The magnitude of a metric space

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Survey paper: arXiv:1606.00095

The aim of this talk

Explain magnitude, a numerical invariant of metric spaces

Magnitude of metric spaces:

- has its origins in category theory
- is closely related to . . .
  - geometric measure
  - maximum entropy
  - quantification of biodiversity
  - potential analysis
- may be relevant to data analysis. . . ?

Plan

1. Where magnitude comes from

2. The magnitude of a finite metric space

    3. Digression: entropy and diversity

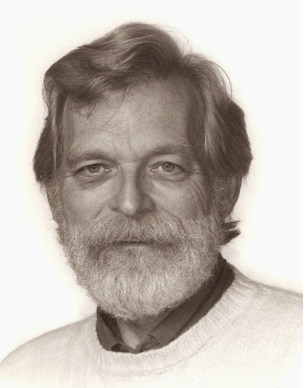
4. The magnitude of a compact metric space

5. Magnitude encodes geometric information

6. Magnitude encodes dimension

1. Where magnitude comes from

Schanuel on how to think about Euler characteristic



Stephen Schanuel, 'Negative sets have Euler characteristic and dimension' (1991):

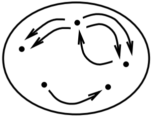
> *Euler's analysis, which demonstrated that in counting suitably 'finite' spaces one can get well-defined negative integers, was a revolutionary advance in the idea of cardinal number—perhaps even more important than Cantor's extension to infinite sets, if we judge by the number of areas in mathematics where the impact is pervasive.*

How is Euler characteristic χ similar to cardinality?

- On finite discrete spaces, χ *equals* cardinality
- $\chi(X \cup Y) = \chi(X) + \chi(Y) - \chi(X \cap Y)$, under suitable hypotheses
- $\chi(X \times Y) = \chi(X) \times \chi(Y)$.

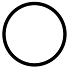
Categories and spaces

A category is a directed graph ('objects' and 'arrows'), together with a rule for composing arrows and an identity arrow on each object.



Every category $\mathbf{A}$ gives rise in a canonical way to a topological space $B\mathbf{A}$, called its classifying space.

E.g.:

- If $\mathbf{A} = (\bullet \quad \bullet \quad \bullet)$ then $B\mathbf{A} = (\bullet \quad \bullet \quad \bullet)$ (discrete space).
- If $\mathbf{A} = \left(\bullet \rightrightarrows \bullet \right)$ then $B\mathbf{A} = S^1 =$  .

The Euler characteristic of a category

We *could* define the Euler characteristic of a category $\mathbf{A}$ to be the Euler characteristic of its classifying space $B\mathbf{A}$ (at least, when $\chi(B\mathbf{A})$ is defined).

For finite $\mathbf{A}$, there is an equivalent combinatorial definition:

Given a category $\mathbf{A}$, let $Z_{\mathbf{A}}$ be the matrix whose rows and columns are indexed by the objects of $\mathbf{A}$, and with entries

$$Z_{\mathbf{A}}(a, b) = \text{number of arrows from } a \text{ to } b.$$

When $Z_{\mathbf{A}}$ is invertible, the Euler characteristic of $\mathbf{A}$ is

$$\chi(\mathbf{A}) = \sum_{\text{objects } a,b} Z_{\mathbf{A}}^{-1}(a, b) \ \in \mathbb{Q}$$

—the sum of all the entries of the inverse matrix of $Z_{\mathbf{A}}$.

Theorem: $\chi(\mathbf{A}) = \chi(B\mathbf{A})$, *under finiteness hypotheses.*

A general definition of size

Categories are a special case of a more general concept: *enriched categories*.

(I won't give the definition.)

The definition of Euler characteristic generalizes smoothly from categories to enriched categories, where it is renamed as *magnitude*.

(I won't give the definition.)

So, one can speak of the magnitude of an enriched category.

This has connections to Möbius inversion in combinatorics, invariants of associative algebras, a new graded homology theory for graphs, ...

Metric spaces are also a special case of enriched categories.

So, we can speak of the magnitude of a metric space.

I *will* give the definition—explicitly!

2. The magnitude of a finite metric space

The definition

Let A be a finite metric space.

Write Z_A for the $A \times A$ matrix with entries

$$Z_A(a, b) = e^{-d(a,b)}$$

$(a, b \in A)$. (Why $e^{-\text{distance}}$? Because $e^{-(x+y)} = e^{-x}e^{-y}$.)

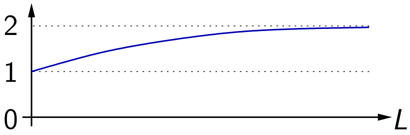
If Z_A is invertible (which it is if $A \subseteq \mathbb{R}^n$), the magnitude of A is

$$|A| = \sum_{a,b \in A} Z_A^{-1}(a, b) \ \in \mathbb{R}$$

—the sum of all the entries of the inverse matrix of Z_A.

First examples

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

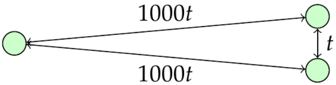


- If $d(a, b) = \infty$ for all $a \neq b$ then $|A| = \text{cardinality}(A)$.

Slogan: Magnitude is the 'effective number of points'.

Example: a 3-point space (Willerton)

Take the 3-point space

$A =$ 

- When t is small, A looks like a 1-point space.

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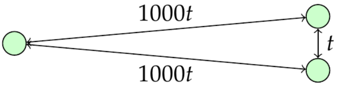
$A =$ 

- When t is small, A looks like a 1-point space.
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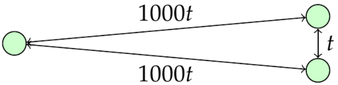
$A =$ 

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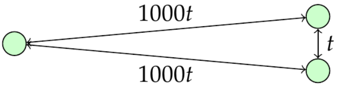
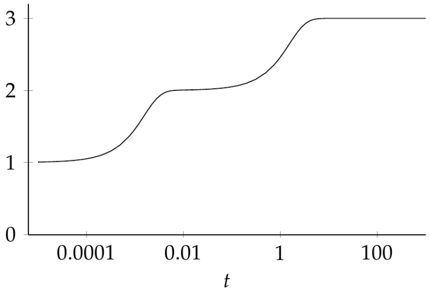
$A =$ 

- When t is small, A looks like a 1-point space.
- When t is moderate, A looks like a 2-point space.
- When t is large, A looks like a 3-point space.

Indeed, the magnitude of A as a function of t is:



Magnitude functions

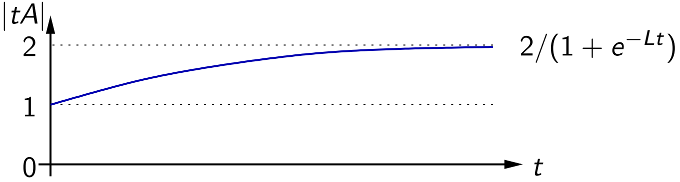
Magnitude assigns to each metric space not just a *number*, but a *function*.

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

The magnitude function of a metric space A is the partially-defined function

$$\begin{array}{ccc} (0,\infty) & \to & \mathbb{R} \\ t & \mapsto & |tA|. \end{array}$$

E.g.: the magnitude function of $A = (\bullet \xleftarrow{} L \xrightarrow{} \bullet)$ is



A magnitude function has only finitely many singularities (none if $A \subseteq \mathbb{R}^n$).

It is increasing for $t \gg 0$, and $\lim_{t\to\infty} |tA| = \text{cardinality}(A)$.

3. Digression:
entropy and diversity

Shannon and Rényi entropies

Let A be a finite set and $\mathbf{p} = \big(p(a)\big)_{a \in A}$ a probability distribution on A.

The Shannon entropy of $\mathbf{p}$ is

$$H_1(\mathbf{p}) = -\sum_{a \in A} p(a) \log p(a).$$

This is the limiting case as $q \to 1$ of the Rényi entropy of order $q \in [0, \infty]$:

$$H_q(\mathbf{p}) = \frac{1}{1-q} \log \sum_{a \in A} p(a)^q.$$

Now suppose that A carries a metric. We can define more generally:

$$H_q^{\mathrm{met}}(\mathbf{p}) = \frac{1}{1-q} \log \sum_{a \in A} p(a) \cdot (Z_A \mathbf{p})(a)^{q-1}$$

where $Z_A \mathbf{p}$ is the matrix Z_A times the column vector $\mathbf{p}$.

E.g.: when all distances are ∞, H_q^{met} reduces to H_q.

Discovery (with Christina Cobbold) Most of the biodiversity measures most commonly used in ecology are special cases of H_q^{met}.

Maximum entropy and magnitude

Let A be a finite *set*. Let's try to maximize $\exp H_q(\mathbf{p})$ over all $\mathbf{p}$. Facts:

- There is a single distribution $\mathbf{p}$ maximizing $\exp H_q(\mathbf{p})$ for all $q \in [0, \infty]$ simultaneously. (It's the uniform distribution.)
- Moreover, $\sup_{\mathbf{p}} \big(\exp H_q(\mathbf{p})\big)$ is the same for all q. It's the cardinality of A.

More generally, let A be a finite *metric space*. Can we maximize $\exp H_q^{\mathrm{met}}(\mathbf{p})$?

Theorem:

- There is a single distribution $\mathbf{p}$ maximizing $\exp H_q^{\mathrm{met}}(\mathbf{p})$ for all $q \in [0, \infty]$ simultaneously. (It's not uniform!)
- Moreover, $\sup_{\mathbf{p}} \big(\exp H_q^{\mathrm{met}}(\mathbf{p})\big)$ is the same for all q.
  It's closely related to the magnitude of A.
  (In fact, it's equal to the magnitude of a certain subspace of A.)

Moral: magnitude $\approx$ maximum entropy.

End of digression

4. The magnitude of a compact metric space

The definition

A metric space X is positive definite if for every finite $A \subseteq X$, the matrix Z_A is positive definite.

E.g.: $\mathbb{R}^n$ with the Euclidean or taxicab metric, hyperbolic space, any ultrametric space.

Theorem (Meckes)

All sensible ways of extending the definition of magnitude from finite metric spaces to compact positive definite spaces are equivalent.

E.g.: For a compact positive definite space A, we can define

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

Or equivalently, we can choose a sequence (B_n) of finite subsets with $B_n \to A$ in the Hausdorff metric, then define $|A| = \lim_{n\to\infty} |B_n|$.

The definition can also be expressed directly, without using finite approximations.

Example: the magnitude of a box

The straight line $[0, L]$ of length L has magnitude $1 + \frac{1}{2}L$.

So $[0, L]$ has magnitude function

Euler characteristic length

dimension

$$t \mapsto |t[0, L]| = |[0, tL]| = \boxed{1} + \tfrac{1}{2}\boxed{L} \cdot t^{\boxed{1}}$$

For metric spaces A and B, let $A \times_1 B$ be their 'ℓ_1 product', given by

$$d_{A \times_1 B}\big((a, b), (a', b')\big) = d_A(a, a') + d_B(b, b').$$

Lemma $|A \times_1 B| = |A|\,|B|$.

It follows that the rectangle $[0, L_1] \times_1 [0, L_2]$ has magnitude function

$$t \mapsto \boxed{1} + \tfrac{1}{2}\boxed{(L_1 + L_2)}t + \tfrac{1}{4}\boxed{L_1 L_2}t^{\boxed{2}}$$

dimension

area

Euler characteristic semiperimeter

So, the magnitude function of a rectangle knows its Euler characteristic, perimeter, area and dimension!

5. Magnitude encodes geometric information

Convex sets

Write $\ell_1^n = \mathbb{R} \times_1 \cdots \times_1 \mathbb{R}$ (that is, $\mathbb{R}^n$ with the taxicab metric).

Theorem *Let $A \subseteq \ell_1^n$ be a convex body. Then its magnitude function $t \mapsto |tA|$ is a polynomial whose degree is $\dim A$ and whose coefficients are certain geometric measures of A (e.g. top coeff $= 2^{-n}\,\mathrm{vol}(A)$).*

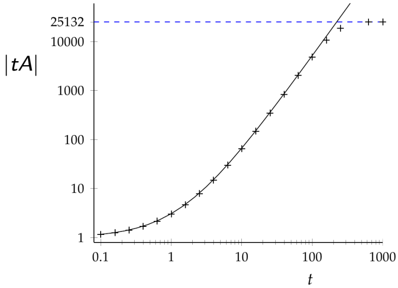
Conjecture (with Willerton) *For convex $A \subseteq \mathbb{R}^2$ with Euclidean metric,*

$$|tA| = \chi(A) + \frac{1}{4}\,\mathrm{perimeter}(A) \cdot t + \frac{1}{2\pi}\,\mathrm{area}(A) \cdot t^2.$$

Can test this numerically using finite approximations.

E.g.: (Willerton)
Let A be the unit 2-disc, approximated by 25132 points.

The magnitude function of A is:



Other spaces

Two sample theorems:


Theorem (Juan-Antonio Barceló & Tony Carbery) *For compact $A \subseteq \mathbb{R}^n$,*

$$\mathrm{vol}(A) = c_n \lim_{t \to \infty} \frac{|tA|}{t^n}$$

where c_n is a known constant.

Theorem (Willerton) *The magnitude function of a homogeneous Riemannian n-manifold M is given asymptotically as $t \to \infty$ by*

$$|tM| = a_n \,\mathrm{vol}(M) \cdot t^n + b_n \,\mathrm{tsc}(M) \cdot t^{n-2} + O(t^{n-4})$$

where a_n and b_n are known constants and tsc *denotes total scalar curvature.*

E.g. when $n = 2$:

$$|tM| = \tfrac{1}{2\pi}\,\mathrm{area}(M) \cdot t^2 + \chi(M) + O(t^{-2}).$$

6. Magnitude encodes dimension

Dimension is the asymptotic growth of magnitude

We've seen that in various examples, the magnitude function $t \mapsto |tA|$ is a polynomial (asymptotically, at least) whose degree is the dimension of A.

The (asymptotic) growth of a function $f\colon (0,\infty) \to \mathbb{R}$ is $\displaystyle\lim_{t\to\infty} \frac{\log f(t)}{\log t} \in \mathbb{R}$.

E.g.: The growth of a polynomial is its degree.

The Minkowski dimension of a metric space A is

$$\lim_{\varepsilon\to 0} \frac{\log(\text{number of } \varepsilon\text{-balls needed to cover } A)}{\log(1/\varepsilon)} \in \mathbb{R}^+.$$

This is one of several notions of fractional dimension, usually equal to the Hausdorff dimension.

Theorem (Meckes) *For compact subsets of $\mathbb{R}^n$, the Minkowski dimension is equal to the growth of the magnitude function.*

So, Minkowski dimension can be recovered from magnitude.

Dimension at different scales (Willerton)

Consider a long thin rectangle: 

- At small scales, it looks 0-dimensional.

Dimension at different scales (Willerton)

Consider a long thin rectangle: 

- At small scales, it looks 0-dimensional.
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- At small scales, it looks 0-dimensional.
- At medium scales, it looks 1-dimensional.
- At large scales, it looks 2-dimensional.

The magnitude function sees all this!

Here's how. . .

Dimension at different scales (Willerton)

For a function $f\colon (0,\infty) \to \mathbb{R}$, the instantaneous growth of f at $t \in (0,\infty)$ is

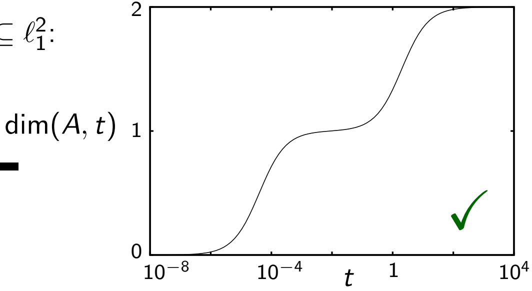
$$\frac{d(\log f(t))}{d(\log t)} = \text{slope of the log-log graph of } f \text{ at } t.$$

E.g.: If $f(t) = Ct^n$ then $\frac{d(\log f(t))}{d(\log t)} = n$ for all t.

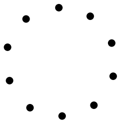
For a space A, the magnitude dimension of A at scale t is

$$\dim(A,t) = \frac{d(\log |tA|)}{d(\log t)}.$$

E.g.: For $A = [0, 50000] \times [0,1] \subseteq \ell_1^2$:

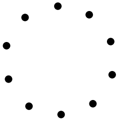


Dimension at different scales

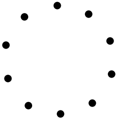
Let $A =$ , with subspace metric from $\mathbb{R}^2$.

- When t is small, tA looks 0-dimensional.

Dimension at different scales

Let $A =$  , with subspace metric from $\mathbb{R}^2$.

- When t is small, tA looks 0-dimensional.
- When t is moderate, tA looks nearly 1-dimensional.



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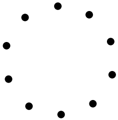
Let $A =$  , with subspace metric from $\mathbb{R}^2$.

- When t is small, tA looks 0-dimensional.
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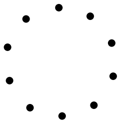
Dimension at different scales

Let $A =$  , with subspace metric from $\mathbb{R}^2$.

- When t is small, tA looks 0-dimensional.
- When t is moderate, tA looks nearly 1-dimensional.
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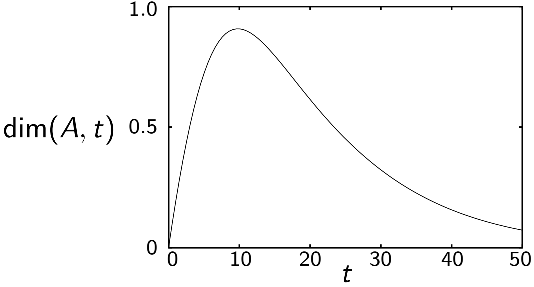
The magnitude function picks all this up.

Indeed, here's the magnitude dimension of A at different scales:



Summary

The idea of magnitude

Philosophically: magnitude is part of a large family of 'invariants of size' spanning mathematics. Other members of this family are cardinality, Euler characteristic, measure, entropy, ...

Explicitly: to get the magnitude $|A|$ of a finite metric space A, invert the matrix $\left(e^{-d(a,b)}\right)_{a,b\in A}$ then add up all its entries.

Interpretation 1: The magnitude of a finite space can be thought of as the 'effective number of points'.

Interpretation 2: It is also very closely related to the maximum entropy of a probability distribution on the space (using a metric-sensitive notion of entropy).

The geometric content of magnitude

The definition of magnitude extends smoothly to compact sets in $\mathbb{R}^n$.

Given a metric space A, we should consider all its rescalings tA.

The magnitude function of A is $|tA|$ as a function of t.

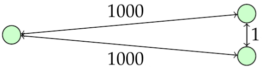
The magnitude function of A contains *lots* of information about A.

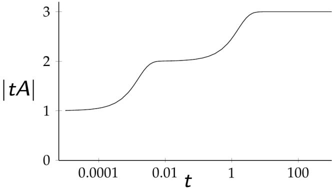
E.g.:

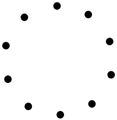
- for compact subsets of $\mathbb{R}^n$, it knows the volume
- for compact subsets of $\mathbb{R}^n$, it knows the Minkowski dimension
- in other contexts, it knows invariants such as Euler characteristic, total scalar curvature, perimeter, intrinsic volumes, ...

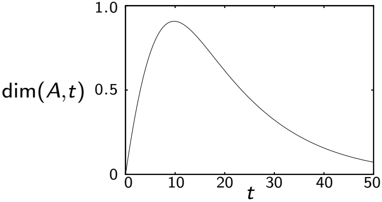
Why am I talking about magnitude at ATMCS?

Because of the role played by finite metric spaces, e.g.

$A =$ 



$A =$ 



Because every time my collaborator Simon Willerton speaks on this, someone asks ‘Is this related to persistent homology?’

And mainly: to find out whether this theory may be resonant — or even useful — to you.