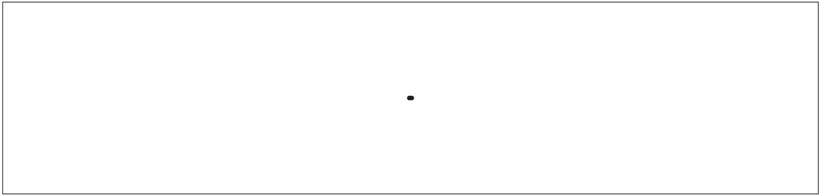
Measuring metric spaces: short sightedness and population diversity

Simon Willerton

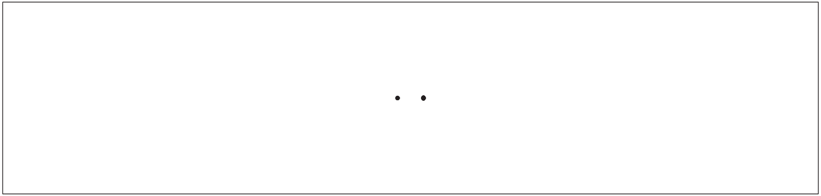
1: Defining the cardinality

Measuring a metric space



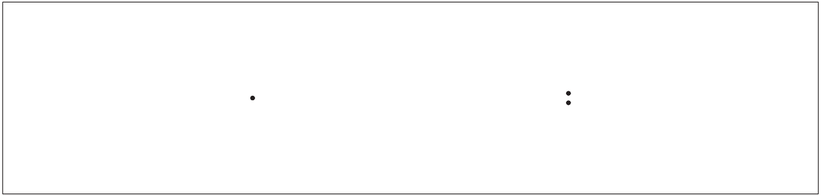
How many things are there?

Measuring a metric space



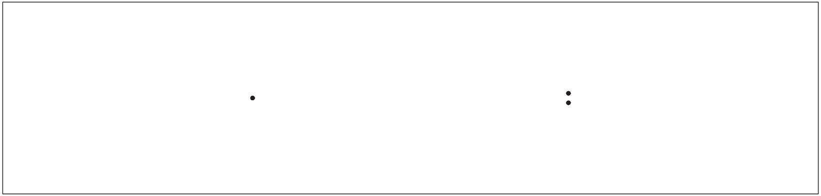
How many things are there?

Measuring a metric space



How many things are there?

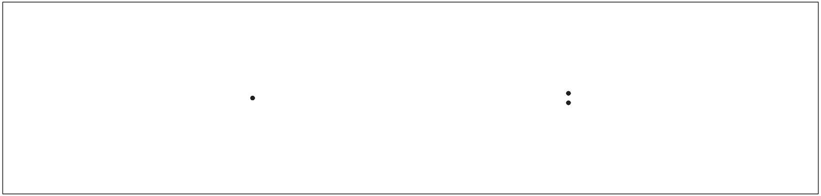
Measuring a metric space



How many things are there?

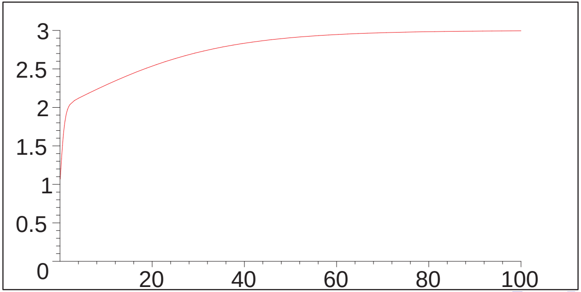
We want to measure the ‘size’ of a set of points with distances.

Measuring a metric space

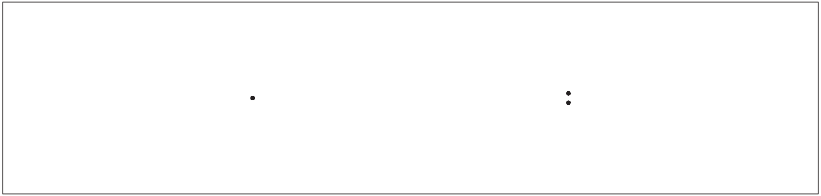


How many things are there?

We want to measure the ‘size’ of a set of points with distances.

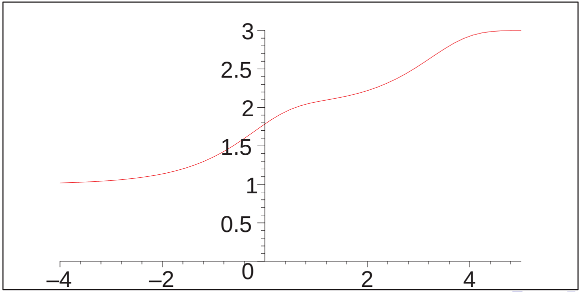


Measuring a metric space



How many things are there?

We want to measure the ‘size’ of a set of points with distances.



Metric spaces

Definition

A metric space is a set X with a 'distance' $d_{ij} \in [0, \infty]$ between each pair of points $i, j \in X$ such that

- triangle inequality: $d_{ik} \leq d_{ij} + d_{jk}$
- no self-distance: $d_{ii} = 0$ for all $i \in X$
- separation: if $i \neq j$ then $d_{ij} \neq 0$
- symmetry: $d_{ij} = d_{ji}$

Metric spaces

Definition

A metric space is a set X with a 'distance' $d_{ij} \in [0, \infty]$ between each pair of points $i, j \in X$ such that

- triangle inequality: $d_{ik} \leq d_{ij} + d_{jk}$
- no self-distance: $d_{ii} = 0$ for all $i \in X$
- separation: if $i \neq j$ then $d_{ij} \neq 0$
- symmetry: $d_{ij} = d_{ji}$

Example

- Euclidean distances between points

Metric spaces

Definition

A metric space is a set X with a 'distance' $d_{ij} \in [0, \infty]$ between each pair of points $i, j \in X$ such that

- triangle inequality: $d_{ik} \leq d_{ij} + d_{jk}$
- no self-distance: $d_{ii} = 0$ for all $i \in X$
- separation: if $i \neq j$ then $d_{ij} \neq 0$
- symmetry: $d_{ij} = d_{ji}$

Example

- Euclidean distances between points
- 'Difference' between species in a population

Metric spaces

Definition

A metric space is a set X with a 'distance' $d_{ij} \in [0, \infty]$ between each pair of points $i, j \in X$ such that

- triangle inequality: $d_{ik} \leq d_{ij} + d_{jk}$
- no self-distance: $d_{ii} = 0$ for all $i \in X$
- separation: if $i \neq j$ then $d_{ij} \neq 0$
- symmetry: $d_{ij} = d_{ji}$

Example

- Euclidean distances between points
- 'Difference' between species in a population
- Distance in an evolutionary tree

Metric spaces

Definition

A metric space is a set X with a 'distance' $d_{ij} \in [0, \infty]$ between each pair of points $i, j \in X$ such that

- triangle inequality: $d_{ik} \leq d_{ij} + d_{jk}$
- no self-distance: $d_{ii} = 0$ for all $i \in X$
- separation: if $i \neq j$ then $d_{ij} \neq 0$
- symmetry: $d_{ij} = d_{ji}$

Note

Not every metric space is embeddable in Euclidean space.

Defining the cardinality (I)

Definition

If X is a finite metric space then (try to) define the cardinality $|X|$ as follows.

Defining the cardinality (I)

Definition

If X is a finite metric space then (try to) define the cardinality $|X|$ as follows.

1. Define the closeness (or similarity) matrix Z by $Z_{ij} := e^{-d_{ij}}$.
   [Z is symmetric with entries in $[0, 1]$ and 1s on the diagonal.]

Defining the cardinality (I)

Definition

If X is a finite metric space then (try to) define the cardinality $|X|$ as follows.

1. Define the closeness (or similarity) matrix Z by $Z_{ij} := e^{-d_{ij}}$.
   [Z is symmetric with entries in $[0, 1]$ and 1s on the diagonal.]
2. Invert Z (if possible).

Defining the cardinality (I)

Definition

If X is a finite metric space then (try to) define the cardinality $|X|$ as follows.

1. Define the closeness (or similarity) matrix Z by $Z_{ij} := e^{-d_{ij}}$.
   [Z is symmetric with entries in $[0, 1]$ and 1s on the diagonal.]
2. Invert Z (if possible).
3. Define $|X|$ as the sum of the entries of Z^{-1}.

Defining the cardinality (I)

Definition

If X is a finite metric space then (try to) define the cardinality $|X|$ as follows.

1. Define the closeness (or similarity) matrix Z by $Z_{ij} := e^{-d_{ij}}$.
   [Z is symmetric with entries in $[0, 1]$ and 1s on the diagonal.]
2. Invert Z (if possible).
3. Define $|X|$ as the sum of the entries of Z^{-1}.

For $t \in (0, \infty)$ let tX be X scaled by a factor of t.

Defining the cardinality (I)

Definition

If X is a finite metric space then (try to) define the cardinality $|X|$ as follows.

1. Define the closeness (or similarity) matrix Z by $Z_{ij} := e^{-d_{ij}}$.
   [Z is symmetric with entries in $[0, 1]$ and 1s on the diagonal.]
2. Invert Z (if possible).
3. Define $|X|$ as the sum of the entries of Z^{-1}.

For $t \in (0, \infty)$ let tX be X scaled by a factor of t.
Define the cardinality function of X to be $|tX|$.

Defining the cardinality (I)

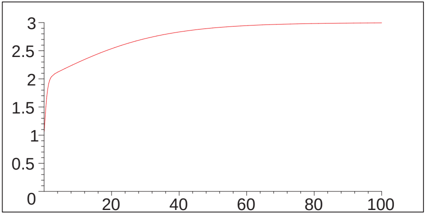
Definition

If X is a finite metric space then (try to) define the cardinality $|X|$ as follows.

1. Define the closeness (or similarity) matrix Z by $Z_{ij} := e^{-d_{ij}}$.
   [Z is symmetric with entries in $[0, 1]$ and 1s on the diagonal.]
2. Invert Z (if possible).
3. Define $|X|$ as the sum of the entries of Z^{-1}.

For $t \in (0, \infty)$ let tX be X scaled by a factor of t.
Define the cardinality function of X to be $|tX|$.

Example



Some obvious conjectures

Conjecture

- *Every finite metric space has a cardinality.*

Some obvious conjectures

Conjecture

- *Every finite metric space has a cardinality.*
- $|tX|$ *is an increasing function of* t.

Some obvious conjectures

Conjecture

- *Every finite metric space has a cardinality.*
- $|tX|$ *is an increasing function of* t.
- *If* X *has* n *points then* $1 \leq |X| \leq n$.

Some obvious conjectures

Conjecture

- *Every finite metric space has a cardinality.*
- $|tX|$ *is an increasing function of* t.
- *If* X *has* n *points then* $1 \leq |X| \leq n$.
- *If all distances are finite then* $|tX| \to 1$ *as* $t \to 0$.

Some obvious conjectures

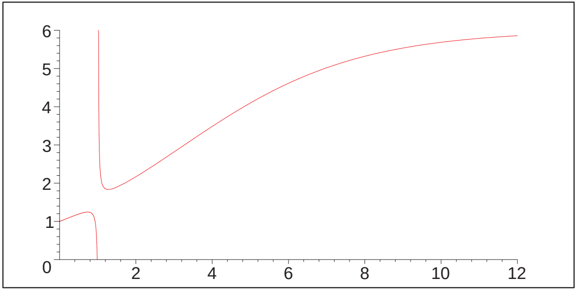
Conjecture

- *Every finite metric space has a cardinality.*
- $|tX|$ *is an increasing function of* t.
- *If* X *has* n *points then* $1 \leq |X| \leq n$.
- *If all distances are finite then* $|tX| \to 1$ *as* $t \to 0$.
- *If* X *has* n *points then* $|tX| \to n$ *as* $t \to \infty$.

Some obvious conjectures

Conjecture

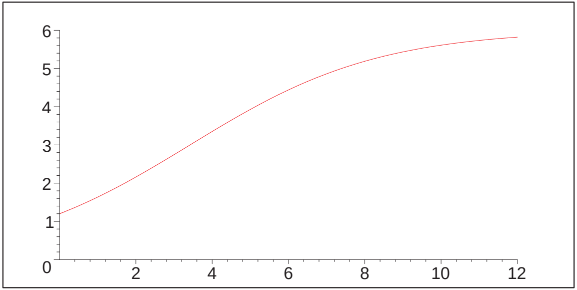
- *Every finite metric space has a cardinality.*
- $|tX|$ *is an increasing function of* t.
- *If* X *has* n *points then* $1 \leq |X| \leq n$.
- *If all distances are finite then* $|tX| \to 1$ *as* $t \to 0$.
- *If* X *has* n *points then* $|tX| \to n$ *as* $t \to \infty$.



Some obvious conjectures

Conjecture

- *Every finite metric space has a cardinality.*
- $|tX|$ *is an increasing function of* t.
- *If* X *has* n *points then* $1 \leq |X| \leq n$.
- *If all distances are finite then* $|tX| \to 1$ *as* $t \to 0$.
- *If* X *has* n *points then* $|tX| \to n$ *as* $t \to \infty$.



Some obvious conjectures

Conjecture

- *Every finite metric space has a cardinality.*
- $|tX|$ *is an increasing function of* t.
- *If* X *has* n *points then* $1 \leq |X| \leq n$.
- *If all distances are finite then* $|tX| \to 1$ *as* $t \to 0$.
- *If* X *has* n *points then* $|tX| \to n$ *as* $t \to \infty$.

Theorem

For any X *with* n *points there exists a* t_0 *such that for* $t > t_0$ *the cardinality* $|tX|$ *exists, is increasing and tends to* n *as* $t \to \infty$.

Defining the cardinality (II)

Definition

Given a finite metric space X, a weighting on X is a number $w_i \in \mathbb{R}$ for each point $i \in X$ such that

$$\sum_{j \in X} e^{-d_{ij}} w_i = 1 \quad \text{for all } i \in X, \qquad \text{i.e.} \quad Zw = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix}.$$

Defining the cardinality (II)

Definition

Given a finite metric space X, a weighting on X is a number $w_i \in \mathbb{R}$ for each point $i \in X$ such that

$$\sum_{j \in X} e^{-d_{ij}} w_j = 1 \quad \text{for all } i \in X, \qquad \text{i.e.} \quad Zw = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix}.$$

If X has a weighting w then define $|X| := \sum_i w_i$.

Defining the cardinality (II)

Definition

Given a finite metric space X, a weighting on X is a number $w_i \in \mathbb{R}$ for each point $i \in X$ such that

$$\sum_{j \in X} e^{-d_{ij}} w_j = 1 \quad \text{for all } i \in X, \qquad \text{i.e.} \quad Zw = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix}.$$

If X has a weighting w then define $|X| := \sum_i w_i$.

Theorem

- *If a weighting exists then it is unique.*

Defining the cardinality (II)

Definition

Given a finite metric space X, a weighting on X is a number $w_i \in \mathbb{R}$ for each point $i \in X$ such that

$$\sum_{j \in X} e^{-d_{ij}} w_i = 1 \quad \text{for all } i \in X, \qquad \text{i.e.} \quad Zw = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix}.$$

If X has a weighting w then define $|X| := \sum_i w_i$.

Theorem

- *If a weighting exists then it is unique.*
- *If Z is invertible then $w_i := \sum_j (Z^{-1})_{ij}$ is a weighting.*

Defining the cardinality (II)

Definition

Given a finite metric space X, a weighting on X is a number $w_i \in \mathbb{R}$ for each point $i \in X$ such that

$$\sum_{j \in X} e^{-d_{ij}} w_j = 1 \quad \text{for all } i \in X, \qquad \text{i.e.} \quad Zw = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix}.$$

If X has a weighting w then define $|X| := \sum_i w_i$.

Theorem

- *If a weighting exists then it is unique.*
- *If Z is invertible then $w_i := \sum_j (Z^{-1})_{ij}$ is a weighting.*

Defining the cardinality (II)

Definition

Given a finite metric space X, a weighting on X is a number $w_i \in \mathbb{R}$ for each point $i \in X$ such that

$$\sum_{j \in X} e^{-d_{ij}} w_i = 1 \quad \text{for all } i \in X, \qquad \text{i.e.} \quad Zw = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix}.$$

If X has a weighting w then define $|X| := \sum_i w_i$.

Theorem

- *If a weighting exists then it is unique.*
- *If Z is invertible then $w_i := \sum_j (Z^{-1})_{ij}$ is a weighting.*

Note

- The weights do not have to be positive!

2: Diversity measures and cardinality

Diversity measures (preliminaries)

Definition

- A probability metric space is a finite metric space X with $p_i \in [0, 1]$ for each $i \in X$ such that $\sum p_i = 1$.

Diversity measures (preliminaries)

Definition

- A probability metric space is a finite metric space X with $p_i \in [0, 1]$ for each $i \in X$ such that $\sum p_i = 1$.
- The mean closeness of $i \in X$ is

$$\sum_j e^{-d_{ij}} p_j = (Zp)_i.$$

This is a measure of the amount of stuff near i.

Diversity measures (preliminaries)

Definition

- A probability metric space is a finite metric space X with $p_i \in [0, 1]$ for each $i \in X$ such that $\sum p_i = 1$.
- The mean closeness of $i \in X$ is

$$\sum_j e^{-d_{ij}} p_j = (Zp)_i.$$

  This is a measure of the amount of stuff near i.
- A surprise function is a decreasing function $\sigma\colon [0, 1] \to [0, \infty]$ with $\sigma(1) = 0$.

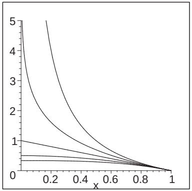
Diversity measures (preliminaries)

Definition

- A probability metric space is a finite metric space X with $p_i \in [0,1]$ for each $i \in X$ such that $\sum p_i = 1$.
- The mean closeness of $i \in X$ is

$$\sum_j e^{-d_{ij}} p_j = (Zp)_i.$$

  This is a measure of the amount of stuff near i.
- A surprise function is a decreasing function $\sigma\colon [0,1] \to [0,\infty]$ with $\sigma(1) = 0$.



Example

There is a useful family σ_α of surprise functions.

$$\sigma_\alpha(p) := \frac{1 - p^{\alpha-1}}{\alpha - 1} \qquad \alpha \in [0,\infty)$$

Diversity measures (definition)

Definition

If (X, p) is a probability metric space then the α-diversity (or expected α-surprise) is

$$D_\alpha(X, p) := \sum p_i \sigma_\alpha((Zp)_i).$$

Diversity measures (definition)

Definition

If (X, p) is a probability metric space then the α-diversity (or expected α-surprise) is

$$D_\alpha(X, p) := \sum p_i \sigma_\alpha((Zp)_i).$$

The α-cardinality $|(X, p)|_\alpha$ is the 'number' of distinct equi-probable species that would give the same expected α-surprise.

Diversity measures (definition)

Definition

If (X, p) is a probability metric space then the α-diversity (or expected α-surprise) is

$$D_\alpha(X, p) := \sum p_i \sigma_\alpha((Zp)_i).$$

The α-cardinality $|(X, p)|_\alpha$ is the 'number' of distinct equi-probable species that would give the same expected α-surprise.

Example

$$|(X, p)|_0 = \sum \frac{p_i}{(Zp)_i} \qquad |(X, p)|_1 = \frac{1}{\prod (Zp)_i{}^{p_i}}$$

$$|(X, p)|_2 = \frac{1}{p^T Zp} \qquad |(X, p)|_\infty = \frac{1}{\max\{(Zp)_i\}}$$

Diversity measures and cardinality

Note

In the case of a discrete space (all the points infinitely far apart), for all α the α-cardinality is maximized by the uniform probability and takes value n.

Diversity measures and cardinality

Note

In the case of a discrete space (all the points infinitely far apart), for all α the α-cardinality is maximized by the uniform probability and takes value n.

Theorem

If X is a finite metric space with a positive weighting w, then $\overline{p}_i := \frac{w_i}{|X|}$ is a probability measure and

$$|(X, \overline{p})|_\alpha = |X| \qquad \textit{for all } \alpha.$$

Diversity measures and cardinality

Note

In the case of a discrete space (all the points infinitely far apart), for all α the α-cardinality is maximized by the uniform probability and takes value n.

Theorem

If X is a finite metric space with a positive weighting w, then $\overline{p}_i := \frac{w_i}{|X|}$ is a probability measure and

$$|(X, \overline{p})|_\alpha = |X| \qquad \textit{for all } \alpha.$$

In many cases $|X|$ maximizes the cardinality.

Diversity measures and cardinality

Note

In the case of a discrete space (all the points infinitely far apart), for all α the α-cardinality is maximized by the uniform probability and takes value n.

Theorem

If X is a finite metric space with a positive weighting w, then $\overline{p}_i := \frac{w_i}{|X|}$ is a probability measure and

$$|(X, \overline{p})|_\alpha = |X| \qquad \text{for all } \alpha.$$

In many cases $|X|$ maximizes the cardinality.

So it looks like a weighting on a metric space is analogous to the uniform distribution on a set of points.

3: Cardinality and continuous metric spaces

Approximating continuous metric spaces

Try to define the cardinality of a nice subset of Euclidean space by approximating with a finite set of points.

Approximating continuous metric spaces

Try to define the cardinality of a nice subset of Euclidean space by approximating with a finite set of points.

Example

Let L_a be a line segment of length a.

Approximating continuous metric spaces

Try to define the cardinality of a nice subset of Euclidean space by approximating with a finite set of points.

Example

Let L_a be a line segment of length a.
Approximate by a set of points: take $\sum_1^{n-1} d_i = a$ and let X_d be

$$\bullet \overset{d_1}{\longleftrightarrow} \bullet \overset{d_2}{\longleftrightarrow} \bullet \ldots \bullet \overset{d_{n-1}}{\longleftrightarrow} \bullet$$

$$|X_d| = \left(\sum \tanh d_i\right) + 1$$

Approximating continuous metric spaces

Try to define the cardinality of a nice subset of Euclidean space by approximating with a finite set of points.

Example

Let L_a be a line segment of length a.
Approximate by a set of points: take $\sum_1^{n-1} d_i = a$ and let X_d be

$$\bullet \overset{d_1}{\longleftrightarrow} \bullet \overset{d_2}{\longleftrightarrow} \bullet \ldots \bullet \overset{d_{n-1}}{\longleftrightarrow} \bullet$$

$$|X_d| = \left(\sum \tanh d_i\right) + 1 \to a + 1 \qquad \text{as } \max\{d_i\} \to 0.$$

Approximating continuous metric spaces

Try to define the cardinality of a nice subset of Euclidean space by approximating with a finite set of points.

Example

Let L_a be a line segment of length a.
Approximate by a set of points: take $\sum_1^{n-1} d_i = a$ and let X_d be

$$\bullet \overset{d_1}{\longleftrightarrow} \bullet \overset{d_2}{\longleftrightarrow} \bullet \ldots \bullet \overset{d_{n-1}}{\longleftrightarrow} \bullet$$

$$|X_d| = \left(\sum \tanh d_i\right) + 1 \to a + 1 \qquad \text{as } \max\{d_i\} \to 0.$$

So we can define the cardinality of the length a line segment

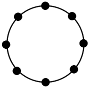
$$|L_a| = a + 1$$

Approximating the circle

Let C_a be the circle of circumference a (with the metric induced from $\mathbb{R}^2$).

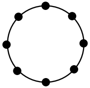
Approximating the circle

Let C_a be the circle of circumference a (with the metric induced from $\mathbb{R}^2$).
Approximate by a symmetric set of points:



Approximating the circle

Let C_a be the circle of circumference a (with the metric induced from $\mathbb{R}^2$). Approximate by a symmetric set of points:

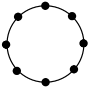


Find that as the number of points tends to infinity we can define

$$|C_a| = \frac{1}{\int_0^1 e^{-2aD(s)} ds}$$

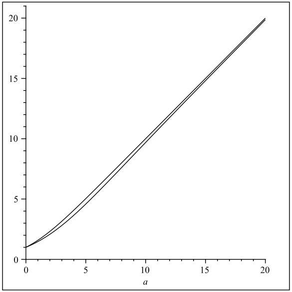
Approximating the circle

Let C_a be the circle of circumference a (with the metric induced from $\mathbb{R}^2$). Approximate by a symmetric set of points:



Find that as the number of points tends to infinity we can define

$$|C_a| = \frac{1}{\int_0^1 e^{-2aD(s)} ds}$$



$$|C_a| \to 1 \quad \text{as } a \to 0$$

$$|C_a| - a \to 0 \quad \text{as } a \to \infty$$

Intrinsic volume

Definition

An invariant valuation μ on (polyconvex) subsets of $\mathbb{R}^m$ is a (continuous, motion invariant) $\mathbb{R}$-valued function such that

- $\mu(A \cup B) = \mu(A) + \mu(B) - \mu(A \cap B)$.

Intrinsic volume

Definition

An invariant valuation μ on (polyconvex) subsets of $\mathbb{R}^m$ is a (continuous, motion invariant) $\mathbb{R}$-valued function such that

- $\mu(A \cup B) = \mu(A) + \mu(B) - \mu(A \cap B)$.

Theorem (Hadwiger's Theorem)

There is a canonical basis $\{\mu_m, \ldots, \mu_0\}$ of invariant valuations on subsets of $\mathbb{R}^m$ and these have the scaling property $\mu_i(tA) = t^i \mu_i(A)$.

Intrinsic volume

Definition

An invariant valuation μ on (polyconvex) subsets of $\mathbb{R}^m$ is a (continuous, motion invariant) $\mathbb{R}$-valued function such that

- $\mu(A \cup B) = \mu(A) + \mu(B) - \mu(A \cap B)$.

Theorem (Hadwiger's Theorem)

There is a canonical basis $\{\mu_m, \ldots, \mu_0\}$ of invariant valuations on subsets of $\mathbb{R}^m$ and these have the scaling property $\mu_i(tA) = t^i \mu_i(A)$.

Example

- $\mu_m =$ usual (Lebesgue) volume
- $\mu_{m-1} = \frac{1}{2}$"surface area"
- $\mu_0 =$ Euler characteristic

Intrinsic volume

Definition

An invariant valuation μ on (polyconvex) subsets of $\mathbb{R}^m$ is a (continuous, motion invariant) $\mathbb{R}$-valued function such that

- $\mu(A \cup B) = \mu(A) + \mu(B) - \mu(A \cap B)$.

Theorem (Hadwiger's Theorem)

There is a canonical basis $\{\mu_m, \ldots, \mu_0\}$ *of invariant valuations on subsets of* $\mathbb{R}^m$ *and these have the scaling property* $\mu_i(tA) = t^i \mu_i(A)$.

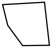
Example

- $\mu_m =$ usual (Lebesgue) volume
- $\mu_{m-1} = \frac{1}{2}$"surface area"
- $\mu_0 =$ Euler characteristic

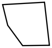
Theorem

The Wills function $W(A) := \mu_m(A) + \mu_{m-1}(A) + \cdots + \mu_0(A)$
is multiplicative: $W(A \times B) = W(A) \times W(B)$.

Asymptotic conjecture

A		$W(A)$
finite collection of points		(number of points)
closed interval		(length) $+ 1$
polygon		(perimeter)
filled polygon		(area) $+ \frac{1}{2}$(perimeter) $+ 1$
unit ball in $\mathbb{R}^3$		$\frac{4}{3}\pi + 2\pi + 4 + 1$

Asymptotic conjecture

A		$W(A)$
finite collection of points		(number of points)
closed interval		(length) $+ 1$
polygon		(perimeter)
filled polygon		(area) $+ \frac{1}{2}$(perimeter) $+ 1$
unit ball in $\mathbb{R}^3$		$\frac{4}{3}\pi + 2\pi + 4 + 1$

Conjecture

The cardinality can be defined for any compact subset of $\mathbb{R}^n$ and

$$|tA| - W(tA) \to 0 \quad as \quad t \to \infty.$$