MEASURING DIVERSITY: AXIOMS AND CHALLENGES

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ABSTRACT

The concept of diversity is widely used in various applications: from image or molecule generation to recommender systems. Thus, being able to properly measure diversity is important. This paper addresses the problem of quantifying diversity for a set of objects. First, we make a systematic review of existing diversity measures and explore their undesirable behavior in some cases. Based on this review, we formulate three desirable properties (axioms) of a reliable diversity measure: monotonicity, uniqueness, and continuity. We show that none of the existing measures has all three properties and thus these measures are not suitable for quantifying diversity. Then, we construct two examples of measures that have all the desirable properties, thus proving that the list of axioms is not self-contradicting. Unfortunately, the constructed examples are too computationally complex for practical use, thus we pose an open problem of constructing a diversity measure that has all the listed properties and can be computed in practice.

1 INTRODUCTION

Diversity of a collection of objects is a concept that is widely used in practice: image generation models are required to generate a diverse sample of images for a given prompt, recommender systems are required to output a diverse set of suggestions for a query, molecule generation models often aim at generating a collection of structurally diverse molecules with a given property. Diversity can also play an important role in assessing how representative is a given dataset, e.g., in molecule generation (Xie et al., 2023) or neural algorithmic reasoning (Veličković & Blundell, 2021; Mahdavi et al., 2023). Thus, being able to quantify diversity is important.

Traditional methods of assessing diversity may differ across domains and tasks. In the image generation domain, diversity ensures that at least some of the generated images can fit a user's preference. The average of pairwise distances between the output images is commonly used as a measure of diversity. For instance, Ruiz et al. (2023) compute diversity as the average LPIPS similarity between the output objects, while Saharia et al. (2022) compute the average pairwise SSIM between the first output sample and the remaining samples. Similarly, in recommender systems, diversity ensures that at least some of the model outputs can fit a user's preference. The average pairwise distance between the outputs is a popular diversity measure in this domain (Alhijawi et al., 2022). Another way of assessing diversity is via the determinantal point process (DPP) approach that defines diversity as the determinant of the similarity matrix (Wilhelm et al., 2018). In the molecule generation domain, the typical task is to generate a diverse collection of molecules with some predefined properties. The underlying goal is to explore the whole space of such possible molecules and pick the best candidates, so diversity of the output collection ensures that generated molecules are not clustered in one area, while other areas are unexplored. A common diversity measure here is also the average pairwise distance between the outputs (Du et al., 2022), although sometimes the percentage of unique generated molecules is reported (Hoogeboom et al., 2022). Finally, in a recent paper on generating structurally diverse graphs (Velikonivtsev et al., 2024), a new measure called *energy* is proposed as a better and more reliable alternative to the average pairwise distance.

Note that in all the examples above, diversity can also be thought of as *coverage*: the goal is to cover different areas of the space of potentially valid outputs. Thus, in this paper, we use the terms *diversity* and *coverage* interchangeably. In the literature, there have been a few attempts to analyze, compare, or suggest better measures of diversity (Xie et al., 2023; Friedman & Dieng, 2023; Velikonivtsev et al., 2024). However, as we show in this paper, the problem is still underexplored.

We limit the scope of our research to the following setup: we are given a collection of abstract objects and their pairwise distances (or pairwise similarities). We define diversity measure as a function that takes this collection as an input and returns some value as an output.

First, we examine the existing diversity measures by providing examples of their undesirable behavior. Namely, we show that existing measures may either lead to unexpected results when comparing diversity of two datasets (i.e., assigning a higher score to a clearly less diverse dataset) or lead to degenerate solutions when being optimized. Motivated by these observations and previous studies on diversity, we formulate three properties (axioms) that a good diversity measure should have. *Monotonicity* requires that increasing pairwise distances between the objects increases diversity value. *Uniqueness* requires that having a duplicate in the collection is worse for diversity than having any non-duplicate object instead. The last property is *continuity* which requires diversity to be a continuous function of pairwise distances. We support the necessity of these properties with examples of abnormal behavior of diversity measures that do not have some of them. After that, we check which of the existing measures have what properties, and find out that none has all three. Then, we prove that the list of axioms is not self-contradicting by constructing two examples of measures that satisfy all of them. Unfortunately, the proposed measures are too computationally expensive (NP-hard) to be used in practice. Finally, we discuss why finding a diversity measure that has all three desirable properties and is computationally manageable is a non-trivial task. We leave the question of whether there exists a computationally feasible measure satisfying all the required axioms for future studies.

2 Measuring diversity

In this section, we describe existing diversity measures. We assume that we are given a collection of n (possibly duplicated) objects $X = (x_1, \dots, x_n)$ and pairwise distances (dissimilarities) between them such that $d_{ij} \geq 0$ and $d_{ij} = 0$ iff x_i and x_j coincide. For generality purposes, we do not require the triangle inequality to be satisfied by d_{ij}.

Table 1: Known diversity measures

Measure	Formula
Average	$\frac{2}{n(n-1)} \sum_{i<j} d_{ij}$
SumAverage	$\frac{1}{n} \sum_{i<j} d_{ij}$
Diameter	$\max_{i<j} d_{ij}$
SumDiameter	$\sum_i \max_{j \neq i} d_{ij}$
Bottleneck	$\min_{i<j} d_{ij}$
SumBottleneck	$\sum_i \min_{j \neq i} d_{ij}$
Energy(γ), $\gamma > 0$	$-\frac{1}{n(n-1)} \sum_{i<j} \frac{1}{d_{ij}^{\gamma}}$
#Circles(t), $t \geq 0$	$\max_{C \subseteq [n]} \lvert C \rvert$ s.t. $d_{ij} > t \, \forall \, i \neq j \in C$
Unique	$\max_{C \subseteq [n]} \frac{\lvert C \rvert}{n}$ s.t. $d_{ij} > 0 \, \forall \, i \neq j \in C$
Vendi Score	$\exp\left(-\sum_{i=1}^{n} \lambda_i \log(\lambda_i)\right)$
DPP	$\det(S)$
RKE	$-\log\left(\frac{1}{n^2} \sum_{i,j}^{n} s_{ij}^2\right)$
Species(q), $1 \neq q \geq 0$	$\left(\sum_{i=1}^{n} \left(\sum_{j=1}^{n} s_{ij}\right)^{q-1}\right)^{\frac{1}{1-q}}$

Table 1 lists existing diversity measures that we cover in our study. As discussed above, arguably the most straightforward and widely-used way to quantify diversity is via the *average pairwise distance* between the elements. Other simple alternatives are the *minimum* and *maximum* pairwise distances (often referred to as Bottleneck and Diameter, respectively). Xie et al. (2023) argue that none of the simple measures are suitable for diversity quantification and propose #Circles(t) that is defined as the maximal number of non-intersecting circles of radius $t/2$ (for some $t > 0$) with centers in elements of X. A measure called Energy(γ) is proposed by Velikonivtsev et al. (2024) as a better alternative to the above measures. For $\gamma = 1$, this measure equals the energy of a system of equally charged particles.

The remaining four measures are defined in terms of pairwise similarities s_{ij} instead of pairwise distances. All these measures require s_{ij} to be a positive semi-definite similarity function and usually require $s_{ii} = 1$. Vendi Score is proposed by Friedman & Dieng (2023) and is calculated via the formula specified in Table 1, where $\lambda_1, \dots, \lambda_n$ are the eigenvalues of the scaled similarity matrix S/n and S is the $n \times n$ matrix with entries s_{ij}. The simplest DPP-based measure is computed as the determinant of the similarity matrix S.[1] The Rényi Kernel Entropy Mode Count (RKE) is proposed

[1]In practice, more complex DPP-based diversity measures can be used (Wilhelm et al., 2018). For instance, when such measures are applied to recommender systems, the relevance scores of objects w.r.t user queries are usually mixed into the similarity matrix, which we do not do here since we only consider diversity.

by (Jalali et al., 2023) and is defined as the negative logarithm of the average squared similarity. Finally, *diversity of order* q is proposed by Leinster & Cobbold (2012) to measure the diversity of a population consisting of several species. In our work, we refer to this measure as Species(q). Here, the parameter q is any nonnegative number not equal to 1. When applied to our setup (all elements having equal weights), the measure Species(q) can be written as specified in Table 1 (up to a constant multiplier).

Some previous works on measuring diversity analyze and compare measures based on properties they do or do not satisfy. We review these works in Section 4.4.

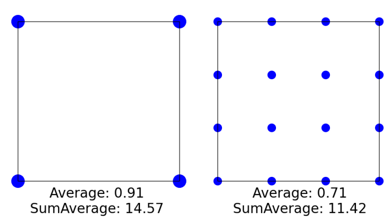
3 Drawbacks of popular diversity measures

In this section, we discuss why none of the measures defined above can be reliably used to quantify diversity. For this, we show intuitive examples of an undesirable behavior for each measure. These examples serve as the main motivation for our research and for the axioms we choose.

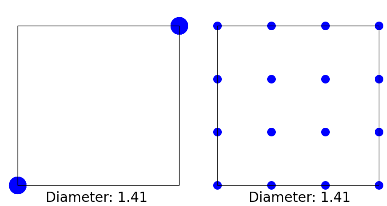
We start with discussing two usage scenarios of diversity measures. First, a diversity measure can be applied to a given dataset to quantify its diversity. Thus, it should be able to identify which dataset is more diverse. For instance, when choosing between two recommendation algorithms, one can be interested in comparing diversity of the retrieved sets of items. Second, diversity can be used as a goal of an optimization process. For instance, Velikonivtsev et al. (2024) generate sets of graphs that are maximally diverse. During the generation process, the authors iteratively modify the set of graphs by accepting modifications that improve a given diversity measure. Thus, a good diversity measure should lead to diverse configurations of elements when being optimized.

Below we examine the diversity measures listed in Table 1 from these two perspectives: *comparison* and *optimization*. We say that a measure exhibits undesirable behavior w.r.t. *comparison* if there exists a pair of datasets, such that the first one is more diverse according to our intuitive perception of diversity, yet the diversity measure assigns the higher value to the second one. We say that a measure exhibits undesirable behavior w.r.t. *optimization* if the dataset with maximal diversity according to this measure is not maximally diverse according to our intuitive perception of diversity. Note that if a measure exhibits undesirable behavior w.r.t. optimization, it also exhibits undesirable behavior w.r.t. comparison. Indeed, if a measure assigns the highest value to some not intuitively diverse set, this means that it assigns a lower value to some dataset that is intuitively diverse, thus exhibiting undesirable behavior w.r.t. comparison. The opposite is not necessarily true: some measures can be suitable for optimization while being unable to reliably compare two non-optimal configurations.

Note that we limit our research to the simple case when the number of elements n is fixed, thus in the examples below all the configurations are of the same size.

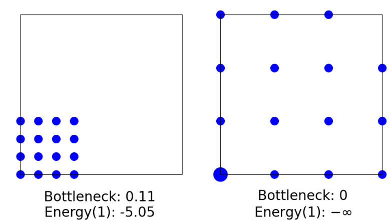


Average and SumAverage Since Average and SumAverage differ only by a constant factor, we consider them together. Consider two configurations of 16 points in the unit square with Euclidean distance (in the configuration on the left, each of the square's angles contains 4 coinciding points). For the left configuration, Average equals 0.91, which is the maximal value among all possible configurations. For the right configuration, Average equals 0.71. Since the right configuration is intuitively more diverse, this example shows undesirable behavior of Average w.r.t. both comparison and optimization. Informally, maximizing Average pushes all points to the boundary of the space, leaving central areas empty.

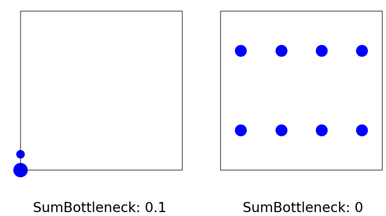


Diameter and SumDiameter Again, consider two configurations of 16 points in the unit square (in the left configuration, two of the square's angles contain 8 coinciding points each). Diameter for both configurations is 1.41, which is the maximal value among all possible configurations. Since the right configuration is intuitively more diverse, this example shows undesirable behavior of Diameter w.r.t. both comparison and optimization. Note that once a configuration contains two points at the maximal distance from each other (in our case 1.41), the positions of all other points do not influence Diameter. While SumDiameter is expected to be a better diversity measure (it takes more distances into account), the same example works to show its undesirable behavior w.r.t. comparison and optimization since the left configuration has the maximal possible SumDiameter value. Indeed, if there are points x_1 and x_2 with maximal distance between them, we can make all other points coincide with x_1 or x_2, thus maximizing SumDiameter.

Bottleneck Bottleneck assigns any configuration without duplicates a higher diversity value than any configuration with duplicates. Consider two configurations of 16 points in the unit square (in the right configuration, the bottom-left angle contains 2 coinciding points). For the left configuration, Bottleneck equals 0.11, and for the right configuration, Bottleneck equals 0. Since the right configuration is intuitively more diverse, we see undesirable behavior of Bottleneck w.r.t. comparison.



SumBottleneck To a lesser extent, SumBottleneck has the same drawbacks as a Bottleneck. Consider two configurations of 16 points in the unit square (in the left configuration, 15 points coincide in the corner of the square, and in the right configuration, each point has one duplicate). For the left configuration, Bottleneck equals 0.1, and for the right configuration, Bottleneck equals 0. Since the right configuration is intuitively more diverse, we see undesirable behavior of Bottleneck w.r.t. comparison.



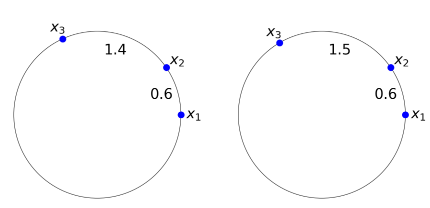
Energy(γ) The drawback of this measure is that in the presence of a duplicate, it has value $-\infty$ and is insensitive to all other pairwise distances. The same example as for Bottleneck demonstrates undesirable behavior of Energy w.r.t. comparison.

Note that the examples for Bottleneck, SumBottleneck, and Energy demonstrate their undesirable behavior only w.r.t. comparison. Intuitively, all these measures behave well w.r.t. optimization since maximizing them enforces more uniform distribution by pushing away the closest elements (the examples for Energy optimization can be found in Velikonivtsev et al. (2024)).

#Circles(t) To use this measure for a reasonable comparison of two collections, one needs to somehow find an appropriate value of t. Indeed, if t is too high, both collections will have diversity 1, and if t is too low, both collections will have diversity equal to their number of unique elements. This complicates the usage of this measure for both comparison and optimization. Also, this measure is discrete and thus difficult to optimize. Finally, the value of this measure is NP-hard to compute, which makes it impractical.

Unique Since this measure does not take into account the pairwise distances between objects, it is essentially unsuitable for comparison or optimization. Indeed, all collections with pairwise distinct objects have the same diversity value 1.

Vendi Score Consider points on a circle with cosine similarity. Suppose the points x_1, x_2, x_3 are arranged on a circle in this order, the distance from x_1 to x_2 is 0.6 radians, the distance from x_2 to x_3 is 1.4 radians. Now, we move x_3 by 0.1 away from x_1 and x_2. Intuitively, we expect that decreasing the similarity between x_3 and other elements must increase diversity. But the Vendi Score decreases from 1.941 to 1.916, which is an example of undesirable behavior w.r.t. comparison.

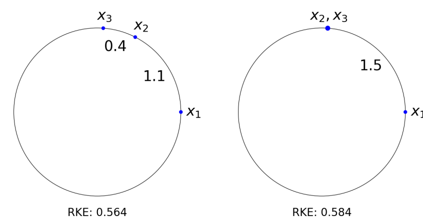


DPP Consider two positive semidefinite symmetric matrices:

$$K_1 = \begin{pmatrix} 1 & 0.2 & 0.6 \\ 0.2 & 1 & 0.7 \\ 0.6 & 0.7 & 1 \end{pmatrix}, \quad K_2 = \begin{pmatrix} 1 & 0.3 & 0.6 \\ 0.3 & 1 & 0.7 \\ 0.6 & 0.7 & 1 \end{pmatrix}. \tag{1}$$

The matrices K_1 and K_2 differ by increasing s_{12} from 0.2 to 0.3. Intuitively, we expect that increasing similarity between any two elements must decrease diversity. But $\det(K_1) = 0.278$ and $\det(K_2) = 0.312 > 0.278$, which is an example of undesirable behavior of the DDP-based measure w.r.t. comparison.

RKE and Species(q) Consider points on a circle with cosine similarity. Suppose the points x_1, x_2, x_3 are arranged on a circle in this order, the distance from x_1 to x_2 is 1.1 radians, the distance from x_2 to x_3 is 0.4 radians. Now, we make x_2 to be a duplicate of x_3. Intuitively, we expect that such change must decrease diversity. But the RKE increases from 0.564 to 0.584, which is an example of undesirable behavior w.r.t. comparison. The same example illustrates the undesirable behavior w.r.t. comparison for Species(q) for various q (see Appendix B).



4 AXIOMATIC APPROACH TO DIVERSITY MEASURES

Motivated by our analysis in Section 3, we formulate a list of properties (axioms) that a reliable diversity measure is expected to satisfy. First, we formally define diversity measures, then formulate the desirable properties and discuss which existing measures satisfy which properties, and finally review desirable properties suggested in previous studies and discuss how they relate to our setup.

4.1 FORMAL DEFINITION OF DIVERSITY MEASURE

Assume that we are given a collection of n (possibly duplicating) objects $X = (x_1, \ldots, x_n)$ and pairwise distances between them d_{ij}, which satisfy the following conditions:

1. $\forall i, j : d_{ij} \geq 0$ and $\forall i : d_{ii} = 0$;
2. if $d_{ij} = 0$, then $\forall k : d_{ik} = d_{jk}$;
3. $\forall i, j : d_{ij} = d_{ji}$.

In terms of objects, the first property requires that the distance between any two objects is nonnegative, and distance from an object to itself is 0. The second property requires that if two objects coincide, then they must have equal distances to any other object. The third property is symmetry of distance. Note that for generality, we do not require the triangle inequality to be satisfied by d_{ij}.

A diversity measure is a function that takes as input any such set of n objects and their pairwise distances and outputs a real number. We assume that diversity depends only on distances d_{ij} and does not depend on the nature of the objects x_i itself. So, the input of our function can be fully described as $n \times n$ matrix D with entries d_{ij}. Denote by D_n a subset of all $n \times n$ matrices satisfying the three properties described above. Then, the diversity function is a function from D_n to $\mathbb{R}$. Since diversity is usually measured for a *multiset* of objects, we also require *permutation invariance*: if we permute (or rename) the objects in X (with correspondingly permuting the rows and columns of D), the value of diversity should not change. Thus, we get the following definition.

Definition 4.1. A *diversity function* is a permutation invariant function from D_n to $\mathbb{R}$.

Note that we assume the number of elements n to be fixed. Thus, we do not aim to determine how diversity should behave when the size of the dataset changes. Our paper shows that even for this (simpler) case is non-trivial to construct a suitable diversity measure.

4.2 AXIOMS FOR DIVERSITY

In this section, we formulate three axioms that we require for a reliable diversity measure.

Axiom 1 (Monotonicity). *A diversity function must be strictly monotonously increasing with respect to all its arguments.*

In other words, if we increase one or several pairwise distances while keeping all other distances fixed, the value of diversity must increase. This axiom is natural to require since it represents the meaning of diversity: the more objects $x_1, \ldots, x_n$ differ from each other, the higher diversity we expect. This property is analogous to monotonicity in Velikonivtsev et al. (2024), but has one important difference: we do not require the objects of X to be pairwise distinct for monotonicity to hold. This difference is critical for being able to compare datasets: we want to be able to tell which configuration is more diverse even if they have duplicates. Otherwise, we may get a measure with undesirable behavior, as shown by the example for Bottleneck and Energy in Section 3.

Axiom 2 (Uniqueness). *Suppose we are given two collections of objects (and their pairwise distances) which differ only by one element: $x_1, \ldots, x_{n-1}, x_n$ and $x_1, \ldots, x_{n-1}, x'_n$. Suppose x'_n coincide with at least one of $x_1, \ldots, x_{n-1}$, while x_n does not coincide with any of $x_1, \ldots, x_{n-1}$. Then, the diversity of the first collection must be higher than the diversity of the second collection.*[2]

This property reflects our intuition that having a duplicate (x'_n) in the multiset is worse for diversity than having a unique element (x_n) instead. Informally, we can say that having x'_n does not help the multiset to cover any new part of the space since a copy of x'_n is already present, while having x_n covers some new area. Uniqueness allows one to avoid an undesirable behavior when the collection with duplicates has higher diversity than an intuitively more diverse collection without duplicates or even when the maximal diversity is achieved by a degenerate configuration (which happens to Average and Diameter, as shown in Section 3). Let us note that the difference between our variant of Uniqueness and the analogous property in Velikonivtsev et al. (2024) is that we do not require all objects in X to be distinct. As for monotonicity, this modification is important for being able to compare datasets even when they have duplicated elements.

Axiom 3 (Continuity). *A diversity function must be continuous.*

This property was not present in previous works, but it is natural to require and we find it critical for a reliable diversity measure. Indeed, in Appendix A we show that there are examples of discontinuous functions that satisfy monotonicity and uniqueness while still exhibiting undesirable behavior. Thus, having only monotonicity and uniqueness is not sufficient.

4.3 PROPERTIES OF EXISTING MEASURES

Table 2 shows which axioms are satisfied by the existing measures (the proofs can be found in Appendix B). It can be seen that none of the existing measures has all three desirable properties.[3] This leads us to the main question of the paper: does there exist a diversity measure with all three desirable properties? In the next section, we construct two examples of such measures, thus giving a positive answer to this question. We include these measures as well as the computational complexities of all the measures in Table 2.

4.4 DESIRABLE PROPERTIES IN PREVIOUS WORKS

Several papers analyze and compare diversity measures in terms of properties they do or do not satisfy. For instance, Xie et al. (2023) formulate three axioms. The first one requires that diversity of a union of two sets must be higher than the diversity of each of these two sets. The second requires that diversity of a union of two sets should be at most the sum of their diversities. Note that both of these axioms constrain the behavior of diversity when the number of objects changes and thus are

[2]For simplicity, we formulate this property in terms of objects, but it can be straightforwardly reformulated in terms of pairwise distances.

[3]Note that Energy was reported in Velikonivtsev et al. (2024) as having Monotonicity and Uniqueness, but it does not in our case since we have stronger versions of these properties that require them to hold even in the presence of duplicated elements.

Table 2: Properties of diversity measures

Measure	Monotonicity	Uniqueness	Continuity	Complexity
Average	✓	✗	✓	$O(n^2)$
SumAverage	✓	✗	✓	$O(n^2)$
Diameter	✗	✗	✓	$O(n^2)$
SumDiameter	✗	✗	✓	$O(n^2)$
Bottleneck	✗	✗	✓	$O(n^2)$
SumBottleneck	✗	✗	✓	$O(n^2)$
Energy(γ), $\gamma > 0$	✗	✗	✓	$O(n^2)$
#Circles(t), $t \geq 0$	✗	✗	✗	NP-hard
Unique	✗	✓	✗	$O(n)$
Vendi Score	✗	✗	✓	$O(n^3)$
DPP	✗	✗	✓	$O(n^3)$
RKE	✓	✗	✓	$O(n^2)$
Species(q)	✓	✗	✓	$O(n^2)$
MultiDimVolume	✓	✓	✓	NP-hard
IntegralMaxClique	✓	✓	✓	NP-hard

not applied in our setting with a fixed number of objects. The last axiom requires that if we have only two objects in X, then diversity must be strictly monotone w.r.t. the pairwise distance between these objects. Note that one of our requirements (monotonicity, see below) generalizes this axiom.

Friedman & Dieng (2023) propose Vendi Score and list four its properties. One of the properties is called *symmetry* and it is equivalent to our *permutation invariance* that we require for all diversity measures. Another property requires that a diversity measure is maximized when all pairwise similarities are 0 and minimized when all pairwise similarities are 1. This property is generalized by our monotonicity axiom. The remaining two properties consider weighted elements or samples of different sizes and thus do not apply to our setup.

Velikonivtsev et al. (2024) address the problem of generating structurally diverse graphs and discuss what measures of diversity are suitable for optimization. The authors formulate two properties: *monotonicity* and *uniqueness*. Monotonicity requires that for a collection of pairwise different objects increasing any pairwise distance d_{ij} also increases the diversity value. Uniqueness requires that if in the collection of pairwise different objects we replace one object with a duplicate of another object from the collection the diversity must decrease.

Leinster & Cobbold (2012) list several groups of useful properties of diversity of order q. *Partitioning properties* are not applied to our case since we consider the diversity only for a fixed number of objects. From *Elementary properties* group Symmetry property corresponds to our requirement of diversity function to be permutation invariant, and Absent species and Identical species properties are not applicable in our case (since we consider n objects with equal weight and not n probabilities summing to 1). From the group of properties named *Effect of species similarity on diversity*, the only property applicable in our case is Monotonicity, which is equivalent to our Monotonicity axiom.

To sum up, among the properties from previous works, the ones applicable in our setting are monotonicity (in stronger form from Velikonivtsev et al. (2024) and Leinster & Cobbold (2012) or weaker forms from Xie et al. (2023) and Friedman & Dieng (2023)) and uniqueness, given that permutation invariance is already incorporated in our definition of a diversity function.

5 Diversity measures with all desirable properties

In this section, we construct two different examples of permutation-invariant measures that have all three desirable properties.

MultiDimVolume For a given k, $2 \leq k \leq n$, and a given submultiset S of size k of the multiset $X = (x_1, \dots, x_n)$, calculate the product of all pairwise distances between the elements of S. Note that this product equals zero if at least two elements of S coincide. Then, for a given k, we take the maximum of such products over all submultisets of size k of X and denote this maximum as $m_k(X)$. We define the diversity of X as $\sum_{k=2}^{n} m_k(X)$. Putting the above into one formula, we get:

$$\mathrm{Diversity}(X) := \sum_{k=2}^{n} \max_{\substack{S \subseteq X \\ |S|=k}} \left(\prod_{\substack{x_i, x_j \in S \\ i<j}} d_{ij} \right). \tag{2}$$

The intuition behind this formula is that for a set S of size k, the product of all pairwise distances between the elements of S can be thought of as an analog of k-dimensional volume of S (analogy comes from the fact that if two elements of S coincide, then the volume degrades to zero). Thus, $m_k(X)$ is the maximal 'volume' of a k-dimensional subset of X.

In Appendix C, we prove that MultiDimVolume satisfies all the axioms. Unfortunately, computing $\mathrm{Diversity}(X)$ in Equation (2) is NP-hard since calculating MultiDimVolume allows one to solve the problem of finding the size of the maximal clique in a graph, and this problem is known to be NP-hard. We refer to Appendix C for the formal proof.

Let us also note that there are multiple ways to define diversity based on the values $m_k(X)$. Indeed, we can consider $\sum_{k=2}^{n} f(m_k(X))$, where f is an arbitrary continuous monotone function. In particular, one may consider $\mathrm{Diversity}(X) = \sum_{k=2}^{n} m_k(X)^{\frac{2}{k(k-1)}}$. This modification is natural since each summand is a product of $k(k-1)/2$ terms. We call this modification a Normalized MultiDimVolume, or Normalized MDV for short. It follows from the proof in Appendix C that all such modifications satisfy all the desirable properties.

IntegralMaxClique For a given threshold $t \geq 0$, we construct the following graph. The nodes are $x_1, \ldots, x_n$. Two nodes x_i and x_j are connected by an edge iff $d_{ij} \geq t$, and we assign d_{ij} as a weight of this edge. We find a clique (complete subgraph) in this graph with the maximal number of nodes. If there are several such cliques, we pick the one with the maximal total weight of edges. For the chosen clique, we calculate the total weight of its edges and denote it by $w_t(X)$. Then, we define diversity as

$$\mathrm{Diversity}(X) := \int_0^{+\infty} w_t(X)\, dt. \tag{3}$$

This integral is finite since $w_t(X)$ is bounded by $\sum_{i<j} d_{ij}$, and if $t > \max_{i<j} d_{ij}$, then the constructed graph has no edges and $w_t(X) = 0$.

The intuition behind this formula is that $m_t(X)$ can be interpreted as the maximal diversity of a subset of X with the restriction that its elements should be at distance t or more from each other.

In Appendix D, we prove that IntegralMaxClique satisfies all the axioms. Unfortunately, computing $\mathrm{Diversity}(X)$ in Equation (3) is NP-hard since, similarly to MultiDimVolume, calculating IntegralMaxClique allows one to solve the problem of finding the size of the maximal clique in a graph. We refer to Appendix D for the formal proof.

By constructing the two examples above, we prove that three desirable properties from our list do not contradict each other. Unfortunately, the constructed examples are too computationally complex for most practical applications.

As shown above, there are various (NP-hard) diversity measures satisfying all the axioms. While none of them can be ruled out based on their theoretical properties, these measures are different and thus may disagree in some cases. However, we expect them to better agree with our intuition of diversity. To show that this is indeed the case, we analyze how MultiDimVolume, Normalized MDV and IntegralMaxClique work on synthetic examples shown to be difficult for other measures in Section 3. The results can be found in Appendix G.

6 DISCUSSION

In the previous section, we prove that the three axioms listed in Section 4.2 are not self-contradicting. However, we have not been able to construct a measure that satisfies these axioms and is computationally feasible to be applied in practice. We pose this as an important open problem to be addressed in future studies.

Let us provide some intuition on why it is hard to combine monotonicity, uniqueness, and continuity in one function. We first formulate the following proposition that shows an additional restriction that these three axioms imply.

Proposition 6.1. *Suppose a diversity function has uniqueness and continuity. Let $x_1, \dots, x_k$ be a set of k pairwise different objects. Let C be a multiset of $n-k$ objects, each of which coincides with one of $x_1, \dots, x_k$. Then, diversity of the multiset $\{x_1, \dots, x_k\} \cup C$ is the same for all such C.*

We prove this proposition in Appendix E. Informally, Proposition 6.1 states that the diversity of a set does not depend on which elements are duplicated. This agrees well with our intuition: duplicates do not give any additional elements and thus are not supposed to affect diversity. On the other hand, constructing a measure that is continuous while 'ignoring' duplicates is tricky since the object's property of being a duplicate is discontinuous. Indeed, we can move a duplicate by any small $\epsilon > 0$ and it stops being a duplicate, so our measure should no longer 'ignore' it. In MultiDimVolume, we address this problem by incorporating products of pairwise distances within subgraphs: any duplicate zeros the corresponding products and thus the placement of a duplicate does not affect the result. In IntegralMaxClique, we use a threshold t to filter out small edges, and thus duplicates do not affect the value for all $t > 0$.

The next proposition states that a diversity function satisfying all the axioms cannot be expressed in a certain form. This particular form is motivated by the approach in Velikonivtsev et al. (2024): the authors iteratively improve diversity of a set by updating one element at a time. Thus, they decompose a considered diversity function into the fitness of one element and diversity of the rest of the elements. Such decomposition would allow one to make quick updates of diversity (in linear time) when only one element is updated. In the proposition below, we show that for a proper diversity measure such decomposition cannot exist if we assume *additive* aggregation.

Proposition 6.2. *Assume that a diversity function can be decomposed in the following way:*

$$\mathrm{Diversity}(X) = F(d_{12}, d_{13}, \dots, d_{1n}) + G(x_2, \dots, x_n),$$

that is, the first term depends only on distances from one object x_1 to all other objects, and the second term depends only on pairwise distances between the objects $x_2, \dots, x_n$. Then, such a diversity function cannot simultaneously satisfy monotonicity, uniqueness, and continuity axioms.

We prove this proposition in Appendix F. This is a negative result showing why it can be difficult to construct a proper diversity measure that is convenient for optimization. Note that, however, this proposition is only proven for the additive aggregations, thus other options are potentially possible.

NP-hard measures in practice Finally, let us note that NP-hard diversity measures can still be used in practice if a set of items that need to be evaluated is sufficiently small. For instance, if a recommender service returns a set of $k = 100$ items and we want to measure diversity of this set, then an NP-hard measure having all the desirable properties can potentially be used. Examples of diversity measures constructed in Section 5 demonstrate that there are several different options that can be used (since there are two measures that may also have variations still satisfying all the properties). We cannot rule out any of these measures based on their theoretical properties. Thus, a decision on which measure should be used may depend on a particular application.

7 CONCLUSION

In this paper, we reviewed existing diversity measures and demonstrated via intuitive examples that these measures cannot be reliably used for evaluating diversity. Based on these examples and previous research on diversity measures, we formulated three simple axioms (desirable properties) for a reliable diversity measure: monotonicity, uniqueness, and continuity. It turns out that none of the previously known measures has all these properties. We constructed two diversity measures that have all the desirable properties, thus proving that the axioms do not contradict each other. Unfortunately, the constructed examples are too computationally complex for practical use.

We leave for future research an important open problem of constructing a diversity measure that has all three desirable properties and is computationally feasible or proving that such a measure cannot exist. While our study does not answer this question, we believe that it gives some important insights into measures of diversity that are frequently used in practice. Being aware of what shortcomings a particular measure has, one can use it more wisely. For instance, we cannot advise using Energy for comparing diversities of arbitrary datasets, while it can be safely used as a target for optimization.

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A The necessity of continuity axiom

Let us give an example of a discontinuous diversity measure that has both monotonicity and uniqueness properties but still demonstrates undesirable behavior:

$$\mathrm{Diversity}(X) = \mathrm{Unique}(X) + \left(1 - e^{-\mathrm{Average}(X)}\right). \tag{4}$$

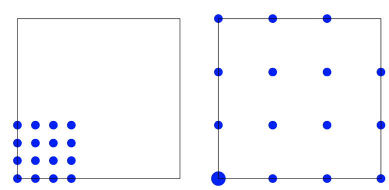
Note that the second term belongs to $[0, 1)$ and equals zero iff $\mathrm{Average}(X) = 0$.

Monotonicity Since the first term is non-strictly monotone and the second term is strictly monotone, the constructed function has the monotonicity property.

Uniqueness Suppose X has a duplicate, and we replace it with any new object not present in X. Then, the first term increases by 1 and the second term changes by less than 1, thus $\mathrm{Diversity}(X)$ increases.

Discontinuity $\mathrm{Diversity}(X)$ (4) is the sum of a discontinuous and a continuous functions and thus is discontinuous.

Undesirable behavior For any configuration, this measure assigns a higher value than to any other configuration with more duplicates. Consider two configurations of 16 points in the unit square (in the right configuration, the bottom-left angle contains 2 coinciding points). For the left configuration, the diversity value is in the interval $[16, 17)$, and for the right configuration, the diversity value is in the interval $[15, 16)$, thus the right configuration has a lower value. Since the right configuration is intuitively more diverse, we see undesirable behavior of the measure w.r.t. comparison.



B Properties of diversity measures: proofs

Let us prove the statements about what measures have what properties, which we indicate in Table 2. Note that for some of the measures, their monotonicity and uniqueness were analyzed in Velikonivtsev et al. (2024). However, since we modified these properties, we need to formally check the new ones.

Average and SumAverage Monotonicity and continuity are trivial. The complexity $O(n^2)$ is also trivial. To prove that uniqueness does not hold, consider the example from Section 3: given 16 points in a square with Euclidean distance, the maximal diversity is achieved when every angle contains 4 objects, and replacing any of these duplicates by any other object will decrease diversity.

Diameter and SumDiameter Consider a collection of three objects with pairwise distances $2, 2, 1$. Increasing distance 1 to 2 does not change the diversity value, thus proving that monotonicity does not hold. For uniqueness, consider the example from Section 3: given 16 points in a square with Euclidean distance, the maximal diversity is achieved when two opposing angles contain 8 objects each, and replacing any of these duplicates by any other object will not increase diversity. Continuity is trivial. Complexity $O(n^2)$ is also trivial.

Bottleneck and Energy(γ) Consider a collection of three objects, where x_1 and x_2 coincide, and $d_{13} = 1$. Increasing d_{13} to 2 will not change the diversity value, thus proving that monotonicity does not hold. Consider a collection of three coinciding objects. Replacing one of them with any other object does not change diversity value, thus proving that uniqueness does not hold. Continuity is trivial. Complexity $O(n^2)$ is also trivial.

SumBottleneck Consider a collection of four objects, where x_1, x_2 coincide, x_3, x_4 coincide, and $d_{13} = 1$. Increasing $d_{13} = d_{23} = d_{14} = d_{24}$ from 1 to 2 (while keeping $d_{12} = d_{34} = 0$) will not change diversity value, thus proving that monotonicity does not hold. Consider a collection of four objects, where x_1, x_2, x_3 coincide and $d_{14} = 10$. Replacing x_3 with a new object that has distance 1 to x_4 will decrease diversity from 10 to 2, thus proving that uniqueness does not hold. Continuity is trivial. Complexity $O(n^2)$ is also trivial.

#Circles(t) Consider a collection of three objects with pairwise distances $4, 3, 2$. Increasing distance 3 to 4 will not change the diversity (for any t), thus proving that monotonicity does not hold. For a given t, consider a collection of two coinciding objects. Replacing the second of them with an object at distance $\frac{t}{10}$ from the first one does not change the diversity value, thus proving that uniqueness does not hold. The lack of continuity is trivial. Let us prove that the complexity of calculating #Circles(t) is NP-hard. The problem of finding the size of the maximal complete subgraph (clique) in an unweighted undirected graph is known to be NP-hard. Consider any unweighted undirected graph G with n nodes. Construct a collection X with n objects corresponding to the nodes of G, the distance between two objects being t if the corresponding nodes are connected and $0.9t$ otherwise. Suppose we computed #Circles(t), then obviously this value is also a size of the maximal clique in G. This proves that calculating #Circles(t) is NP-hard.

Unique Monotonicity, uniqueness, and continuity are trivial. Complexity is also trivial.

To prove the results for Vendi Score, DPP, and DKE, we first need to formulate the axioms in terms of similarities. Monotonicity requires that the measure monotonically increases when some of the pairwise similarities decrease. Uniqueness is formulated in terms of objects, and two objects being duplicates means that they have the maximal similarity value. Finally, continuity can be trivially reformulated.

Vendi Score We first elaborate on the example of a violation of monotonicity from Section 3. Consider points on a circle with cosine similarity. Suppose the points x_1, x_2, x_3 are arranged on a circle in this order, the circle distance from x_1 to x_2 is 0.6 radians, the distance from x_2 to x_3 is 1.4 radians. Now we move x_3 by 0.1 away from x_1 and x_2. Let us see what similarity matrices we have before and after this move:

$$K_1 = \begin{pmatrix} 1 & \cos(0.6) & \cos(2.0) \\ \cos(0.6) & 1 & \cos(1.4) \\ \cos(2.0) & \cos(1.4) & 1 \end{pmatrix}, \quad K_2 = \begin{pmatrix} 1 & \cos(0.6) & \cos(2.1) \\ \cos(0.6) & 1 & \cos(1.5) \\ \cos(2.1) & \cos(1.5) & 1 \end{pmatrix}. \tag{5}$$

Vendi Score of K_1 is 1.941 and Vendi Score of K_2 is $1.916 < 1.941$, which is a violation of monotonicity property.

Now suppose the points x_1, x_2, x_3 are arranged on a circle in this order, the circle distance from x_1 to x_2 is 0.2 radians, the distance from x_2 to x_3 is 0.3 radians. We replace x_2 by a duplicate of x_1. Let us see what similarity matrices we have before and after this replacement:

$$K_1 = \begin{pmatrix} 1 & \cos(0.2) & \cos(0.5) \\ \cos(0.2) & 1 & \cos(0.3) \\ \cos(0.5) & \cos(0.3) & 1 \end{pmatrix}, \quad K_2 = \begin{pmatrix} 1 & 1 & \cos(0.5) \\ 1 & 1 & \cos(0.5) \\ \cos(0.5) & \cos(0.5) & 1 \end{pmatrix}. \tag{6}$$

The corresponding collections of objects differ by replacing x_2 with a copy of x_1, that is, K_1 corresponds to (x_1, x_2, x_3) and K_2 corresponds to (x_1, x_1, x_3). Vendi Score of K_1 is 1.187 and Vendi Score of K_2 is $1.233 > 1.187$, which is a violation of the uniqueness property.

Continuity holds since $\exp\left(-\sum_{i=1}^{n} \lambda_i \log(\lambda_i)\right)$ continuously depends on $\lambda_1, \ldots, \lambda_n$, which continuously depend on the similarity matrix. It is known that the complexity of finding the eigenvalues of a general (positive-semidefinite) matrix is $O(n^3)$, thus the complexity of calculating Vendi Score is also $O(n^3)$.

DPP The example of a violation of monotonicity is shown in Section 3. To obtain the matrix K_1, we can consider three points A, B, C on a unit 2D sphere with pairwise spherical distances between A and B equal to $\arccos(0.6) = 0.927$, between B and C equal to $\arccos(0.7) = 0.795$ and between

A and C equal to $\arccos(0.2) = 1.369$. The similarity is given by the cosine function. For the matrix K_2 we decrease the distance between A and C from $\arccos(0.2) = 1.369$ to $\arccos(0.3) = 1.266$, while keeping the distance between A and B unchanged, and the distance between B and C unchanged.

To prove that uniqueness is violated, consider a collection of three coinciding objects. Replacing one of them with any other object does not change the diversity value, thus proving that uniqueness is violated. Continuity is trivial. It is known that the complexity of finding the determinant of a general (positive-semidefinite) matrix is $O(n^3)$, thus the complexity of calculating $\det(S)$ is also $O(n^3)$.

RKE Monotonicity, continuity, and complexity $O(n^2)$ are trivial. To prove that uniqueness is violated, we elaborate on the example from Section 3. Consider points on a circle with cosine similarity. Suppose the points x_1, x_2, x_3 are arranged on a circle in this order, the distance from x_1 to x_2 is 1.1 radians, the distance from x_2 to x_3 is 0.4 radians. Now, we make x_2 to be a duplicate of x_3. We get the following similarity matrices before and after the modification:

$$K_1 = \begin{pmatrix} 1 & \cos(1.1) & \cos(1.5) \\ \cos(1.1) & 1 & \cos(0.4) \\ \cos(1.5) & \cos(0.4) & 1 \end{pmatrix}, \quad K_2 = \begin{pmatrix} 1 & \cos(1.5) & \cos(1.5) \\ \cos(1.5) & 1 & 1 \\ \cos(1.5) & 1 & 1 \end{pmatrix}. \tag{7}$$

The corresponding collections of objects differ by replacing x_2 with a copy of x_3, that is K_1 corresponds to (x_1, x_2, x_3) and K_2 corresponds to (x_1, x_3, x_3). RKE of K_1 is 0.564 and RKE of K_2 is $0.584 > 0.564$, which is a violation of the uniqueness property.

Species(q) Continuity and complexity $O(n^2)$ are trivial. Monotonicity is trivial for both cases $0 \le q < 1$ and $1 < q$. For violation of uniqueness, we consider the same example as for RKE. We computed Species(q) of the collection x_1, x_2, x_3 and the collection x_1, x_3, x_3 for all q in range $[0, 100]$ with step size 0.001 (excluding $q = 1$ when Species(q) is not defined). For all the considered q, the first collection gets a lower value of Species(q) than the second collection, which is a violation of the uniqueness property.

C Properties of MultiDimVolume

Let us prove that MultiDimVolume has monotonicity, uniqueness, continuity and is NP-hard to compute.

For convenience, we repeat the definition of MultiDimVolume. For a given k, $2 \le k \le n$, and a given submultiset S of size k of the multiset $X = (x_1, \dots, x_n)$, calculate the product of all pairwise distances between the elements of S. Note that this product equals zero if at least two elements of S coincide. Then, for a given k, we take the maximum of such products over all submultisets of size k of X and denote this maximum as $m_k(X)$. We define the diversity of X as $\sum_{k=2}^{n} m_k(X)$. Putting the above into one formula, we get:

$$\text{Diversity}(X) := \sum_{k=2}^{n} \max_{\substack{S \subseteq X \\ |S|=k}} \left(\prod_{\substack{x_i, x_j \in S \\ i<j}} d_{ij} \right). \tag{8}$$

Assume that we are given any distance matrix D (or, equivalently, a collection of objects X). Denote by $\bar{k}$ the maximal k such that $m_k(X)$ is non-zero. Note that by construction X includes exactly $\bar{k}$ pairwise non-coinciding objects and $m_{\bar{k}}(X)$ is the product of pairwise distances between these objects.

Monotonicity We want to prove that MultiDimVolume is strictly monotone in D. Suppose we increase the distance between two objects x_i and x_j by $\epsilon > 0$; that is, we replace d_{ij} by $d_{ij} + \epsilon$. Obviously, for every k, the value of $m_k(X)$ has not decreased. Thus, to prove monotonicity, it is sufficient to prove that at least one of $m_k(X)$ has increased. If x_i and x_j did not coincide before increasing d_{ij}, then after increasing d_{ij} the term $m_{\bar{k}}(X)$ has increased since d_{ij} is one of the multipliers in $m_{\bar{k}}(X)$. If x_i and x_j has coincided before increasing d_{ij}, then after increasing d_{ij} the collection X includes exactly $\bar{k}+1$ non-coinciding objects, and $m_{\bar{k}+1}(X)$ has increased from 0 to some positive value.

Note that for some matrices D we cannot increase only one distance. For instance, if the objects x_1, x_2, x_3 coincide and we increase d_{12} by ϵ, we also need to simultaneously increase d_{13} or d_{23}, otherwise we have $d_{13} = d_{23} = 0, d_{12} > 0$, which implies that x_1 coincides with x_3 and x_2 coincides with x_3, but x_1 and x_2 do not coincide. Clearly, the proof above easily generalizes to the case when we increase several distances simultaneously.

Uniqueness Suppose X includes at least one duplicate. We replace this duplicate with some new object that was not present in X. Then, $m_{\bar{k}+1}(X)$ has increased from 0 to some positive value. Also, for any $k \le \bar{k}$, the values of $m_k(X)$ have not decreased. Thus, $\mathrm{Diversity}(X)$ has increased.

Continuity Note that MultiDimVolume is a composition of product, maximum, and sum that are all continuous functions. A composition of continuous functions is continuous. Thus, MultiDimVolume is continuous.

NP-hard Let us first prove that finding $m_k(X)$ for all k is NP-hard. The problem of finding the size of the maximal complete subgraph (clique) in an unweighted undirected graph is known to be NP-hard. Consider any unweighted undirected graph G with n nodes. Construct a collection X with n objects corresponding to the nodes of G, the distance between two objects being 3 if the corresponding nodes are connected and 2 otherwise. Suppose we computed $m_k(X)$ for all k. Take maximal k such that $m_k(X) = 3^{\frac{k(k-1)}{2}}$. Then k is the size of the maximal clique in G, which concludes the proof.

Although we proved that finding $m_k(X)$ for all k is NP-hard, it does not directly imply that computing MultiDimVolume is NP-hard. Indeed, maybe we can compute MultiDimVolume without directly computing $m_k(X)$ for all k. Let us give a sketch of how to avoid this technical obstacle.

As above, consider a graph X for which we want to find the size of the maximal clique. Construct a collection X with n objects corresponding to the nodes of G, the distance between two objects being $2+\epsilon$ if the corresponding nodes are connected and 2 otherwise, where $\epsilon > 0$ is a small number (we will specify later how small it should be). Consider $m_k(X)$ for some k. It is a product of pairwise distances between some k objects of X. Denote by $0 \le r_k \le \frac{k(k-1)}{2}$ the number of their pairwise distances which are equal to $2+\epsilon$ (so, the remaining $\frac{k(k-1)}{2} - r_k$ distances are equal to 2). This is equivalent to saying that:

$$m_k(X) = (2+\epsilon)^{r_k} 2^{\frac{k(k-1)}{2} - r_k} = 2^{\frac{k(k-1)}{2}} + \epsilon r_k 2^{\frac{k(k-1)}{2}-1} + O\left(\epsilon^2\right).$$

Therefore,

$$\mathrm{Diversity}(X) = \sum_{k=2}^{n} m_k(X) = \left(\sum_{k=2}^{n} 2^{\frac{k(k-1)}{2}}\right) + \epsilon \sum_{k=2}^{n} r_k 2^{\frac{k(k-1)}{2}-1} + O\left(\epsilon^2\right).$$

Note that for a given n, the value of ϵ can be chosen sufficiently small so that the last term $O(\epsilon^2)$ is negligibly small compared to the other two terms.

Now suppose we know $\mathrm{Diversity}(X)$. We also know the term $\sum\limits_{k=2}^{n} 2^{\frac{k(k-1)}{2}}$ and we know ϵ. Thus, we can compute $\sum\limits_{k=2}^{n} r_k 2^{\frac{k(k-1)}{2}-1}$.

We claim that knowing the value $M = \sum\limits_{k=2}^{n} r_k 2^{\frac{k(k-1)}{2}-1}$ we can recover $r_2, r_3, \ldots, r_n$. For this, we note that for any $k = 3, \ldots, n$:

$$2^{\frac{k(k-1)}{2}-1} > \sum_{i=2}^{k-1} \frac{i(i-1)}{2} \cdot 2^{\frac{i(i-1)}{2}-1}. \tag{9}$$

Indeed, this holds for $k = 3$ and it is easy to check that the left-hand side of the inequality grows faster than the right-hand side.

Now, consider $k = n$ and note that the left-hand side of (9) is equal to how much the value of M changes if we change r_n by 1. In turn, the right-hand side of (9) is the upper bound on the sum of all other terms in M. Thus, knowing M we can find the value r_n as the maximum integer number such that $r_n 2^{\frac{k(k-1)}{2}-1} \le M$. After we found r_n, we get rid of the term $r_n 2^{\frac{n(n-1)}{2}-1}$ and can do the same reasoning to find r_{n-1}, and continue until we found all $r_2, \dots, r_n$. After that, we take the maximal k such that $r_k = \frac{k(k-1)}{2}$, this is the size of the maximal clique in G, which concludes the proof.

D Properties of IntegralMaxClique

Let us prove that IntegralMaxClique has monotonicity, uniqueness, continuity and is NP-hard to compute.

For convenience, we repeat the definition of IntegralMaxClique. For a given threshold $t \ge 0$, we construct the following graph. The nodes are $x_1, \dots, x_n$. Two nodes x_i and x_j are connected by an edge iff $d_{ij} \ge t$, and we assign d_{ij} as a weight of this edge. We find a clique (complete subgraph) in this graph with the maximal number of nodes. If there are several such cliques, we pick the one with the maximal total weight of edges. For the chosen clique, we calculate the total weight of its edges and denote it by $w_t(X)$. Then, we define diversity as

$$\mathrm{Diversity}(X) := \int_0^{+\infty} w_t(X)\, dt. \tag{10}$$

Assume that we are given any distance matrix D (or, equivalently, a collection of objects X). Denote by $\bar{d}$ the lowest non-zero pairwise distance between the objects of X. If all pairwise distances are 0, then monotonicity is trivial, so we can assume $\bar{d} > 0$. Note that for $t \le \bar{d}$, the value of $w_t(X)$ is the sum of pairwise distances between all pairwise non-coinciding elements of X.

Monotonicity Assume that we increase the distance between two objects x_i and x_j by $\epsilon > 0$, that is, we replace d_{ij} by $d_{ij} + \epsilon$. Obviously, for every t, the value of $w_t(X)$ has not decreased. If $d_{ij} > 0$, then for all $t \le \bar{d}$ the term d_{ij} is a summand in $w_t(X)$, thus for every $t \le \bar{d}$ the value of $w_t(X)$ has increased at least by ϵ. Therefore, $\mathrm{Diversity}(X)$ has increased by at least $\bar{d}\epsilon$. If $d_{ij} = 0$, then for all $t \le \epsilon$, the value of $w_t(X)$ has increased by at least ϵ (since a new element is added to the maximal clique). Thus, $\mathrm{Diversity}(X)$ has increased by at least ϵ^2.

As for MultiDimVolume, the proof above easily generalizes to the case when we increase several distances simultaneously.

Uniqueness Suppose X includes at least one duplicate. We replace this duplicate with some new object which was not present in X. Suppose the distance from the new object to the nearest object is $r > 0$. Then, for $t \le r$, the value of $w_t(X)$ has increased by at least r, and for every $t > r$, the value of $w_t(X)$ has not decreased. Thus, $\mathrm{Diversity}(X)$ has increased by at least r^2.

Continuity Assume that we increase the distance between two objects x_i and x_j by $\epsilon > 0$, that is, we replace d_{ij} by $d_{ij} + \epsilon$. Let us see how much $\mathrm{Diversity}(X)$ could change. Obviously, for every t, the value of $w_t(X)$ has not decreased. Let us estimate how much $\mathrm{Diversity}(X)$ could increase. We decompose the integral into three parts:

$$\mathrm{Diversity}(X) := \int_0^{+\infty} w_t(X)\, dt = \int_0^{d_{ij}} w_t(X)\, dt + \int_{d_{ij}}^{d_{ij}+\epsilon} w_t(X)\, dt + \int_{d_{ij}+\epsilon}^{+\infty} w_t(X)\, dt. \tag{11}$$

It is easy to prove that for $t \le d_{ij}$, the value of $w_t(X)$ could increase at most by ϵ, thus the first part could increase at most by ϵd_{ij} (since we integrate from 0 to d_{ij}). For the second term, we note that $w_t(X)$ is bounded from above by $\left(\sum_{k<l} d_{kl}\right) + \epsilon$, thus the second term is bounded by $\epsilon \left(\sum_{k<l} d_{kl}\right) + \epsilon^2$ and could increase by at most this value. The third term does not change since for $t > d_{ij} + \epsilon$ the value of $w_t(X)$ does not change.

Therefore, $\text{Diversity}(X)$ has increased by at most $\epsilon d_{ij} + \epsilon \left(\sum_{k<l} d_{kl} \right) + \epsilon^2$. So, if we increase d_{ij} by ϵ, then $\text{Diversity}(X)$ increases by at most ϵc, where c is some constant independent of ϵ (given that $\epsilon < 1$, so the term ϵ^2 is bounded by ϵ). From this, the continuity follows.

NP-hard The problem of finding the size of the maximal complete subgraph (clique) in an unweighted undirected graph is known to be NP-hard. Consider any unweighted undirected graph G with n nodes. Construct a collection X with n objects corresponding to the nodes of G, the distance between two objects being 3 if the corresponding nodes are connected and 2 otherwise. Suppose we computed $\text{Diversity}(X)$. Let us show how to find the size of the maximal clique in G. Note that for $t \le 2$, the value of $w_t(X)$ is the sum of all pairwise distances in X, that is, $\sum_{k<l} d_{kl}$ (which can be computed in $O(n^2)$ time). For $2 < t \le 3$, the value of $w_t(X)$ is $3\frac{s(s-1)}{2}$, where s is the size of the maximal clique in G. For $t > 3$, the value of $w_t(X)$ is 0. So, we get $\text{Diversity}(X) = 2\sum_{k<l} d_{kl} + 3\frac{s(s-1)}{2}$, from which we can find s in constant time. Thus, once we know $\text{Diversity}(X)$, we can find s in $O(n^2)$ time. This proves that calculating $\text{Diversity}(X)$ is NP-hard.

E PROOF OF PROPOSITION 6.1

Let us first recall the statement of the proposition. Suppose a diversity function has uniqueness and continuity. Let $x_1, \ldots, x_k$ be a set of k pairwise different objects. Let C be a multiset of $n - k$ objects, each of which coincides with one of $x_1, \ldots, x_k$. Then, diversity of the multiset $\{x_1, \ldots, x_k\} \cup C$ is the same for all such C.

Consider the following lemma.

Lemma E.1. *Suppose a diversity function has uniqueness and continuity. Let $x_1, \ldots, x_{n-1}$ be any collection of $n-1$ objects. We denote by A_1 the collection of n objects $x_1, \ldots, x_{n-1}, x_1$ and by A_2 the collection of n objects $x_1, \ldots, x_{n-1}, x_2$ (note that A_1 and A_2 differ only by the last object). Then,* $\text{Diversity}(A_1) = \text{Diversity}(A_2)$.

Informally, this lemma says that we can remove the duplicate of x_1 and add the duplicate of x_2 without changing the value of the diversity function. The proposition trivially follows from this lemma, so it is sufficient to prove it.

W.l.o.g., assume that $\text{Diversity}(A_1) - \text{Diversity}(A_2) = \epsilon > 0$. Denote by A_2' the following collection: take A_2 and increase the distance from the last object to all objects by small $\delta > 0$ in such a way that diversity changes by less than $\frac{\epsilon}{2}$ (note that the last object is no longer a duplicate). By continuity it is possible. Then, $\text{Diversity}(A_2')$ is less than $\text{Diversity}(A_2) + \frac{\epsilon}{2}$. Thus, $\text{Diversity}(A_2') < \text{Diversity}(A_1)$. However, by uniqueness, we have $\text{Diversity}(A_2') > \text{Diversity}(A_1)$ since the last object of A_2' is not a duplicate, and the last object of A_1 is a duplicate. So, we get a contradiction which concludes the proof of the lemma.

F PROOF OF PROPOSITION 6.2

We need to prove that a diversity function satisfying all the axioms cannot be decomposed in the following form:

$$\text{Diversity}(X) = F(d_{12}, d_{13}, \ldots, d_{1n}) + G(x_2, \ldots, x_n).$$

Suppose we increase d_{12} (and d_{21}) by some Δ. Then, diversity will increase by the following value:

$$F(d_{12} + \Delta, d_{13}, \ldots, d_{1n}) + G(x_2, \ldots, x_n) - F(d_{12}, d_{13}, \ldots, d_{1n}) - G(x_2, \ldots, x_n) = \\ = F(d_{12} + \Delta, d_{13}, \ldots, d_{1n}) - F(d_{12}, d_{13}, \ldots, d_{1n}). \quad (12)$$

Note that by permutation invariance we can decompose $\text{Diversity}(X)$ based not on x_1, but on x_2:

$$\text{Diversity}(X) = F(d_{21}, d_{23}, \ldots, d_{2n}) + G(x_1, x_3, \ldots, x_n). \quad (13)$$

Using this decomposition, we see that when we increase d_{12} (and d_{21}) by Δ, the diversity increases by the following value:

$$F(d_{21}+\Delta, d_{23}, \ldots, d_{2n}) + G(x_1, x_3, \ldots, x_n) - F(d_{21}, d_{23}, \ldots, d_{2n}) - G(x_1, x_3, \ldots, x_n) = \\ = F(d_{21}+\Delta, d_{23}, \ldots, d_{2n}) - F(d_{21}, d_{23}, \ldots, d_{2n}) \quad (14)$$

Combining the results of (13) and (14), we get:

$$F(d_{12}+\Delta, d_{13}, \ldots, d_{1n}) - F(d_{12}, d_{13}, \ldots, d_{1n}) = F(d_{21}+\Delta, d_{23}, \ldots, d_{2n}) - F(d_{21}, d_{23}, \ldots, d_{2n}).$$

Note that the left part depends on $d_{13}, \ldots, d_{1n}$, while the right part does not depend on these variables. Similarly, the right part depends on $d_{23}, \ldots, d_{2n}$, while the left part does not depend on these variables. This means that both parts actually do not depend on any of $d_{13}, \ldots, d_{1n}$ and $d_{23}, \ldots, d_{2n}$, so they depend only on d_{12} (or d_{21}, which is the same) and Δ. Thus, we proved that if we increase d_{12} by Δ, the diversity changes by some value that depends only on d_{12} and Δ and does not depend on other pairwise distances. By permutation invariance, for any d_{ij} the analogous statement is true. From these statements, it easily follows that

$$\text{Diversity}(X) = h(d_{12}) + h(d_{13}) + \ldots = \sum_{i<j}^{n} h(d_{ij}),$$

where we have the same function h applied to all distances by permutation invariance.

Consider the following collection: the first $n-1$ objects are duplicates of one element, and the last object is at distance 1 from them. So, there are $n-1$ pairwise distances of 1 and $\frac{(n-1)(n-2)}{2}$ distances of 0. Thus, diversity is $(n-1)h(1) + \frac{(n-1)(n-2)}{2}h(0)$. Using Proposition 6.1, we can move one of the duplicates in such a way that now it duplicates the last object, and diversity should not change. Now, there are $2(n-2)$ pairwise distances of 1, and $\frac{(n-2)(n-3)}{2} + 1$ distances of 0. Thus, diversity is $2(n-2)h(1) + \left(\frac{(n-2)(n-3)}{2} + 1\right) h(0)$. So, we get

$$(n-1)h(1) + \frac{(n-1)(n-2)}{2}h(0) = 2(n-2)h(1) + \left(\frac{(n-2)(n-3)}{2} + 1\right) h(0),$$

from which we get $(n-3)h(1) = (n-3)h(0)$, which implies $h(1) = h(0)$ (given that $n > 3$). Monotonicity implies that h is strictly monotone, which contradicts $h(1) = h(0)$, which concludes the proof.

G Comparing the measures on synthetic examples

In this section, we show how MultiDimVolume, Normalized MDV, and IntegralMaxClique work on synthetic examples shown to be difficult for other measures in Section 3. Our intuition is that in Figure 1, the diversity of Example 1 is greater than the diversity of examples 2 and 3, the diversity of Example 4 is greater than the diversity of Example 5, and the diversity of Example 6 is greater than the diversity of Example 7. We report the values of MultiDimVolume, Normalized MDV, and IntegralMaxClique in Figure 1. All three new measures correctly compare each pair of the examples mentioned above, as we report in Table 3, where we also report the results for other distance-based measures. We do not include similarity-based measures since there is no uniquely defined similarity function for the collections of points in Figure 1. We also do not report the results for #Circles(t) since they depend on the choice of t.

Table 3: Behavior of measures for examples in the Figure 1

Measure	$1 > 2$	$1 > 3$	$4 > 5$	$6 > 7$
Average	✗	✗	✓	✓
SumAverage	✗	✗	✓	✓
Diameter	✗	✗	✓	✓
SumDiameter	✗	✗	✓	✓
Bottleneck	✓	✓	✗	✗
SumBottleneck	✓	✓	✓	✗
Energy(γ), $\gamma > 0$	✓	✓	✗	✗
Unique	✓	✓	✗	✓
MultiDimVolume	✓	✓	✓	✓
Normalized MDV	✓	✓	✓	✓
IntegralMaxClique	✓	✓	✓	✓

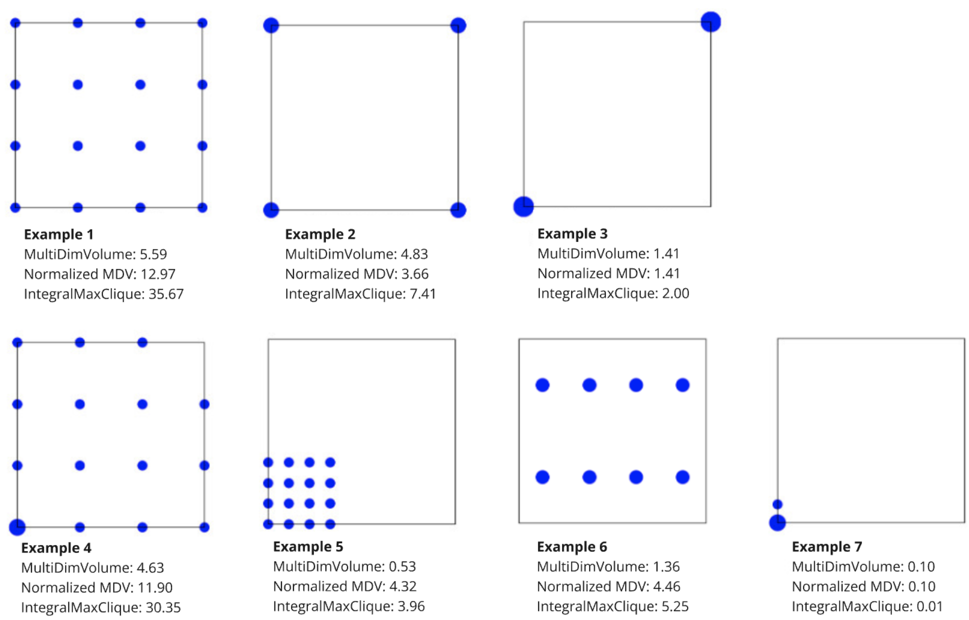


Figure 1: Values of MultiDimVolume, Normalized MDV, and IntegralMaxClique for several distributions