A new axiomatic approach to diversity

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Abstract
The topic of diversity is an interesting subject, both as a purely mathematical concept and also for its applications to important real-life situations. Unfortunately, although the meaning of diversity seems intuitively clear, no precise mathematical definition exists. In this paper, we adopt an axiomatic approach to the problem, and attempt to produce a satisfactory measure.

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1. Introduction

Over the last twenty years, an important problem in conservation biology has been how best to measure the ‘diversity’ of a set of species. This is because diversity has emerged as a leading criterion when prioritising species to be saved from extinction. The topic also has applications in a wide number of other fields, such as linguistics and economics, but in this paper we examine it as a mathematical concept.

There are two distinct challenges. The first is how to accurately evaluate the diversity of any two elements (e.g. species), and the second is how to then use these pairwise-diversities, or ‘distances’, to produce scores for sets of size greater than two. It is the latter, more mathematically interesting problem, that we address here.

Biologists and economists have produced numerous papers (see [1]–[13] and the references therein) investigating various different measures. Some of these are very simple ‘rule of thumb’ methods (e.g. minimum distance [3], maximum distance [2], average distance [12], total distance [2]), while others are more elaborate (e.g. phylogenetic diversity [4], which we shall shortly discuss, or p-median [5]). However, each of these is known to be imperfect, in that they sometimes rank sets in a counter-intuitive order.

The most popular method seems to be phylogenetic diversity (4). Given the tree-like structure of evolutionary relationships, phylogenetic diversity was
developed for the specialised case when the pairwise-diversities induce a tree-metric, with the score of a set of organisms being defined to be the length of the minimal subtree connecting them. For example, given the tree shown in Figure 1, the sets \(\{u, v, w\}\) and \(\{u, v, x\}\) score 14 and 22, respectively, and so

![Figure 1: An example of phylogenetic diversity.](image)

the latter would be considered as the more diverse.

One problem with phylogenetic diversity is that, in practice, the pairwise-diversities will often not induce a tree-metric. Moreover, even with a tree-metric, sets can still sometimes get ranked in an undesirable order. For example, in Figure 1 the set \(\{u, x, y\}\) would score more than the set \(\{u, w, y\}\) (20 compared to 19), even though \(w\) is very different from both \(u\) and \(y\), while \(x\) is very similar to \(y\). Indeed, adding \(w\) to the set \(\{u, y\}\) does not increase the phylogenetic diversity score at all, which seems strongly counter-intuitive!

It is the object of this paper to introduce a new axiomatic approach to diversity, in an attempt to produce a measure that never disagrees with intuition (furthermore, we shall only assume that the pairwise-diversities satisfy the properties of a metric, and not necessarily a tree-metric). Such an idea has already been discussed in [9] and [2], but the axioms suggested were not completely satisfactory, and hence resulted in some undesirable measures being accepted (for example, it is shown that the unique way to satisfy the axioms of [2] is to rank sets according to their maximum distance).

To avoid confusion, we should mention in passing that there are a number of papers (see, for example, [13], or [7]) in which the term ‘diversity’ is used to mean the total number of features contained by a set (e.g. the number of different books possessed by a set of libraries). Also, there is an unrelated section of the literature (see, for example, [8] or [1]) which uses the term to refer to a type of entropy. In most situations, these definitions are not consistent with the notion of diversity explored in this paper (although there have been some attempts to unify the different approaches, see e.g. [8] or [11]).

Finally, it is worth remarking that, even without the biological motivation, the question under discussion in this paper seems very natural — given two collections of points in a metric space, which is the more spread out? It seems surprising that the topic has never previously been investigated by mathematicians.
The remainder of the paper is divided into four main sections. In the first, Section 2, we propose four basic axioms that any sensible diversity measure should satisfy. In Section 3, we then present some measures that fulfill all these requirements (the first such measures ever to be produced). In Section 4, we discuss one further property that a perfect diversity measure should be expected to satisfy, and finally, in Section 5, we present a new measure that seems to have all these properties.

2. Axioms

Throughout the rest of this paper, we shall assume that we are given a complete weighted graph, where the edge-weights denote the pairwise-diversities of the vertices (this is slightly different from the tree-like structure of Figure 1). We will henceforth refer to these pairwise-diversities as ‘distances’, and we shall assume that they satisfy the properties of a metric. Our aim is to construct a way to use these distances to give a score for the overall diversity of any subset of our collection of vertices. To that end, we will spend this section proposing four axioms that any satisfactory diversity measure, $D$, should satisfy.

We start with three properties that are hoped to be intuitively natural:

**Axiom 1.** For any non-empty set of vertices $S$, we have $D(S \cup \{x\}) \geq D(S)$ for all $x$, with equality if and only if $x \in S$.

**Axiom 2.** For any two vertex-sets $S = \{s_1, s_2, \ldots, s_n\}$ and $T = \{t_1, t_2, \ldots, t_n\}$ satisfying $D(\{t_i, t_j\}) \geq D(\{s_i, s_j\})$ for all $i$ and $j$, we have $D(T) \geq D(S)$, with equality if and only if $D(\{t_i, t_j\}) = D(\{s_i, s_j\})$ for all $i$ and $j$.

**Axiom 3.** Continuity. Given any set of vertices $S = \{s_1, s_2, \ldots, s_n\}$ and any $\epsilon > 0$, there exists a $\delta(S, \epsilon) > 0$ such that, for any set of vertices $T = \{t_1, t_2, \ldots, t_n\}$ satisfying $|D(\{t_i, t_j\}) - D(\{s_i, s_j\})| < \delta$ for all $i$ and $j$, we have $|D(T) - D(S)| < \epsilon$.

It is worth observing that two other desirable properties follow automatically from these axioms. First, note that Axiom 1 implies $D(\{x\}) = 0$ for all $x$.

**Corollary 1.** $D(\{x\}) = 0$ for all $x$.

Secondly, it follows from applying Axiom 3 to the sets $S = \{s_1, s_2, \ldots, s_n, s_n\}$ and $T = \{s_1, s_2, \ldots, s_n, x\}$ (and using the triangle inequality) that we have continuity when adding a new vertex:

**Corollary 2.** Given a set of vertices $S = \{s_1, s_2, \ldots, s_n\}$ and an $\epsilon > 0$, there exists a $\delta(S, \epsilon) > 0$ such that, for any vertex $x$ satisfying $D(\{x, s_n\}) < \delta$, we have $D(S \cup \{x\}) < D(S) + \epsilon$. 

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Our fourth axiom is motivated by the principle that consistent results ought to be obtained regardless of differences in the scale used to measure the original distances. For example, if we wish to compare the diversity of the locations of stars in two different galaxies, then the resultant ranking should not depend on whether the distances were measured in light-years or kilometres. In other words, multiplying all our original distances by some constant $c$ should not affect whether or not $D(S) > D(T)$ for any sets $S$ and $T$:

**Axiom 4.** Scaling. *Given four sets of vertices $S = \{s_1, s_2, \ldots, s_n\}$, $S' = \{s'_1, s'_2, \ldots, s'_n\}$, $T = \{t_1, t_2, \ldots, t_k\}$ and $T' = \{t'_1, t'_2, \ldots, t'_k\}$, if $D(\{s_i, s_j\}) = cD(\{s'_i, s'_j\})$ for all $i$ and $j$ and $D(\{t_i, t_j\}) = cD(\{t'_i, t'_j\})$ for all $i$ and $j$, for some constant $c > 0$, then $D(S') > D(T')$ if and only if $D(S) > D(T)$.*

By considering the case when $|T| = 2$, this implies the following:

**Corollary 3.** *Given two sets $S = \{s_1, s_2, \ldots, s_n\}$ and $S' = \{s'_1, s'_2, \ldots, s'_n\}$, if $D(\{s'_i, s'_j\}) = cD(\{s_i, s_j\})$ for all $i$ and $j$, for some constant $c > 0$, then $D(S') = cD(S)$.*

There is also an ‘equidistance’ axiom that we will discuss (extensively) in Section 4.

Note that it is implicit in our whole approach that the diversity score ought to be a function only of the distances. While this is certainly sensible if the vertices represent points in Euclidean space, since the set of distances uniquely defines the set of points (up to translations, rotations and reflections), it is perhaps less clear for some other scenarios.

For example, consider the points $u, v, w, x, y$ shown in Table 1 and suppose that we wish to choose one new vertex, either $x$ or $y$, to add to the set $\{u, v, w\}$. Since $x$ and $y$ both have (Hamming) distance exactly 2 from all the other points, it is automatic with our approach that they would be considered as equally good, i.e. the diversity of the set $\{u, v, w, x\}$ would equal the diversity of the set $\{u, v, w, y\}$. However, since these two sets have fundamental differences (one is four-dimensional and one is three-dimensional), it could be argued that forcing their diversity scores to be equal is, while hardly ridiculous, rather heavy-handed. Nevertheless, we shall turn a blind eye to such objections, as it is difficult to know how to proceed otherwise.

| Points | Co-ordinates |
|--------|-------------|
| $u$    | 1 0 0 0     |
| $v$    | 0 1 0 0     |
| $w$    | 0 0 1 0     |
| $x$    | 0 0 0 1     |
| $y$    | 1 1 1 0     |

Table 1: A selection of points on a four-dimensional cube.
3. New diversity measures

In the previous section, we proposed four axioms that any diversity measure should satisfy. Although the problem seems fairly natural, it is surprisingly difficult to construct a measure that fulfills all these requirements (indeed, every method suggested in the existing literature fails either Axiom 1 or Axiom 2). However, in this section we shall now present a simple system for obtaining measures that do satisfy all four axioms. This is not the end of the story, though, and in Section 4 we shall argue that these measures are still not satisfactory.

Given a real-valued function \( f \), let us define the measure \( D_f \) recursively (from our given distances) by using the equation

\[
D_f(S) = f(S) + \max_{T \subset S, |T| = |S| - 1} \{ D_f(T) \}
\]

for all vertex-sets \( S \) of size greater than two. Let us call the function \( f \) suitable if: (a) \( f \) is a continuous function of the distances; (b) if any of the distances are 0, then \( f = 0 \); (c) if none of the distances are 0, then \( f \) is strictly positive and is a monotonically strictly increasing function of the distances; and (d) \( f \) is ‘scale-invariant’ in the sense of Axiom 4. For example, we could choose \( f(\{s_1, s_2, \ldots, s_n\}) \) to be \( \left( \prod_{1 \leq i < j \leq n} D(\{s_i, s_j\}) \right)^{1/2} \) or \( \left( \sum_{1 \leq i < j \leq n} \frac{1}{D(\{s_i, s_j\})} \right)^{-1} \), or any linear combination of these. We will now see that \( D_f \) satisfies the axioms if \( f \) is suitable:

**Theorem 4.** The diversity measure \( D_f \) defined in equation (1) satisfies Axioms 1–4 if the function \( f \) is suitable.

**Proof** It is immediately clear by induction that \( D_f \) satisfies Axioms 2–4, so it only remains to show that Axiom 1 is satisfied. To do this, we need to prove that (i) adding a vertex already in the set does not alter the score, and (ii) adding a vertex not already in the set strictly increases the score.

We shall proceed by induction. Suppose that (i) and (ii) both hold when adding a vertex to any set of size less than \( k \) (note that the base step is a direct consequence of the fact that the distances satisfy the properties of a metric), and let us now consider the case when we are adding a vertex \( s_{k+1} \) to a set \( S = \{s_1, s_2, \ldots, s_k\} \) of size exactly \( k \).

First, let us work towards (i) by supposing (without loss of generality) that \( s_{k+1} = s_k \). By part (b) of the definition of suitability, we then have \( f(S \cup \{s_{k+1}\}) = 0 \) and so \( D_f(S \cup \{s_{k+1}\}) = \max_{i \leq k+1} \{ D_f\left( (S \cup \{s_{k+1}\}) \setminus s_i \right) \} \).

Hence, it suffices to prove that \( D_f\left( (S \cup \{s_{k+1}\}) \setminus s_i \right) \) is maximised by taking \( i \in \{k, k+1\} \). But note that, for \( i < k \), the induction hypothesis implies \( D_f\left( (S \cup \{s_{k+1}\}) \setminus s_i \right) = D_f(S \setminus s_i) \leq D_f(S) \), and so we are done.

Now let us work towards (ii) by supposing that \( s_{k+1} \notin S \). If the vertices of \( S \) are all distinct, then \( f(S \cup \{s_{k+1}\}) > 0 \) and the result is clear. If not, then
let $S'$ denote a maximally sized subset of $S$ with vertices that are all distinct. By the induction hypothesis, we have $D_f(S' \cup \{s_k+1\}) > D_f(S')$. But note that, by a combination of the induction hypothesis and (i), the left-hand side is $D_f(S \cup \{s_k+1\})$ and the right-hand side is $D_f(S)$.

One particular choice for a suitable function would be to take

$$f(\{s_1, s_2, \ldots, s_n\}) = \frac{\binom{n}{2}}{\sum_{1 \leq i < j \leq n} D(\{s_i, s_j\})},$$

(2)

as this has the aesthetically pleasing property that it will always be equal to 1 for the ‘regular’ case when the distances are all 1 (and hence $D_f(S)$ will be equal to $|S| - 1$ for this case). However, this is a personal choice and is certainly not an axiom!

4. The equidistance axiom

In the previous section, we saw a scheme for generating diversity measures that satisfy Axioms 1–4. However, as briefly mentioned earlier, there is also a fifth axiom that is necessary — that of equidistance. In this section, we shall explain why such an axiom is desirable and discuss how to define it. We will start with the case when we just have graphs of order three, which we shall see only requires a small modification to our previous measures; then we will investigate a seemingly natural way to extend the concept to graphs of arbitrary order, which we shall see actually produces an intriguing contradiction; and finally we will propose a more careful definition. In Section 5, we shall then describe a pretty measure that appears to always give nice results.

Let us imagine that we have two vertices $x$ and $y$ that are distance 1 apart, and that we wish to add one more vertex to this set. Suppose that we are free to choose any element from $\{z : D(\{x, z\}) + D(\{y, z\}) = 2\}$. It seems intuitive that the overall diversity score ought to be greater the more equidistant the new vertex is between $x$ and $y$. Unfortunately, this is actually not true for the diversity measure defined at the end of the last section, where we use the suitable function of equation (2) in recursion (1), since we know that the regular unit triangle scores 2, whereas the triangle with lengths $1$, $\frac{1}{2}$ and $\frac{3}{2}$ scores $\frac{3}{2} + \max\{1, \frac{1}{2}, \frac{3}{2}\} = \frac{11}{4} + \frac{3}{2} > 2$. This example establishes the need for a new axiom:

**Axiom 5.** Three-vertex equidistance. Given two sets $S = \{s_1, s_2, s_3\}$ and $T = \{t_1, t_2, t_3\}$, if $D(t_1, t_2) = D(s_1, s_2)$ and $D(t_1, t_3) + D(t_2, t_3) = D(s_1, s_3) + D(s_2, s_3) = \lambda$, but $|D(t_1, t_3) - \frac{\lambda}{2}| < |D(s_1, s_3) - \frac{\lambda}{2}|$ (and $|D(t_2, t_3) - \frac{\lambda}{2}| < |D(s_2, s_3) - \frac{\lambda}{2}|$), then $D(T) > D(S)$.

One way to approach the problem of trying to satisfy Axiom 5 would be to find a suitable function $f$ for which the partial derivative with respect to the
maximum distance (when the total distance is fixed) is always less than −1, thus offsetting the contribution to $D_T$ of the $\max_{T \subseteq S: |T|=2} \{D(T)\}$ term.

However, a neater solution is to instead develop a separate diversity measure for sets of size three that does satisfy Axiom 5 (and also Axioms 1–4) and then simply use the recursion of equation (1) on this (it can be checked that Theorem 4 will still hold). For example, we could set

$$D(\{s_1, s_2, s_3\}) = g(\{s_1, s_2, s_3\}) + \frac{1}{2} \sum_{1 \leq i < j \leq 3} D(\{s_i, s_j\}),$$

where $g$ is any suitable function that also satisfies Axiom 5. It is simple to see that $D(\{s_1, s_2, s_3\})$ satisfies Axioms 2–5, and Axiom 1 (for the case when we are comparing sets of size three with sets of size two) follows from using the triangle inequality on the second term. An aesthetically pleasing choice, if we then use recursion (1) with the suitable function defined in equation (2), is to take $g(\{s_1, s_2, s_3\}) = 3 \left( \sum_{1 \leq i < j \leq 3} \frac{1}{D(\{s_i, s_j\})} \right)^{-1}$, so that

$$D(\{s_1, s_2, s_3\}) = \frac{3}{2} \left( \sum_{1 \leq i < j \leq 3} \frac{1}{D(\{s_i, s_j\})} \right)^{-1} + \frac{1}{2} \sum_{1 \leq i < j \leq 3} D(\{s_i, s_j\}). \quad (3)$$

Of course, we really need something more general than just the three-vertex rule of Axiom 5. For example, consider the two four-vertex sets, $S$ and $S'$, depicted in Figure 2. It seems intuitive that $S'$ should be considered as more diverse than $S$, as the position of $s'_4$ is equidistant in relation to $s_1$, $s_2$ and $s_3$. Unfortunately, the diversity measure that we have just defined gives $D(S') = 3$ and $D(S) = \frac{6}{\frac{1}{2} + 1 + 1 + 1 + 1} + D(\{s_1, s_2, s_4\}) = \frac{4}{3} + \frac{1}{\frac{1}{2} + 1 + 1} + \frac{1}{2} \left( \frac{4}{3} + \frac{1}{3} + 1 \right) = \frac{97}{30} > 3$.

One natural way to extend Axiom 5 to any number of vertices is the following:

'**Axiom** 5' Strong equidistance. Given two sets $S = \{s_1, s_2, \ldots, s_n\}$ and $T = \{t_1, t_2, \ldots, t_n\}$, if $D(t_i, t_j) = D(s_i, s_j)$ for all $i, j < n$ and $\sum_{i<j} D(t_i, t_j) = \sum_{i<j} D(s_i, s_j)$, then $D(T) = D(S)$.

Figure 2: Two four-vertex sets, $S$ and $S'$. 

1. maximum
2. $D_T$
3. $\{D(T)\}$
4. $\max_{T \subseteq S: |T|=2} \{D(T)\}$
5. $D_T$
6. $g$
7. $\{s_1, s_2, s_3\}$
8. $D(\{s_1, s_2, s_3\})$
9. $g(\{s_1, s_2, s_3\})$
10. $\frac{1}{2} \sum_{1 \leq i < j \leq 3} D(\{s_i, s_j\})$
11. $D(\{s_1, s_2, s_3\})$
12. $g(\{s_1, s_2, s_3\})$
13. $3 \left( \sum_{1 \leq i < j \leq 3} \frac{1}{D(\{s_i, s_j\})} \right)^{-1}$
14. $\frac{3}{2} \left( \sum_{1 \leq i < j \leq 3} \frac{1}{D(\{s_i, s_j\})} \right)^{-1}$
15. $\frac{1}{2} \sum_{1 \leq i < j \leq 3} D(\{s_i, s_j\})$
16. $D(\{s_1, s_2, s_3\})$
17. $\frac{3}{2} \left( \sum_{1 \leq i < j \leq 3} \frac{1}{D(\{s_i, s_j\})} \right)^{-1} + \frac{1}{2} \sum_{1 \leq i < j \leq 3} D(\{s_i, s_j\})$
18. $D(\{s_1, s_2, s_3\})$
19. $\frac{3}{2} \left( \sum_{1 \leq i < j \leq 3} \frac{1}{D(\{s_i, s_j\})} \right)^{-1}$
20. $\frac{1}{2} \sum_{1 \leq i < j \leq 3} D(\{s_i, s_j\})$
21. $D(\{s_1, s_2, s_3\})$
22. $\frac{3}{2} \left( \sum_{1 \leq i < j \leq 3} \frac{1}{D(\{s_i, s_j\})} \right)^{-1} + \frac{1}{2} \sum_{1 \leq i < j \leq 3} D(\{s_i, s_j\})$
23. $D(\{s_1, s_2, s_3\})$
24. $\frac{3}{2} \left( \sum_{1 \leq i < j \leq 3} \frac{1}{D(\{s_i, s_j\})} \right)^{-1} + \frac{1}{2} \sum_{1 \leq i < j \leq 3} D(\{s_i, s_j\})$
25. $D(\{s_1, s_2, s_3\})$
26. $\frac{3}{2} \left( \sum_{1 \leq i < j \leq 3} \frac{1}{D(\{s_i, s_j\})} \right)^{-1} + \frac{1}{2} \sum_{1 \leq i < j \leq 3} D(\{s_i, s_j\})$
27. $D(\{s_1, s_2, s_3\})$
28. $\frac{3}{2} \left( \sum_{1 \leq i < j \leq 3} \frac{1}{D(\{s_i, s_j\})} \right)^{-1} + \frac{1}{2} \sum_{1 \leq i < j \leq 3} D(\{s_i, s_j\})$
continuity (Axiom 3), there exists a set \( S \). Consider the sets constructed from \( S \) such that when we wish to add a new vertex, it perhaps does not cover all desirable situations. For example, let us now recall our original four-vertex example of Figure 2. The intuition that it was desirable for the fourth vertex to be equidistant in relation to \( s_1, s_2 \) and \( s_3 \) perhaps stems from the fact that these other three vertices were all in symmetric positions to begin with. Hence, it seems sensible that a satisfactory equidistance axiom should have to take into account such symmetry considerations (note that this was not necessary for the three-vertex case, since every set of size two is automatically symmetric).

Another fault with ‘Axiom’ 5′ is that, by only considering the case when we wish to add a new vertex, it perhaps does not cover all desirable situations. For example, consider the sets \( S \) and \( T \) shown in Figure 3. It seems intuitive that

\[
\sum_{i<n} D(s_i, s_n) = \lambda, \quad \text{but} \quad D(t_i, t_n) - \frac{\lambda}{n-1} \leq D(s_i, s_n) - \frac{\lambda}{n-1} \quad \text{for all} \quad i < n,
\]

then \( D(T) \geq D(S) \), with equality if and only if there is equality in \((*)\) for all \( i < n \).

Unfortunately, as we shall now see, it turns out that this strong version actually leads to inconsistencies with our earlier axioms!:

Theorem 5. ‘Axiom’ 5′ is inconsistent with Axioms 1–3.

Proof Let the vertex-sets \( S = \{s_1, s_2, s_3\}, T = \{t_1, t_2, t_3\} \) and \( U_n = \{u_1, u_2, u_3\} \) be as shown in Figure 3. By Axiom 2, we have \( D(S) > D(T) \) and so, by continuity (Axiom 3), there exists a \( k \) such that \( D(S) > D(U_k) \).

Now consider the set \( U'_k = \{u_1, u_2, \ldots, u_{k+2}\} \supset U_k \) constructed from \( U_k \) by setting \( D(\{u_2, u_l\}) = 0 \) for all \( l \geq 4 \) (i.e. adding in \( k - 1 \) extra copies of \( u_2 \)) and, similarly, the set \( S' = \{s_1, s_2, \ldots, s_{k+2}\} \) constructed from \( S \) by setting \( D(\{s_2, s_1\}) = 0 \) for all \( l \geq 4 \) (i.e. adding in \( k - 1 \) extra copies of \( s_2 \)).

If we assume the strong equidistance of ‘Axiom’ 5′, then \( D(U'_k) > D(S') \). But, by Axiom 1 \( D(U'_k) = D(U_k) \) and \( D(S') = D(S) \). Hence, we find that \( D(U_k) > D(S) \), and so we have a contradiction. \( \square \)

Note that (with a bit of care to ensure that the triangle inequality is not violated during the proof) a form of this example still produces a contradiction even if we alter the strong equidistance ‘axiom’ to include the condition \( D(t_i, t_n) = D(s_i, s_n) \) for all \( i \geq 3 \) as well as \( \sum_{i<n} D(t_i, t_n) = \sum_{i<n} D(s_i, s_n) \). This seems very surprising!

However, let us now recall our original four-vertex example of Figure 2. The intuition that it was desirable for the fourth vertex to be equidistant in relation to \( s_1, s_2 \) and \( s_3 \) perhaps stems from the fact that these other three vertices were all in symmetric positions to begin with. Hence, it seems sensible that a satisfactory equidistance axiom should have to take into account such symmetry considerations (note that this was not necessary for the three-vertex case, since every set of size two is automatically symmetric).

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Now consider the set \( U'_k = \{u_1, u_2, \ldots, u_{k+2}\} \supset U_k \) constructed from \( U_k \) by setting \( D(\{u_2, u_l\}) = 0 \) for all \( l \geq 4 \) (i.e. adding in \( k - 1 \) extra copies of \( u_2 \)) and, similarly, the set \( S' = \{s_1, s_2, \ldots, s_{k+2}\} \) constructed from \( S \) by setting \( D(\{s_2, s_1\}) = 0 \) for all \( l \geq 4 \) (i.e. adding in \( k - 1 \) extra copies of \( s_2 \)).

If we assume the strong equidistance of ‘Axiom’ 5′, then \( D(U'_k) > D(S') \). But, by Axiom 1 \( D(U'_k) = D(U_k) \) and \( D(S') = D(S) \). Hence, we find that \( D(U_k) > D(S) \), and so we have a contradiction. \( \square \)

Note that (with a bit of care to ensure that the triangle inequality is not violated during the proof) a form of this example still produces a contradiction even if we alter the strong equidistance ‘axiom’ to include the condition \( D(t_i, t_n) = D(s_i, s_n) \) for all \( i \geq 3 \) as well as \( \sum_{i<n} D(t_i, t_n) = \sum_{i<n} D(s_i, s_n) \). This seems very surprising!

However, let us now recall our original four-vertex example of Figure 2. The intuition that it was desirable for the fourth vertex to be equidistant in relation to \( s_1, s_2 \) and \( s_3 \) perhaps stems from the fact that these other three vertices were all in symmetric positions to begin with. Hence, it seems sensible that a satisfactory equidistance axiom should have to take into account such symmetry considerations (note that this was not necessary for the three-vertex case, since every set of size two is automatically symmetric).

Another fault with ‘Axiom’ 5′ is that, by only considering the case when we wish to add a new vertex, it perhaps does not cover all desirable situations. For example, consider the sets \( S \) and \( T \) shown in Figure 3. It seems intuitive that
$T$ should be thought of as the more diverse, since the edges $t_3t_2$ and $t_3t_4$ are in symmetric positions, but this would not have been covered by ‘Axiom’ $5$.

Hence, it seems desirable to formulate exactly what we mean by ‘symmetry’ before we attempt to propose another equidistance axiom. With this in mind, we now give two definitions:

**Definition 6.** Let $G$ be called a partial graph if it can be formed from an unlabelled edge-weighted complete graph by deleting some of the edge-weights and, instead, giving (distinct) labels to the associated edges.

For example, the graphs $G_1$ and $G_2$ shown in Figure 5 are two of the partial graphs that can be formed from (the unlabelled version of) the graph representing the set $S$ in Figure 4.

**Definition 7.** Given a partial graph $G$ whose labelled edges are $e_1, e_2, \ldots, e_k$, let us say that $e_1$ is symmetric to $e_l$ in $G$ if there exists a permutation $e_{i_1}, e_{i_2}, \ldots, e_{i_k}$ of the labels for which $i_1 = l$ and relabelling $e_j$ as $e_{i_j}$ for all $j$ does not change $G$.

For example, it can be seen that $e_1$ is symmetric to $e_2$ in $G_2$ (indeed, all edges are symmetric here) by considering the permutation shown in Figure 6. In $G_1$, however, $e_1$ and $e_2$ are not symmetric.

It can be checked that, for each partial graph, symmetry defines an equivalence relation on the labelled edges.
Now that we have defined symmetry, we will return to the issue of formulating a successful equidistance axiom. Our new version comes in two parts, the first of which we present immediately:

**Axiom 5**′′a Symmetric equidistance, part one. Let $G_S$ be an unlabelled edge-weighted complete graph representing the set $S$, and let $G_p$ be a partial graph that can be formed from $G_S$. Let us denote the equivalence classes of the labelled edges in $G_p$ by $E_1 = \{e_{11}, e_{12}, \ldots, e_{1k_1}\}$, $E_2 = \{e_{21}, e_{22}, \ldots, e_{2k_2}\}$, $E_3 = \{e_{31}, e_{32}, \ldots, e_{3k_3}\}$, and $E_l = \{e_{l1}, e_{l2}, \ldots, e_{lk_l}\}$. Now let $G_T$ be the graph formed from $G_p$ by setting $w_{G_T}(e_{ij}) = \frac{1}{k_i} \sum_{e \in E_i} w_{G_S}(e)$ for all $i$ and $j$ (i.e. averaging out the weights of all the edges in each equivalence class) and let $T$ be the set represented by $G_T$ (it can be checked that $G_T$ will satisfy the triangle inequality). Then $D(T) \geq D(S)$, with equality if and only if $T = S$.

For example, Axiom 5"a could be applied to the graphs $G_S$, $G_p$ and $G_T$ shown in Figure 7.

![Figure 6: A permutation of the edges of $G_2$.](image)

![Figure 7: An example of Axiom 5"a.](image)

It is a deliberate decision to only state Axiom 5"a for the case when the edges in each equivalence class are completely evenly weighted in $G_T$, rather than just more evenly weighted than in $G_S$, in order to take care that the axiom is not stronger than our intuition. For example, consider the sets $S$, $T$ and $T'$ depicted in Figure 8. It certainly seems reasonable to say that $T$ should be considered more diverse than $S$ (and this can be deduced by applying Axiom 5"a to the relevant four edges), but, in the light of Theorem 5, it is perhaps going too far to claim that $T'$ should also definitely be considered more diverse than $S$ (and,
indeed, this is not implied by Axiom 5′′a).

However, in the case when we are dealing with an equivalence class containing just two edges, a stronger formulation does seem desirable, and this is given in the second part of our axiom:

**Axiom 5′′b** Symmetric equidistance, part two. Let $G_S$ be an unlabelled edge-weighted complete graph representing the set $S$, and let $G_p$ be a partial graph formed from $G_S$ by deleting exactly two of the edge-weights and, instead, labelling the associated edges as $e_1$ and $e_2$. Suppose $e_1$ and $e_2$ are symmetric in $G_p$. Let us define $\lambda := w_{G_S}(e_1) + w_{G_S}(e_2)$, let $G_T$ be any graph formed from $G_p$ by setting $w_{G_T}(e_1)$ and $w_{G_T}(e_2)$ to be values satisfying $w_{G_T}(e_1) + w_{G_T}(e_2) = \lambda$ and $|w_{G_T}(e_1) - \frac{\lambda}{2}| < |w_{G_T}(e_1) - \frac{\lambda}{2}|$ (and $|w_{G_T}(e_2) - \frac{\lambda}{2}| < |w_{G_T}(e_2) - \frac{\lambda}{2}|$), and let $T$ be the set represented by $G_T$ (it can be checked that $T$ will satisfy the triangle inequality). Then $D(T) > D(S)$.

For example, Axiom 5′′b could be applied to the graphs $G_S$, $G_p$ and $G_T$ shown in Figure 9 to give $D(T) > D(S)$.

![Figure 8: A further example of Axiom 5′′a.](image)

![Figure 9: An example of Axiom 5′′b.](image)

Note that we can sometimes obtain useful results by applying Axiom 5′′b successively to different edges. For example, a second application of the axiom could have been used in the previous case to obtain $D(T') > D(S)$, where $T'$ is as depicted in Figure 10.
5. A perfect diversity measure?

In the previous section, we argued the case for a new ‘symmetric equidistance’ axiom. Unfortunately, the intricate nature of this seems to make it extremely difficult to find a satisfactory diversity measure. In particular, the measures suggested in Section 3 seem irreparably distorted by the max\{D(T)\} term, which was critical for satisfying Axiom 1. However, in this section we shall present a possible alternative that appears to give nice results without employing such an expression.

Given a set \( S = \{s_1, s_2, \ldots, s_n\} \), let \( p_{kl} = \frac{1}{\sum_{1 \leq i < j \leq n}} \frac{1}{D(s_i, s_j)} \) for all \( k \neq l \), and define \( D \) recursively by the equation

\[
D(S) = \sum_{1 \leq k < l \leq n} p_{kl} \left( D(\{s_k, s_l\}) + D(S_{kl}) \right),
\]

where \( S_{kl} \) denotes the set formed from \( S \) by ‘merging’ \( s_k \) and \( s_l \) into a new vertex \( s_{kl} \) and setting \( D(\{s_{kl}, s_i\}) = \frac{D((s_k, s_i)) + D((s_l, s_i))}{2} \) for all \( i \) (it can be checked that the distances will still satisfy the properties of a metric).

For example, consider the set \( S = \{s_1, s_2, s_3\} \) illustrated in Figure 11 for which the sets \( S_{12}, S_{13} \) and \( S_{23} \) are also depicted. Here, we would have \( p_{12} = \frac{1}{\frac{2}{13} + \frac{1}{13}} = \frac{3}{13} \) and, similarly, \( p_{13} = \frac{6}{13} \) and \( p_{23} = \frac{4}{13} \). Hence, we would obtain

\[
D(S) = \frac{3}{13} \left( 4 + \frac{2}{3} \right) + \frac{6}{13} \left( 2 + \frac{3}{2} \right) + \frac{4}{13} (3 + 3) = \frac{453}{26}.
\]

For sets of size three, this method simplifies to a nice formula:
Theorem 8. The diversity measure $D$ defined in equation (4) satisfies the formula

$$D(\{s_1, s_2, s_3\}) = \frac{3}{2} \left( \sum_{1 \leq i < j \leq 3} \frac{1}{D(\{s_i, s_j\})} \right)^{-1} + \frac{1}{2} \sum_{1 \leq i < j \leq 3} D(\{s_i, s_j\}).$$

Proof By equation (4), we have

$$D(\{s_1, s_2, s_3\}) = p_{12} \left( D(\{s_1, s_2\}) + D(\{s_1, s_3\}) + D(\{s_2, s_3\}) \right)$$

$$+ p_{13} \left( D(\{s_1, s_3\}) + D(\{s_1, s_2\}) + D(\{s_2, s_3\}) \right)$$

$$+ p_{23} \left( D(\{s_2, s_3\}) + D(\{s_1, s_2\}) + D(\{s_1, s_3\}) \right)$$

$$= p_{12} D(\{s_1, s_2\}) + \frac{p_{12}}{2} \sum_{1 \leq i < j \leq 3} D(\{s_i, s_j\})$$

$$+ p_{13} D(\{s_1, s_3\}) + \frac{p_{12}}{2} \sum_{1 \leq i < j \leq 3} D(\{s_i, s_j\})$$

$$+ p_{23} D(\{s_2, s_3\}) + \frac{p_{12}}{2} \sum_{1 \leq i < j \leq 3} D(\{s_i, s_j\})$$

$$= \frac{p_{12}}{2} D(\{s_1, s_2\}) + \frac{p_{13}}{2} D(\{s_1, s_3\}) + \frac{p_{23}}{2} D(\{s_2, s_3\})$$

$$+ \frac{1}{2} \sum_{1 \leq i < j \leq 3} D(\{s_i, s_j\}),$$

since $p_{12} + p_{13} + p_{23} = 1$

$$= \frac{3}{2} \left( \sum_{1 \leq i < j \leq 3} \frac{1}{D(\{s_i, s_j\})} \right)^{-1} + \frac{1}{2} \sum_{1 \leq i < j \leq 3} D(\{s_i, s_j\}),$$

by definition of $p_{kl}$. \qed

Note that this is the same expression as that given in equation (3) on page 7 and so this measure certainly satisfies all the axioms when a set has size three.

The equations produced for larger sets are much more complicated, and hence more difficult to analyse, but the method appears to always give nice results. For example, with the sets depicted in Figure 2 on page 7 we would obtain

$$D(S) = \frac{1}{15/2} (1 + D(S_{12})) + \frac{1}{15/2} (1 + D(S_{13})) + \frac{3/4}{15/2} \left( \frac{4}{3} + D(S_{14}) \right)$$

$$+ \frac{1}{15/2} (1 + D(S_{23})) + \frac{3/4}{15/2} \left( \frac{4}{3} + D(S_{24}) \right) + \frac{3}{15/2} \left( \frac{1}{3} + D(S_{34}) \right),$$

where $S_{12}, S_{13}, S_{14}, S_{23}, S_{24}$ and $S_{34}$ are as shown in Figure 12.
\[
\frac{2}{15} \left( 1 + \frac{3}{2} \left( \frac{19}{4} \right)^{-1} + \frac{1}{2} \cdot \frac{8}{3} \right) + \frac{2}{15} \left( 1 + \frac{3}{2} \left( \frac{59}{20} \right)^{-1} + \frac{1}{2} \cdot \frac{19}{6} \right) \\
+ \frac{1}{10} \left( \frac{4}{3} + \frac{3}{2} \left( \frac{47}{14} \right)^{-1} + \frac{1}{2} \cdot \frac{17}{6} \right) + \frac{2}{15} \left( 1 + \frac{3}{2} \left( \frac{59}{20} \right)^{-1} + \frac{1}{2} \cdot \frac{19}{6} \right) \\
+ \frac{1}{10} \left( \frac{4}{3} + \frac{3}{2} \left( \frac{47}{14} \right)^{-1} + \frac{1}{2} \cdot \frac{17}{6} \right) + \frac{2}{5} \left( \frac{1}{3} + \frac{3}{2} \left( \frac{19}{7} \right)^{-1} + \frac{1}{2} \cdot \frac{10}{3} \right),
\]
using Theorem \(8\)

\[\approx 2.838,\]

whereas it is simple to see (by induction) that \(D(S') = 3 > D(S)\), as required.

![Diagram](image.png)

Figure 12: The ‘merged’ sets \(S_12, S_13, S_14, S_23, S_24\) and \(S_34\).

by Axiom \(5''a\).

Unfortunately, it seems difficult to prove that the measure always satisfies Axioms 1 and 2, let alone the new equidistance axioms. All experimental results have been positive, however, and so it is very much hoped that other mathematicians will explore this measure further.

6. Concluding remarks

Although many of the properties required of a sensible diversity measure seem simple, we have seen that it is not easy to produce one. In particular, the requirement for such a measure to take into account complicated symmetry considerations (and the fact that it is not obvious precisely what these should be) seems to make the problem rather difficult. Nevertheless, it is hoped that the ideas presented in this paper have gone some way towards building a rigorous framework for diversity, and developing a measure that is truly satisfactory.
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