The magnitude of graphs and finite metric spaces

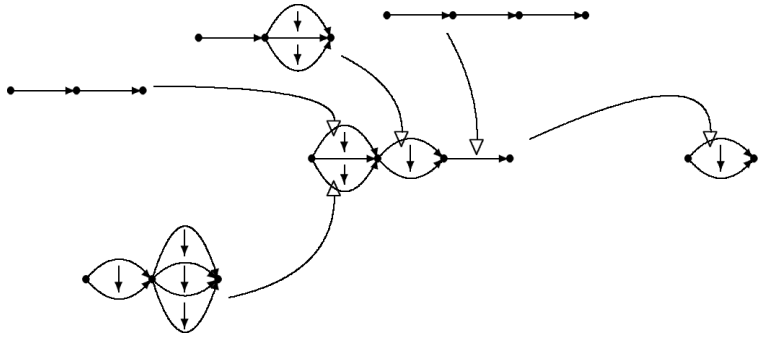
Tom Leinster

Edinburgh

Why am I here?

My PhD thesis was on higher category theory.

(Not the reason I'm here.)



My only qualification in life sciences is an ITEC certificate in Anatomy, Physiology and Body Massage.

(Definitely not the reason I'm here.)

A little of my work has been in ecology; we'll come back to this.

(Not really the reason I'm here.)

Plan

1. Background
2. The magnitude of a finite set of points
3. Diversity
4. The magnitude of a graph
5. The future: magnitude homology

1. Background

Size

For many types of mathematical object, there is a canonical notion of size.

- Sets have cardinality. It satisfies

$$|A \cup B| = |A| + |B| - |A \cap B|$$
$$|A \times B| = |A| \times |B|\,.$$

- Subsets of $\mathbb{R}^n$ have volume. It satisfies

$$\mathrm{vol}(A \cup B) = \mathrm{vol}(A) + \mathrm{vol}(B) - \mathrm{vol}(A \cap B)$$
$$\mathrm{vol}(A \times B) = \mathrm{vol}(A) \times \mathrm{vol}(B).$$

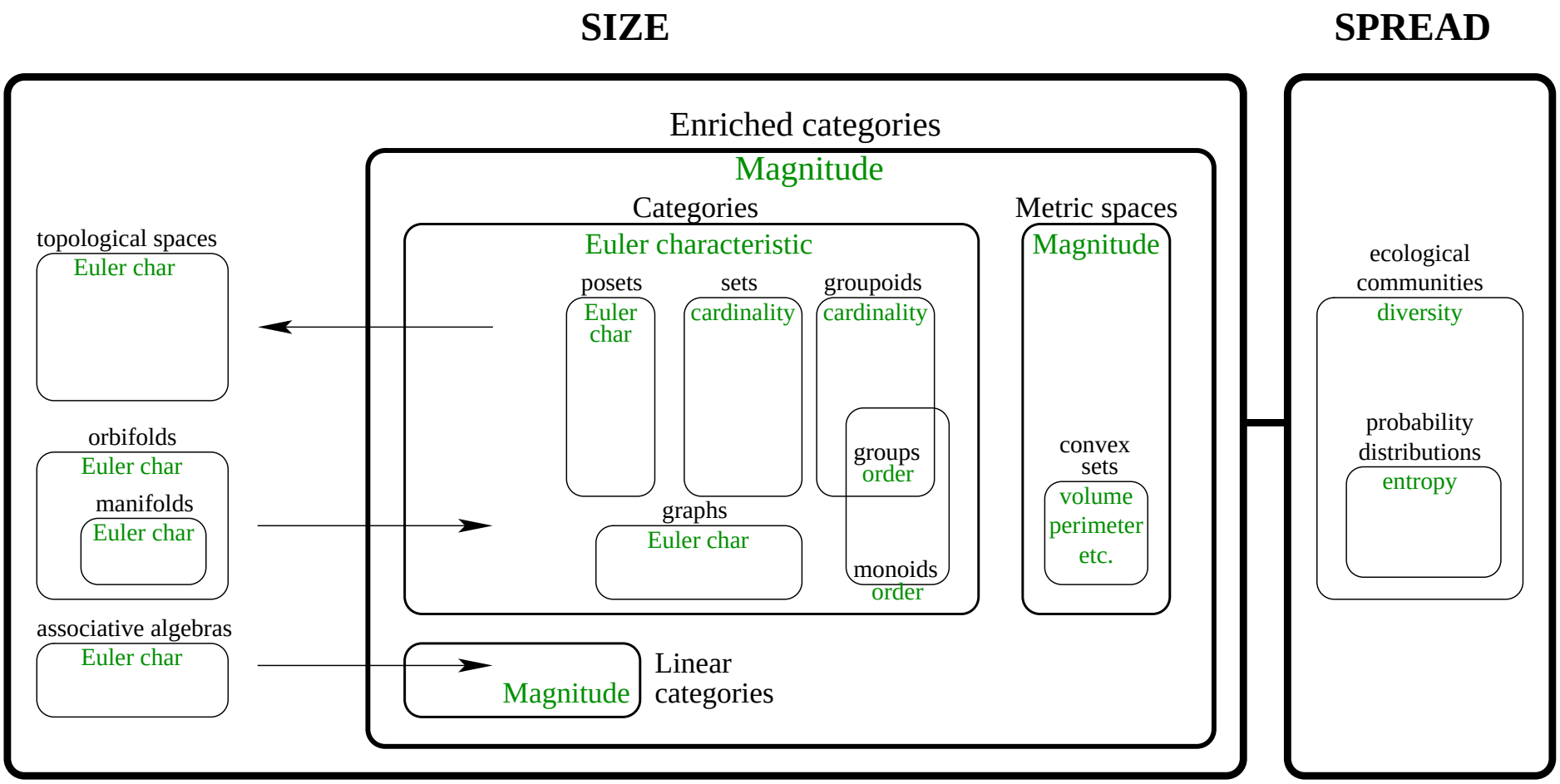
- Topological spaces have Euler characteristic. It satisfies

$$\chi(A \cup B) = \chi(A) + \chi(B) - \chi(A \cap B) \quad \text{(under hypotheses)}$$
$$\chi(A \times B) = \chi(A) \times \chi(B).$$

Challenge Find a general definition of 'size', including these and other examples.

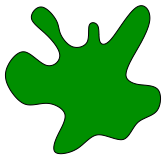
One answer The magnitude of an "enriched category".

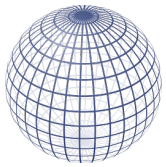
The wide world of magnitude



The magnitude of a compact metric space

Let A be a compact metric space, e.g. a closed bounded subset of $\mathbb{R}^n$.





The magnitude $|A|$ of A is a real number measuring the 'size' of A. (Definition later.)

Olaf, yesterday: 'There is no privileged scale!' So...

Given $t > 0$, write tA for A scaled up by a factor of t.

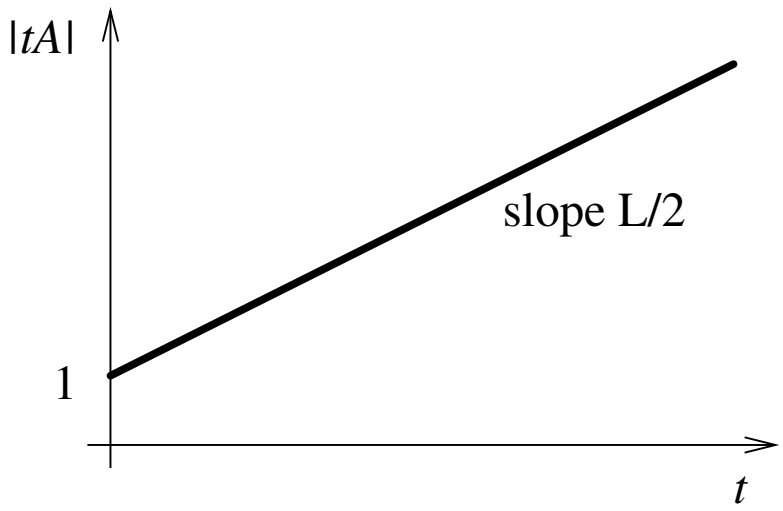
The magnitude function of A is the function $t \mapsto |tA|$.

Thus, magnitude assigns to each space not just a *number*, but a *function*.

The magnitude of a line segment

Example: Let A be a straight line of length L.

The magnitude function of A is



$$t \mapsto |tA| = \boxed{1} + \tfrac{1}{2}\boxed{L} \cdot t^{\boxed{1}}$$

Euler characteristic

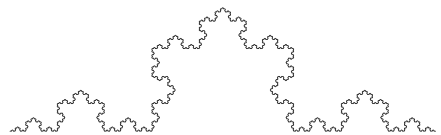
length

dimension

The magnitude of a compact metric space: theorems

Let A be a compact subset of $\mathbb{R}^n$.

Theorem (Meckes) *The asymptotic growth rate of $|tA|$ as $t \to \infty$ is the Minkowski dimension of A.*

E.g. $\left| t$  $\right|$ grows like t^2 and $\left| t$  $\right|$ grows like $t^{1.261\ldots}$, for large t.

Theorem (Barceló and Carbery; Gimperlein and Goffeng) *Under technical hypotheses,*

$$|tA| = c_n \operatorname{vol}_n(A) \cdot t^n + c_{n-1} \operatorname{vol}_{n-1}(\partial A) \cdot t^{n-1} + O(t^{n-2})$$

as $t \to \infty$, where c_n and c_{n-1} are known constants.

E.g. If $n = 3$ then $\operatorname{vol}_n(A)$ and $\operatorname{vol}_{n-1}(\partial A)$ are the volume and surface area of A.

So: if you know the magnitude function of a space, you know its dimension, volume and surface area.

The magnitude of a compact metric space: theorems

Theorem (Willerton) *Let A be a homogeneous Riemannian n-manifold. Then*

$$|tA| = C_n \operatorname{vol}_n(A) \cdot t^n + C_{n-2} \operatorname{TotalScalarCurvature}(A) \cdot t^{n-2} + O(t^{n-4})$$

as $t \to \infty$, where C_n and C_{n-2} are known constants. In particular, when $n = 2$,

$$|tA| = \tfrac{1}{2\pi} \operatorname{area}(A) \cdot t^2 + \chi(A) + O(t^{-2}).$$

Theorem (Barceló and Carbery) *The magnitude of an odd-dimensional Euclidean ball is a rational function of its radius. Specifically:*

$$|tB^1| = 1 + t,$$

$$|tB^3| = \frac{1}{3!}(6 + 12t + 6t^2 + t^3),$$

$$|tB^5| = \frac{1}{5!} \frac{360 + 1080t + 525t^2 + 135t^4 + 18t^5 + t^6}{3 + t}.$$

The moral

For geometrically interesting subsets of $\mathbb{R}^n$, the magnitude function conveys geometrically interesting information.

(Despite—or because of?—its very general, abstract categorical origins.)

What information does the magnitude function contain for *finite* sets of points?

2. The magnitude of a finite set of points

The definition

Let A be a finite metric space with points $1, \dots, n$ and distance d_{ij} from point i to point j.

Write $Z_A = Z$ for the $n \times n$ matrix with entries

$$Z_{ij} = e^{-d_{ij}}.$$

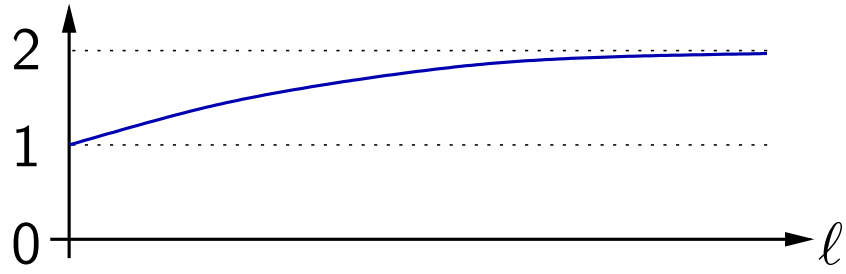
Assuming Z is invertible (which it usually is), the magnitude of A is

$$|A| = \sum_{i,j} (Z^{-1})_{ij}$$

—the sum of all n^2 entries of Z^{-1}.

First examples

- $|\emptyset| = 0$.
- $|\bullet| = 1$.
- $|\bullet \overset{\leftarrow \ell \ \rightarrow}{} \bullet| =$ sum of entries of $\begin{pmatrix} e^{-0} & e^{-\ell} \\ e^{-\ell} & e^{-0} \end{pmatrix}^{-1} = \dfrac{2}{1+e^{-\ell}}$.



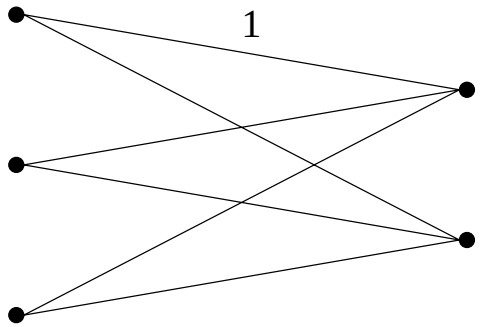
- If $d(i,j) = \infty$ for all $i \neq j$ then $|A| = n$ (number of points).

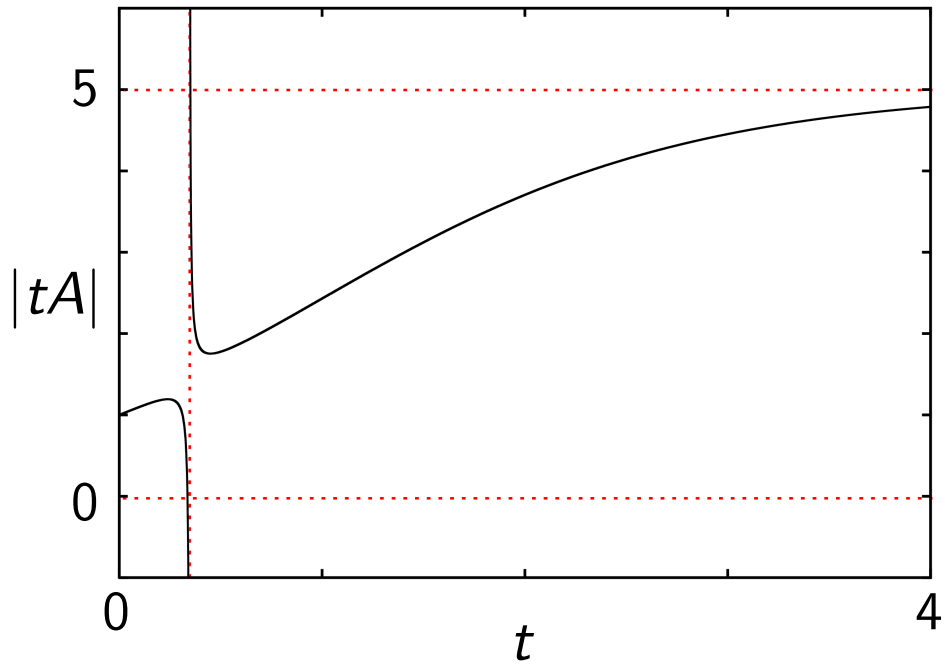
Slogan: Magnitude is the 'effective number of points'
(or clusters, or modules, . . .)

Magnitude functions

Let A be a finite metric space. The magnitude function of A is the (partially-defined) function $t \mapsto |tA| \quad (t > 0)$.

Example:





Properties:

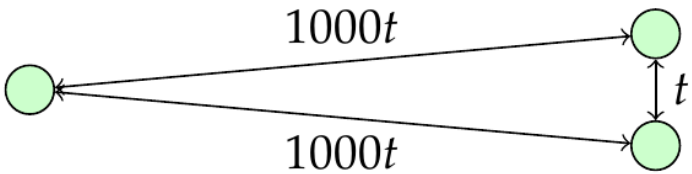
- The magnitude function has only finitely many singularities (none if $A \subseteq \mathbb{R}^n$)
- $\lim_{t\to\infty} |tA|$ is equal to n, the number of points
- $|tA|$ is increasing in t for $t \gg 0$.

Detecting clusters at different scales (Willerton)

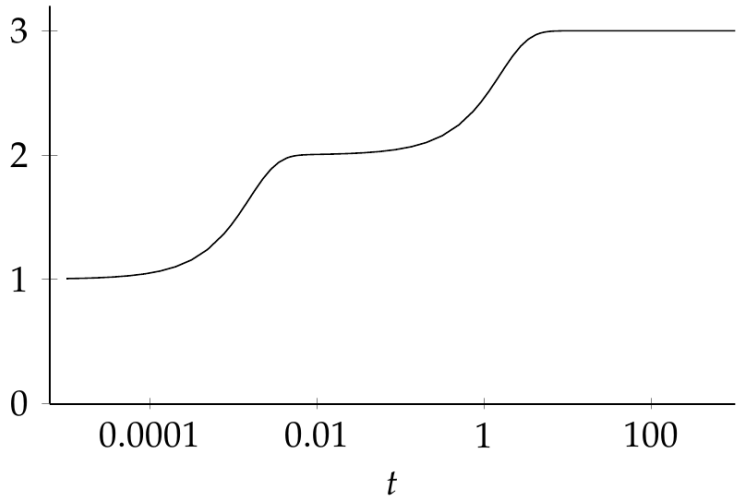
Magnitude: 2.3

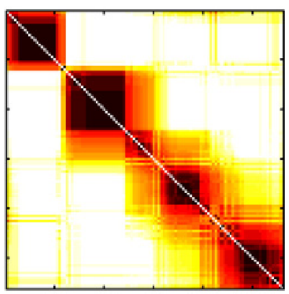
As the points get further apart, the magnitude gets closer to 3.

Precise version: the magnitude function of the 3-point space



is





Rubinov & Sporns

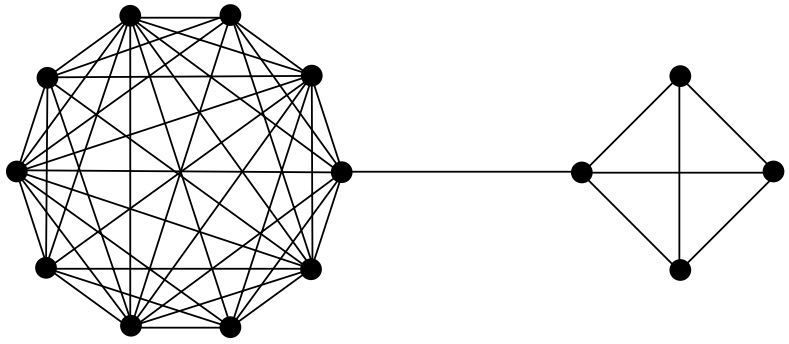
Observation

Magnitude can be seen as 'effective number of clusters', but it's not always an integer! Awkward reality: 'clusters' are ill-defined.

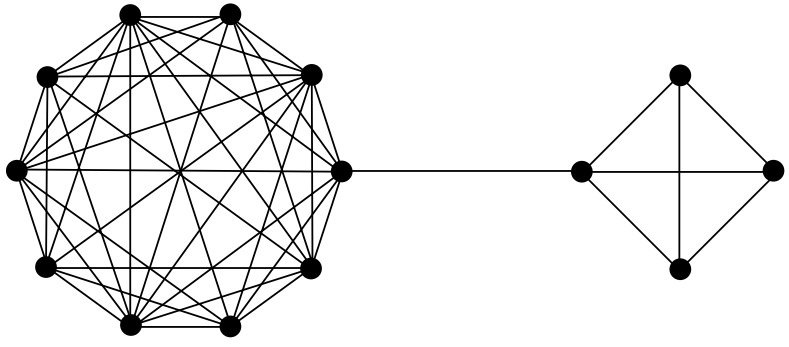
Detecting the critical nodes and edges

View a graph as a metric space: the points are the nodes, and the distance between nodes is the length of a shortest path between them.

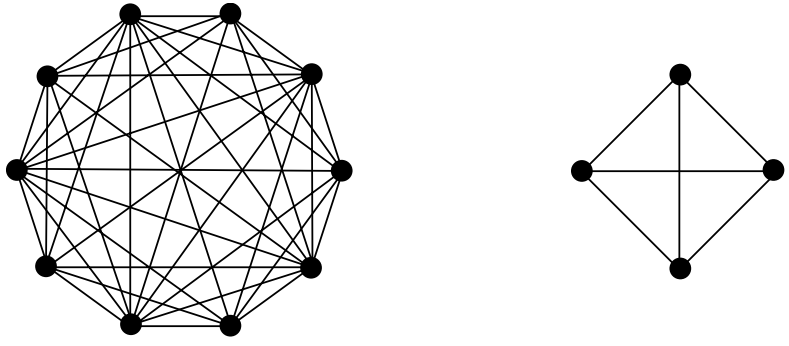
whole graph

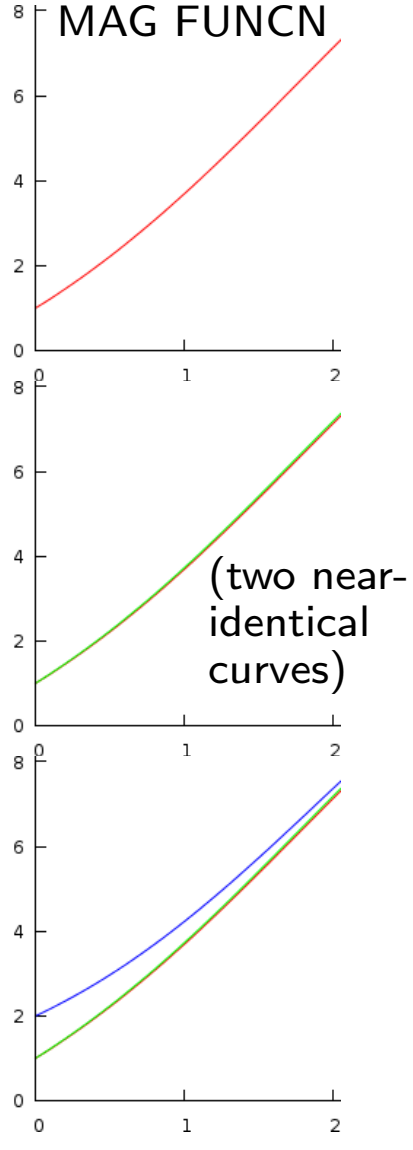


one edge on left deleted



bridge deleted

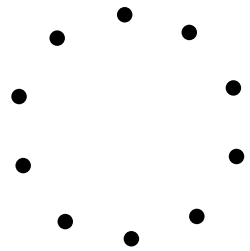


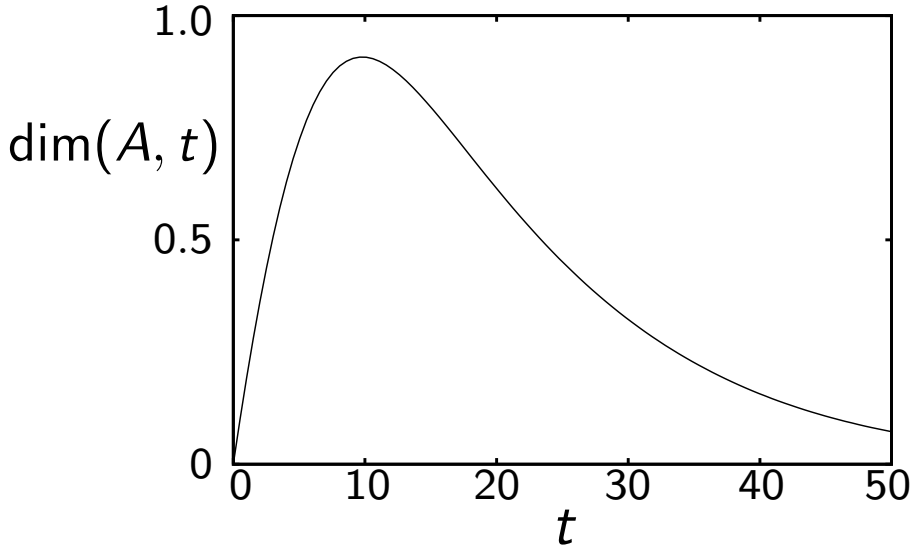


Detecting dimension at multiple scales

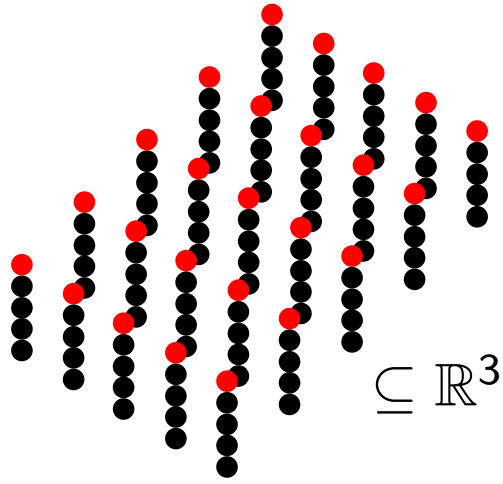
Definition (Willerton) The dimension of A at scale t is $\dim(A, t) = \dfrac{d(\log|tA|)}{d(\log t)}$.

E.g. $A =$

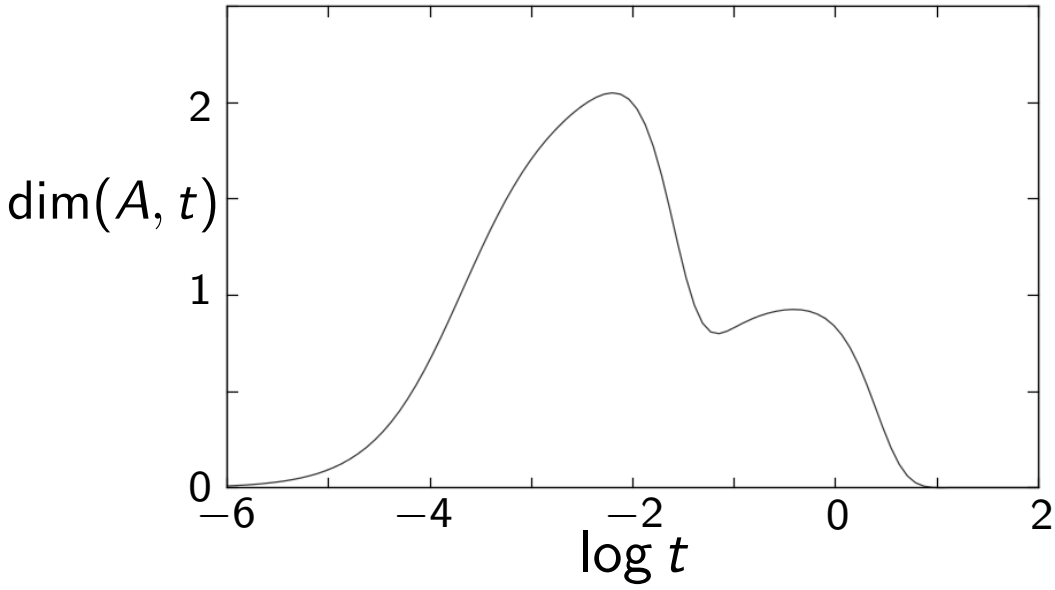




E.g. $A \approx$



$\subseteq \mathbb{R}^3$



grid is $100 \times 100 \times 100$,
with 100:1 ratio of
horizontal:vertical spacing.

An appeal

The only 'results' we have on the ability of magnitude functions to detect features of data-sets are a handful of specific examples. We need:

1. More empirical exploration
2. Theorems. . . or at least, conjectures!

Back to compact spaces

There are several equivalent ways to define the magnitude of a compact metric space X (assuming a technical hypothesis).

The simplest:

$$|X| = \sup\{|A| \ : \ \text{finite } A \subseteq X\}.$$

With this definition, and lots of analysis, we get all the results on geometric invariants stated earlier.

3. Diversity

Joint with Christina Cobbold (*Ecology*, 2012)

A brief history of diversity measurement

Challenge Given a biological community, derive a single real number measuring its 'diversity' (whatever *that* means).

There are practical problems . . . which we'll ignore.

There are statistical problems . . . which we'll ignore.

There are conceptual problems . . . which we'll focus on.

Some conceptual questions:

- How much importance to attach to rare species?
  E.g. there are 8 species of great ape, but 99.99% are humans.
- How to incorporate the varying similarities between species?
  E.g. 10 species of pine vs. 10 very different tree species.

Lots of measures of diversity have been proposed...

688 NATURE April 30, 1949 Vol. 163

Measurement of Diversity

THE 'characteristic' defined by Yule[1] and the 'index of diversity' defined by Fisher[2] are two measures of the degree of concentration or diversity

The third and fourth cumulants of the distribution of l have also been calculated exactly. They indicate that as N increases, the distribution tends to normality except when $\lambda = 1/Z$; in that case the distribution of

VEGETATION OF THE SISKIYOU MOUNTAINS, OREGON AND CALIFORNIA[1]

R. H. WHITTAKER
Biology Department, Brooklyn College, Brooklyn 10, N. Y.

Lots of measures of diversity have been proposed. . .

688 NATURE April 30, 1949 Vol. 163

THE NONCONCEPT OF SPECIES DIVERSITY: A CRITIQUE AND ALTERNATIVE PARAMETERS[1]

STUART H. HURLBERT[2]

Division of Biological Control, Department of Entomology, University of California, Riverside

Abstract. The recent literature on species diversity contains many semantic, conceptual, and technical problems. It is suggested that, as a result of these problems, species diversity has become a meaningless concept, that the term be abandoned, and that ecologists take a

THROUGH THE JUNGLE OF BIOLOGICAL DIVERSITY

Carlo Ricotta

Department of Plant Biology, University of Rome "La Sapienza", Rome, Italy.

Mailing address: Department of Plant Biology, University of Rome "La Sapienza",

About 12.800 results (0,24 seconds)

Lots of measures of diversity have been proposed. . .

688 NATURE

THE NONCONCEPT OF SPECIES DIVE
ALTERNATIVE PARA

STUART H. HURLBE

Division of Biological Control, Department of Entomol

Abstract. The recent literature on species diversity
and technical problems. It is suggested that, as a resu
has become a meaningless concept, that the term be

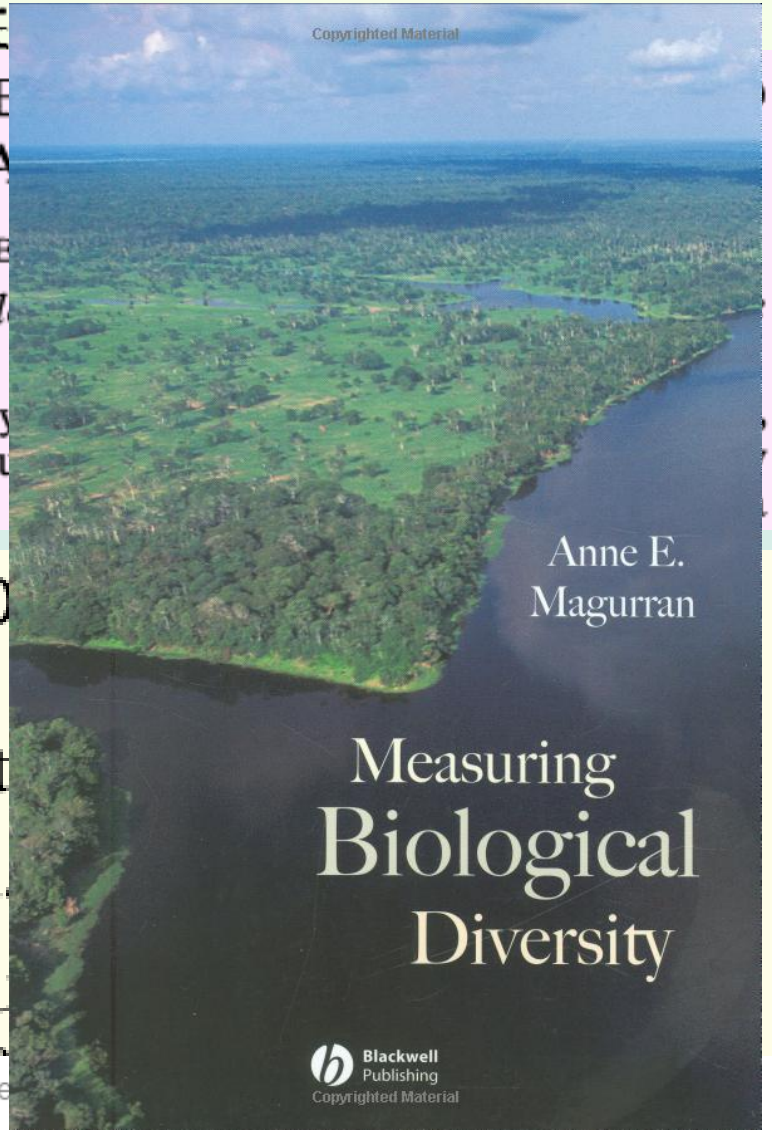
THROUGH THE JUNGLE OF BIO

Carlo Ricott

Department of Plant Biology, University of Rome "

Mailing address: Department of Plant Biology, U
Piazzale Aldo Moro 5, 00185 Roma, Italy. Phone

About 12.800 results (0,24 se



We'll meet a family of measures that encompasses many of them.

Modelling a community

Model a biological community mathematically as follows:

- The organisms are classified into n species.
- They have relative abundances $\mathbf{p} = \begin{pmatrix} p_1 \\ \vdots \\ p_n \end{pmatrix}$ (with $\sum p_i = 1$).
- The similarity between species i and j is $Z_{ij} \in [0, 1]$.
  Here 0 means totally dissimilar and 1 means identical.
  Assume $Z_{ii} = 1$ and $Z_{ij} = Z_{ji}$, so have symmetric $n \times n$ matrix Z.

Similarity can be measured in many ways, including:

- Naive model $Z = I$: distinct species have nothing in common.
- Percentage genetic similarity.
- Taxonomically, e.g. $Z_{ij} = \begin{cases} 1 & \text{if same species} \\ 0.7 & \text{if different species but same genus} \\ 0 & \text{otherwise.} \end{cases}$
- $Z_{ij} = e^{-d_{ij}}$ if (d_{ij}) is a metric on species.

A unifying family of diversity measures

Recap: We model a community by a relative abundance vector $\mathbf{p} = \begin{pmatrix} p_1 \\ \vdots \\ p_n \end{pmatrix}$ and an $n \times n$ similarity matrix Z.

- $(Z\mathbf{p})_i = \sum_j Z_{ij} p_j$ is the expected similarity between a random organism and one of species i. It measures the ordinariness of species i.
- So $1/(Z\mathbf{p})_i$ is the distinctiveness of species i.

A community is diverse if it contains many distinctive individuals.

So one measure of diversity is the average distinctiveness:

$$\sum_i p_i \frac{1}{(Z\mathbf{p})_i}.$$

More generally, it's worth considering the power mean

$$\left(\sum_i p_i \left(\frac{1}{(Z\mathbf{p})_i} \right)^{1-q} \right)^{1/(1-q)}$$

for every real q (but we'll stick to $q \geq 0$).

A unifying family of diversity measures

Definition

The diversity of the community, of order $q \geq 0$, is

$$D_q^Z(\mathbf{p}) = \left(\sum_i p_i (Z\mathbf{p})_i^{q-1} \right)^{1/(1-q)}.$$

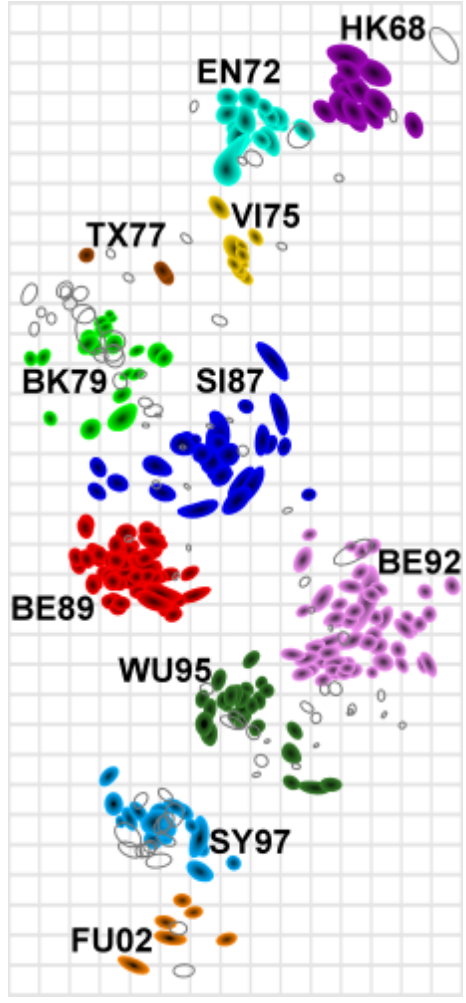
When $q = 1$, this doesn't make sense. Instead, define

$$D_1^Z(\mathbf{p}) = \lim_{q \to 1} D_q^Z(\mathbf{p}) = \exp\Big(-\sum p_i \log(Z\mathbf{p})_i \Big).$$

E.g. Naive model $Z = I$: then $D_1^Z(\mathbf{p}) = \exp(\text{Shannon entropy of } \mathbf{p})$.

Properties of these diversity measures

- This family of diversity measures encompasses many of the measures already defined and used by ecologists, geneticists, etc.
- They behave sensibly when species are reclassified (don't jump suddenly).
- They behave smoothly under change of resolution (e.g. if we go down to the subspecies level).
- They can be used in situations where we *don't have species classifications at all* (often the case for microbial communities).

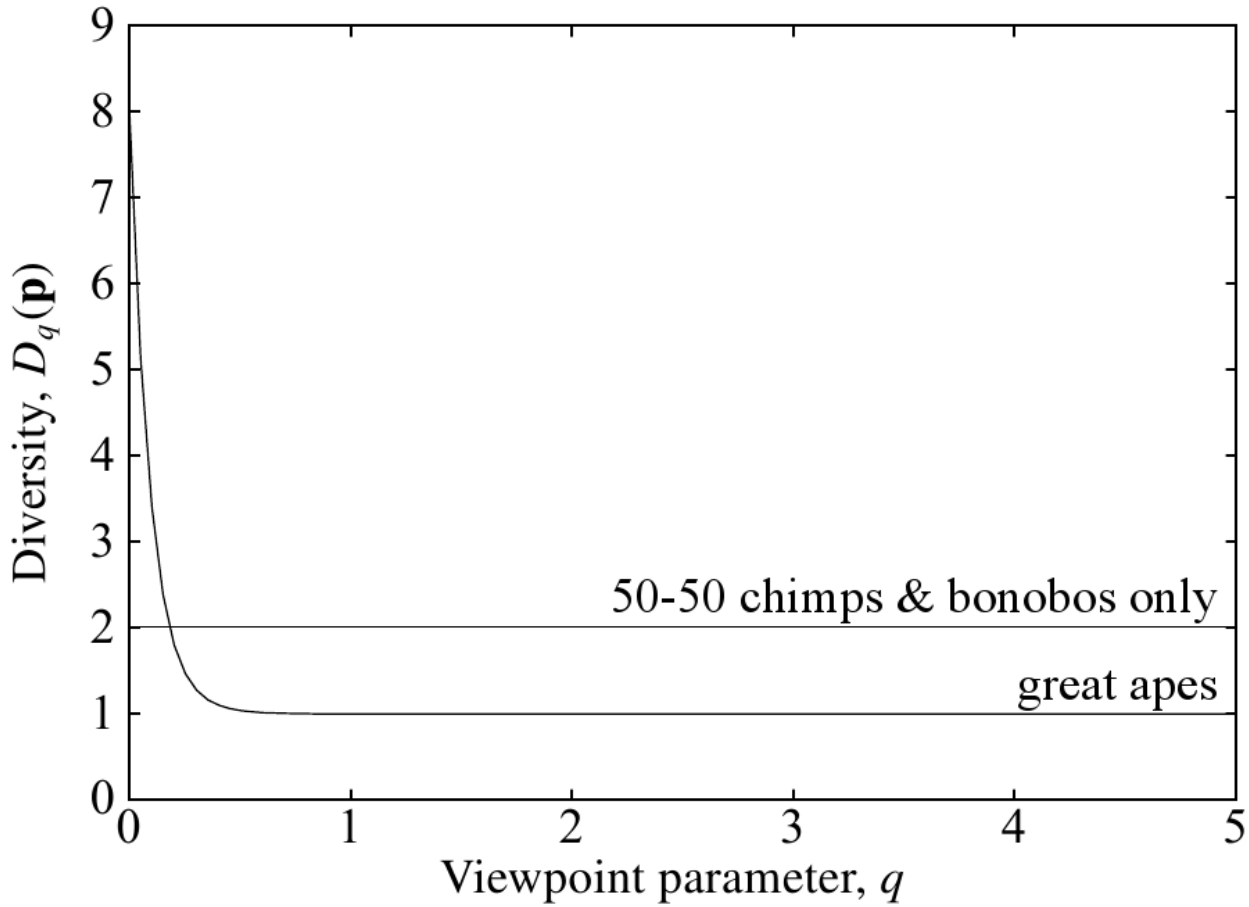


Influenza strains, 1968–2002

Comparing communities

The diversity profile of a community is the graph of $D_q^Z(\mathbf{p})$ against q.

E.g. Great apes worldwide, with naive similarity matrix ($Z = I$):



The parameter q controls the relative emphasis on rare or common species.

Maximizing diversity

Problem: Fix a list of species (i.e. a similarity matrix Z), and suppose we are free to choose their relative abundances $\mathbf{p}$.

- Which distribution $\mathbf{p}$ maximizes the diversity $D_q^Z(\mathbf{p})$?
- What is the value of the maximum diversity, $\sup_{\mathbf{p}} D_q^Z(\mathbf{p})$?

Diversity profiles can cross, so in principle, both answers depend on q.

Theorem (with Mark Meckes, *Entropy*, 2016)

Neither does. That is:

- *There is a single distribution* $\mathbf{p}_{max}$ *maximizing diversity of all orders* q *simultaneously (a 'best of all possible worlds').*
- *The maximum diversity* $D_q^Z(\mathbf{p}_{max})$ *is the same for all* q*. Call it* $D_{max}(Z)$*.*

Consequences of the maximum diversity theorem

Any $n \times n$ similarity matrix Z (e.g. coming from a metric via $Z_{ij} = e^{-d_{ij}}$) gives rise *canonically* to:

- a probability distribution $\mathbf{p}_{\max}$ on $\{1, \ldots, n\}$ (usually unique)
- a real number $D_{\max}(Z)$.

Often, $D_{\max}(Z)$ is equal to the magnitude $|Z| = \sum_{i,j} (Z^{-1})_{ij}$.

It's *always* equal to the magnitude of Z restricted to some subset of $\{1, \ldots, n\}$.

In a slogan:

Magnitude $\approx$ maximum diversity

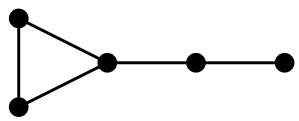
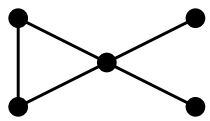
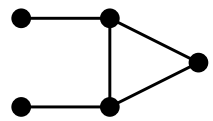
4. Graphs, revisited (briefly)

The magnitude of a graph

We've seen that any graph G can be understood as a special metric space, where all distances are integers.

(For simplicity, I'll stick to undirected graphs—but can do directed.)

Special property of graphs *Write $x = e^{-t}$. Then the magnitude function $t \mapsto |tG|$ is a rational function of x.*

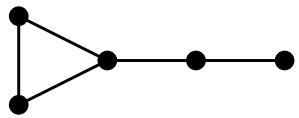
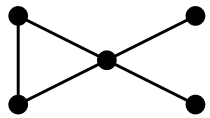
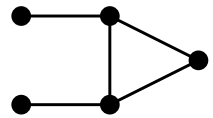
E.g.  ,  and  all have magnitude function

$$\frac{5 + 5x - 4x^2}{(1 + x)(1 + 2x)}.$$

The magnitude of a graph can be studied as a graph invariant, and shares some invariance properties with the Tutte polynomial.

The magnitude of a graph

Lemma *The magnitude function of a graph can also be expressed as a power series with integer coefficients.*

E.g.  ,  and  have magnitude function

$$5 - 10x + 16x^2 - 28x^3 + 52x^4 - 100x^5 + \cdots .$$

In general, the magnitude function of a graph G is

$$c_0 + c_1 x + c_2 x^2 + \cdots$$

where

$$c_0 = \text{number of nodes}$$

$$c_1 = -2 \cdot (\text{number of edges})$$

$$c_2 = \sum_{i,j:d_{ij}=2} \underbrace{\Big((\text{num of configurations } i\text{—}\bullet\text{—}j) - 1\Big)}_{\text{redundancy}}$$

$$+ 6 \cdot (\text{num of triangles}) + 2 \cdot (\text{num of edges}).$$

5. The future: magnitude homology

Two points of view on Euler characteristic

So far: Euler characteristic has been treated as an analogue of cardinality.

Alternatively: Given any homology theory H_* of any kind of object X, can define

$$\chi(X) = \sum_{n=0}^{\infty} (-1)^n \operatorname{rank} H_n(X).$$

Note:

- $\chi(X)$ is a *number*
- $H_*(X)$ is an *algebraic structure*, and functorial in X.

In this sense, homology improves on ("categorifies") Euler characteristic.

The magnitude homology of a graph (Hepworth–Willerton)

There is a definition (omitted) of the magnitude homology of a graph.

It is a *graded* homology theory. That is, for each graph G and integer $k \geq 0$, it gives a *sequence*

$$H_{k,0}(G), H_{k,1}(G), H_{k,2}(G), \dots$$

of abelian groups.

So for each $k \geq 0$, we have a power series

$$\mathrm{rank}(H_{k,0}(G)) + \mathrm{rank}(H_{k,1}(G))x + \mathrm{rank}(H_{k,2}(G))x^2 + \cdots$$

The Euler characteristic $\chi(G)$ for this homology theory is (inevitably) defined as the alternating sum of these power series over $k = 0, 1, \dots$.

Theorem (Hepworth, Willerton) $\chi(G)$ *is exactly the magnitude function of* G*.*

So: magnitude is the Euler characteristic of magnitude homology.

The magnitude homology of a metric space

The definition of magnitude homology can be generalized from graphs to enriched categories (Shulman).

In particular, there is a magnitude homology of metric spaces.

Sample Theorem *For a closed set* $A \subseteq \mathbb{R}^n$,

$$A \text{ is convex} \iff H_1(A) = 0.$$

Otter (2018) has done a comparison of magnitude homology with persistent homology:

- She proves a relationship between persistent homology and a 'blurred version' of magnitude homology...
- but concludes that 'morally, these are very different homology theories', conveying different information.

Summary

Summary

Magnitude is a numerical invariant of metric spaces (e.g. data sets, networks, and the kinds of space that geometers like thinking about).

By considering rescalings, magnitude assigns a function to each space.

- For geometrically interesting spaces, the magnitude function carries geometrically interesting information (volume, dimension, etc).
- For finite spaces, it seems—empirically—to carry multiscale information on number of clusters and dimensionality.

We can also measure the diversity ($\sim$ entropy) of any probability distribution on a finite metric space...

...and magnitude is closely related to maximum diversity.

There is a theory of magnitude homology for metric spaces.

It is related to persistent homology, but expresses different information about the space... Lots to explore here!

References and further reading: www.maths.ed.ac.uk/$\sim$tl/magbib