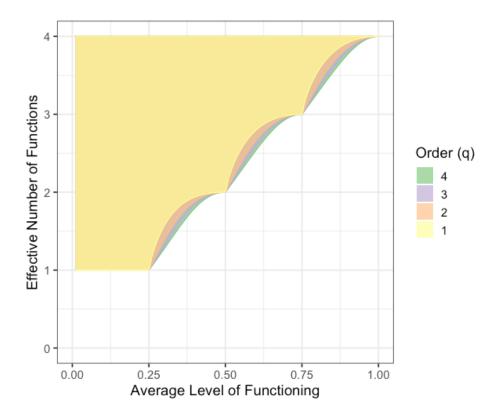


Figure 1. Relationship between ${}^{q}N$ and average level of functions for 4 functions at q = 1,2,3, and 4. Filled areas show the full range of possible values of effective number of functions. Note, areas with a higher order (q) do overlap completely with lower orders, save for the additional edge that is visible.

Most importantly, a combined metric satisfies our definition of multifunctionality. High numbers imply both a high level of function and high functional evenness (i.e., p_i is close to 1/K for all functions). Low values imply that, even if a single function is being optimized, the assemblage of functions as a whole is not performing well. The relationship can also be easily decomposed into its constituent parts for a more detailed examination of its behavior.

Last, from a convenience standpoint, having a single metric allows us to begin to examine it as any other response variable. In the Biodiversity and Ecosystem Functioning world, we might look at additive partitioning in addition to complementary overlap approaches. In global change biology, we can look at stability, resistance, and resilience. The options are open.

A note on standardization

As pointed out in discussions of multifunctionality, how functions are standardized matters (Gamfeldt and Roger 2017, Manning et al. 2018). First is the choice of direction - what implies positive function? When services are being examined explicitly, this is hopefully a straightforward choice - although consider tradeoffs between nutrient cycling rates and storage as a tricky context. Further, not all functions are equally important, particularly in the case of management. Fortunately, choosing an 'optimal' level of function to link to 1 can alleviate this (e.g., if 25% of function is sufficiently high, 25% or higher can be considered a '1'). Functions can also be upweighted or downweighted in the calculation of ^qN so long as $\sum p_i = 1$. Choices for standardization are often best made in the context of a specific system or application and must be transparently justified.

Correlated functions and multifunctionality

A great deal of debate in the multifunctionality literature has sprung from the issue of how to deal with correlations between functions (Bradford et al. 2014a, b, Byrnes et al. 2014b, Manning et al. 2018). As with species diversity, the rationale is that not all functions are equally different and that a metric of true multifunctionality should identify "variables that represent independent aspects of ecosystem functioning" (Manning et al. 2018). As an illustration, consider a scenario where we measure a set of functions, several of which result from a shared mechanism so that they are inextricably linked (for example, growth rate and final biomass). If we want to study the circumstances under which overall multifunctionality is maximized, the results will be disproportionately driven by circumstances maximizing this mechanism influencing the set of correlated functions; thus a naive application of a multifunctionality measure would implicitly upweight the importance of this function cluster over uncorrelated functions.

To address the issue of correlated functions, Manning et al. (2018) proposed performing a cluster analysis of ecosystem functions and building a dendrogram representing the distance matrix between functions. The performance of single functions is then averaged within clusters and multifunctionality is calculated among clusters and not individual functions. This is conceptually very similar to metrics of phylogenetic and functional species diversity that construct phylogenetic trees or dendrograms based on functional similarities and measure species diversity taking into account the dendrogram structure (e.g. Faith's PD, Allen's H, Petchey and Gaston's FD, Rao's Quadratic entropy etc.). The problem is that, as discussed by Chao et al. (2014a), dendrograms are very sensitive to the type of clustering method used and the shape of a dendrogram can vary substantially between different methods (Poos et al. 2009). For the method proposed by Manning et al 2018, it is also unclear at what depth the dendrogram should be cut (i.e., what clusters are considered as independent). Fortunately, extensions of the Hill numbers framework to account for species similarity (e.g., in terms of traits or genetic relatedness) ,(Chao et al. 2014a, 2019) provide a solution to the challenge of evaluating multifunctionality across correlated functions.

To account for correlation among functions in the effective multifunctionality framework, we need to incorporate several concepts from Chao et al. (2019). First, how similar are functions? For this, we need a distance matrix of some sort. If this is based on *a priori* mechanistic information about the underlying processes driving functions (e.g., physiological or evolutionary constraints), so much the better. We often do not have such a matrix. Other options include a matrix derived from principal components or other methods of constructing distance matrices (see Manning et al. 2018). In the absence of such information, a practical choice could be to look at the correlation matrix among functions, R. Defining D = (1 - R)/2 would create a distance matrix where a d_{ij} value of 0 means two functions are inextricably linked (perfectly correlated) while 1 means they trade-off completely ($r_{ij} = -1$). This is one choice, and we suggest that determining the proper way to create a distance matrix between functions for the estimation of effective diversity is an exciting area of research.

With a distance matrix in hand, we need to ask ourselves, how distinct must two functions be before we consider them completely different? This incorporates the threshold τ proposed in Chao et al. (2019). Using this threshold, the distance matrix is truncated such that $d_{ij}(\tau) = \min(d_{ij}, \tau)$. If, for example, $\tau = \min(d_{ij})$, all functions are equally distinct and we recover the results ignoring correlations. If $\tau = 1$ or the maximum distance in the matrix, we fully incorporate information from the distance matrix with no truncation. If $\tau = 0.5$, all negatively correlated functions are as distinct as uncorrelated functions. Chao et al. (2019) recommend using the average weighted pairwise distance between any two functions as τ

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$$d_{mean} = \sum_{i=1}^{K} \sum_{j=1}^{K} d_{ij} p_i p_j \quad (6)$$

as setting τ to d_{mean} yields results that are consistent with comprehensive evaluations of all possible values of τ .

We can then use our truncated distance matrix, $d_{ij}(\tau)$, to define the effective number of underlying functions, qN_u as follows when we are interested in the effective number of underlying "functions". This equation takes advantage of $d_{ij}(\tau)/\tau$ signifying the portion of one function that is distinct from another.

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$${}^{q}N_{u} = \left(\sum_{i=1}^{K} p_{i} \left(\sum_{j=1}^{K} \left[1 - \frac{d_{ij}(\tau)}{\tau}\right] p_{j}\right)^{q-1}\right)^{1/(1-q)}$$
 (7)

In essence, the inner part of the equation is the proportion of function i multiplied by the summed portion of all functions that contribute to the same underlying function. For q=1, we need to use the limit, as before, so

$${}^{q}N_{u} = exp\left(-\sum_{i=1}^{K} p_{i} \log\left(\sum_{j=1}^{K} \left[1 - \frac{d_{ij}(\tau)}{\tau}\right] p_{j}\right)\right)$$
(8)

This effective number of functions can then be used to calculate multifunctionality as above. The average, A, does not need to be modified, because correlations do not systematically bias estimates of the mean (although uncertainty in that mean could be biased downwards by correlations). The correlations only need to be accounted for in the estimate of ^qN..

Discussion

With the framework above in hand, we are hopeful for a proliferation of literature investigating both new and old ideas in multifunctionality. With its ties to theoretically grounded methods of measuring species diversity and its flexibility to encompass some of the real sticking points in the field, we hope that Ecology will embrace this framework moving forward. It produces intuitive I metrics - effective number of functions performing at equal levels, effective multifunction scaled by total level of performance, and standardized versions of both - as well as offers a solution to account for correlated functions. To aid in this advance, see Appendix 2_where we present a worked example in R (R Core Development Team 2008). Over the last decade and a half of its development, the multifunctionality literature has grown slowly, in no small part due to the *ad hoc* nature of the metrics we have developed. We hope that period is at an end.

Further, the metrics presented here are the foundation of a much larger framework that has seen deep exploration in the species diversity world. By embracing this framework for Multifunctionality research, we open up new vistas for ecology. Some are small - what are the consequences and best choices for τ , how we calculate distance matrices, at what scale to evaluate correlation between functions, should we incorporate changes in correlation and distance matrices as an ecological response in and of themselves,

how we standardize functional measurements, and many more. Other new areas of inquiry are quite large. Can we use this framework to begin to address the problem of unmeasured functions as we deal with unmeasured species (Chao et al. 2014b)? Can we use it to think about turnover in multifunctionality across space and time as we do with beta diversity (Chao and Ricotta 2019) or think about partitioning landscape multifunctionality into different components (Jost 2007)? Particularly as we think about global change's impacts on ecosystem services at multiple scales, this framework lays out fruitful avenues for future exploration.

Ultimately, we feel that the proliferation of univariate multifunctionality metrics without strong theoretical underpinning has caused a great deal of confusion about how to measure multifunctionality. We hope that this piece will provide the field of multifunctionality with a way out of its current state of division and confusion. Further, we hope it provides food for additional theory that addresses the causes and consequences of ecosystem multifunctionality, something that is currently sorely lacking but highly relevant to policy and management (e.g., the efforts of the Intergovernmental Science-Policy Platform on Biodiversity and Ecosystem Services). We have been heartened by the idea, leaving the cradle of the field of biodiversity and ecosystem function, and feel that it has the promise to provide a holistic unifying concept for anyone interested in capturing a snapshot of system dynamics in a single meaningful metric with direct ties to the beautifully developing field of diversity partitioning. Much is to be done on honing the particulars of this approach, but we feel it offers a strong theory-driven unified approach that will enable the field of Multifunctionality research to move forward swiftly.

Acknowledgements

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313 **Data Access** 314 --Redacted for review, but see supplementary materials for all relevant code--315 316 References 317 Angelini, C., van der Heide, T., Griffin, J. N., Morton, J. P., Derksen-Hooijberg, M., Lamers, L. P. M., 318 Smolders, A. J. P. and Silliman, B. R. 2015. Foundation species' overlap enhances biodiversity 319 and multifunctionality from the patch to landscape scale in southeastern United States salt 320 marshes. - Proc. R. Soc. B Biol. Sci. 282: 20150421. 321 Binder, S., Isbell, F., Polasky, S., Catford, J. A. and Tilman, D. 2018. Grassland biodiversity can pay. -322 PNAS: 201712874. 323 Bradford, M. A., Wood, S. A., Bardgett, R. D., Black, H. I. J., Bonkowski, M., Eggers, T., Grayston, S. J., 324 Kandeler, E., Manning, P., Setälä, H. and Jones, T. H. 2014a. Discontinuity in the responses of 325 ecosystem processes and multifunctionality to altered soil community composition. - PNAS 111: 326 14478-14483. 327 Bradford, M. A., Wood, S. A., Bardgett, R. D., Black, H. I. J., Bonkowski, M., Eggers, T., Grayston, S. J., 328 Kandeler, E., Manning, P., Setälä, H. and Jones, T. H. 2014b. Reply to Byrnes et al.: Aggregation 329 can obscure understanding of ecosystem multifunctionality. - PNAS 111: E5491–E5491. 330 Brandt, P., Abson, D. J., DellaSala, D. A., Feller, R. and von Wehrden, H. 2014. Multifunctionality and 331 biodiversity: Ecosystem services in temperate rainforests of the Pacific Northwest, USA. - Biol. 332 Conserv. 169: 362–371. 333 Byrnes, J. E. K., Gamfeldt, L., Isbell, F., Lefcheck, J. S., Griffin, J. N., Hector, A., Cardinale, B. J., 334 Hooper, D. U., Dee, L. E. and Emmett Duffy, J. 2014a. Investigating the relationship between 335 biodiversity and ecosystem multifunctionality: challenges and solutions. - Methods Ecol. Evol. 5:

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