

Maximum entropy, uniform measure

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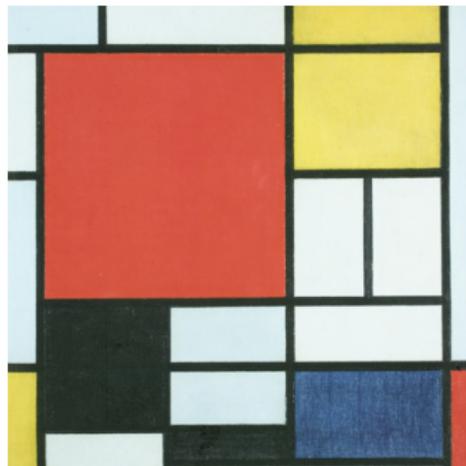
ML@CL Seminar
Cambridge Computer Laboratory
13th November 2020



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Plan

I. Quantifying diversity

II. Diversity and entropy

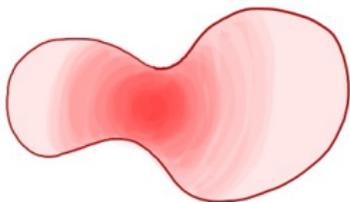
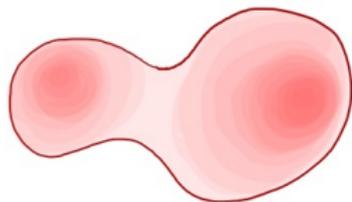
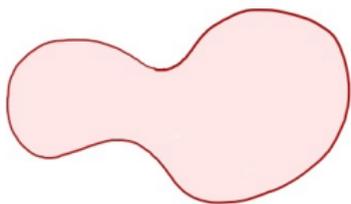
III. Maximizing entropy

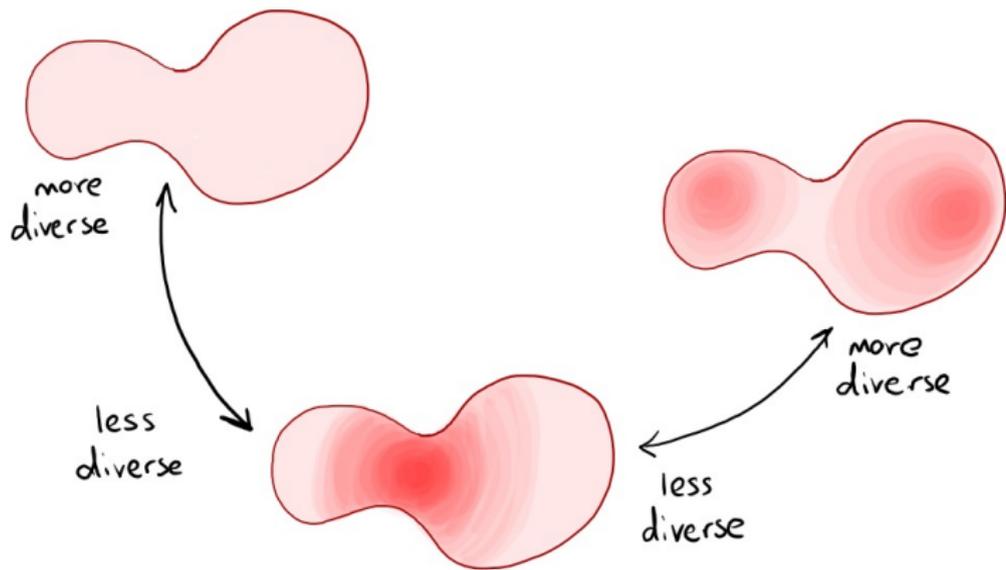
IV. Uniform measure

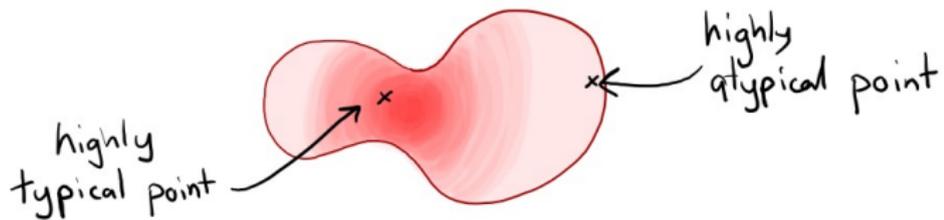
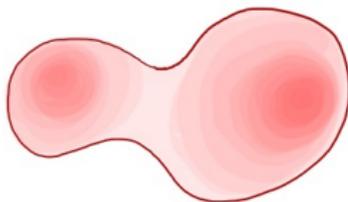
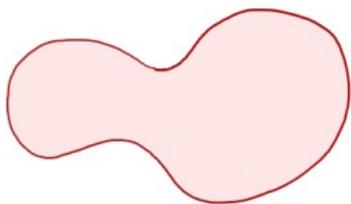
V. Categorical connections

Part I

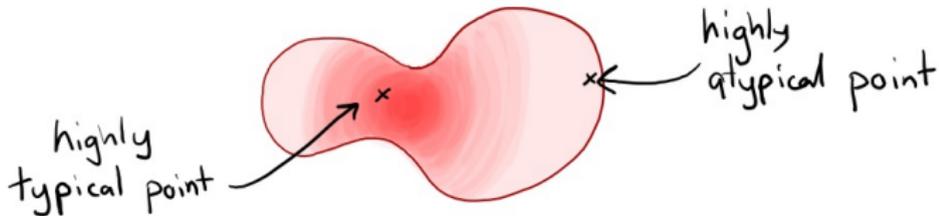
Quantifying Diversity







"Diversity is average atypicality."



Spaces with similarities

Definition

Let X be a compact Hausdorff topological space.

A **similarity kernel** on X is a continuous function $K : X \times X \rightarrow [0, \infty)$ satisfying $K(x, x) > 0$ for all $x \in X$.

The pair (X, K) is called a **space with similarities**.

It's **symmetric** if $K(x, y) = K(y, x)$ for all $x, y \in X$.

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Example

A compact metric space with metric d has similarity kernel

$$K(x, y) = e^{-d(x, y)}.$$

When $X = \mathbb{R}^d$ this is the **Laplace kernel**.

Typicality functions

Definition

Let (X, K) be a space with similarities.

For each probability distribution μ on X , and each $x \in X$, define

$$(K\mu)(x) = \int K(x, -) d\mu \in [0, \infty).$$

The function $K\mu : X \rightarrow [0, \infty)$ is the **typicality function** of μ .

The **atypicality function** of μ is $1/K\mu$.

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Example

If X is a compact metric space, the typicality function of μ is given by

$$(K\mu)(x) = \int e^{-d(x,y)} d\mu(y).$$

Diversity

Definition

Let (X, K) be a space with similarities, and μ a probability distribution on X . For $q \in [0, \infty)$ not equal to 1, the **diversity of order q** of μ is

$$D_q^K(\mu) = \left(\int \left(\frac{1}{K\mu} \right)^{1-q} d\mu \right)^{1/(1-q)} .$$

At $q = 1, \infty$ this expression takes its limiting values.

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Example

If X is a compact metric space, then

$$D_q(\mu) = \left(\int \left(\int e^{-d(x,y)} d\mu(x) \right)^{q-1} d\mu(y) \right)^{1/(1-q)}.$$

Part II

Diversity and Entropy

Diversity on finite sets

Equip the set $X = \{x_1, \dots, x_n\}$ with the similarity kernel K (a matrix). Let $\mu = (\mu_1, \dots, \mu_n)$ be a probability distribution on X .

The diversity of order q of μ is

$$D_q^K(\mu) = \left(\sum_{\text{supp}\mu} (K\mu)_i^{q-1} \mu_i \right)^{1/(1-q)} .$$

Diversity on finite sets

Equip the set $X = \{x_1, \dots, x_n\}$ with the similarity kernel $K = I$.
Let $\mu = (\mu_1, \dots, \mu_n)$ be a probability distribution on X .

The diversity of order q of μ is

$$D_q^!(\mu) = \left(\sum_{\text{supp}\mu} \mu_i^q \right)^{1/(1-q)} = \exp(H_q(\mu))$$

where H_q is the **Rényi entropy** of order q .

Diversity on finite sets

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$$D_q^I(\mu) = \left(\sum_{\text{supp} \mu} \mu_i^q \right)^{1/(1-q)} = \exp(H_q(\mu))$$

where H_q is the **Rényi entropy** of order q .

In particular,

$$D_1^I(\mu) = \exp\left(-\sum \mu_i \log \mu_i\right) = \exp(\mathbf{Shannon}(\mu)).$$

Entropy in ecology

To ecologists, $\exp(H_q(\mu))$ is known as the **Hill number** of order q .

The Hill numbers are used as measures of **ecological diversity**.

Strategy Model an ecological community by a set of species X and a distribution μ on X , representing the relative abundances of species.

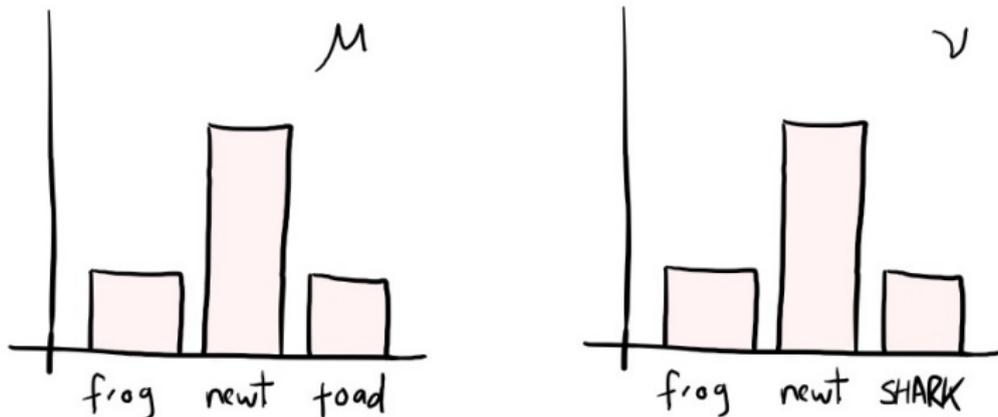
Then take the Hill number

$$\exp(H_q(\mu)) = D_q^I(\mu)$$

to quantify the 'diversity' of the community.

Entropy in ecology

Problem The Hill numbers don't see similarities between species.



$$H_q(\mu) = H_q(\nu)$$

Similarity-sensitive diversity

Solution (Cobbold and Leinster, 2012)

Record **pairwise similarities** of the species in a matrix, K . Define the **similarity-sensitive diversity of order q** to be

$$D_q^K(\mu) = \left(\sum_{\text{supp}\mu} (K\mu)_i^{q-1} \mu_i \right)^{1/(1-q)} .$$

This is where our diversity measures originate.

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This is where our diversity measures originate.

For example,

$$D_2^K = \frac{1}{\text{expected similarity of two individuals chosen at random}}$$

while

$$D_2^I = \frac{1}{\text{probability that they're of the same species}}.$$

Similarity-sensitive entropy

In the general setting of a space with similarities, we **define**

$$\text{entropy} := \log(\text{diversity}).$$

Definition

Let (X, K) be a space with similarities, and μ a distribution on X . For $q \in [0, \infty]$, the **entropy of order q** of μ is $H_q^K(\mu) = \log D_q^K(\mu)$.

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Example

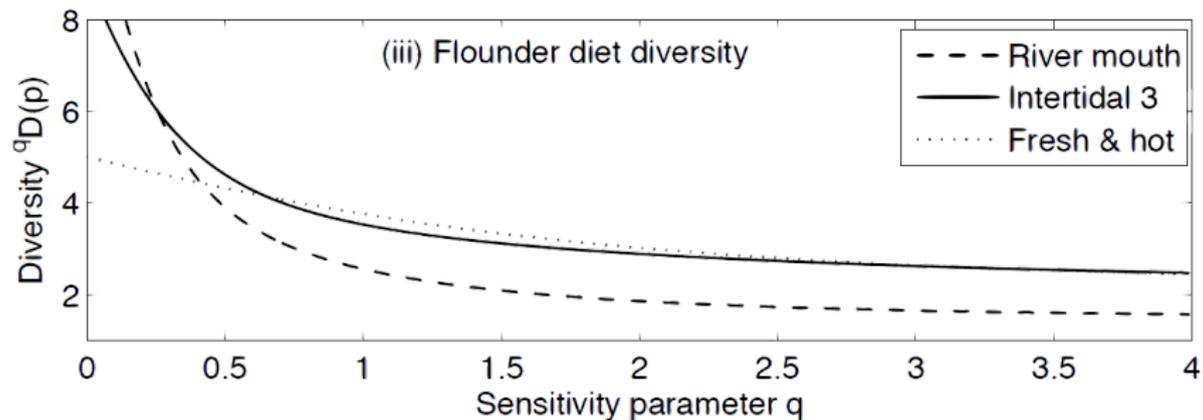
If X is a compact metric space, then

$$H_1(\mu) = - \int \log \left(\int e^{-d(x,y)} d\mu(x) \right) d\mu(y).$$

Part III

Maximizing Diversity and Entropy

The parameter q matters!



Leinster and Cobbold, *Measuring Diversity...*, Ecology 93 (2012)

A maximum entropy theorem

Theorem (Leinster and Roff, 2019)

Let (X, K) be a symmetric space with similarities.

- 1. There exists a probability distribution μ on X that maximises $D_q^K(\mu)$ and $H_q^K(\mu)$ for all $q \in [0, \infty]$ at once.*
- 2. The maximum diversity $\sup_{\mu} D_q^K(\mu)$ and maximum entropy $\sup_{\mu} H_q^K(\mu)$ are independent of $q \in [0, \infty]$.*

A maximum entropy theorem

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2. The maximum diversity $\sup_{\mu} D_q^K(\mu)$ and maximum entropy $\sup_{\mu} H_q^K(\mu)$ are independent of $q \in [0, \infty]$.

- If μ maximises H_q^K for one q , it maximises for all q .
- In general μ need not be unique, but if K is positive-definite, it is.
- So every compact subset of \mathbb{R}^n has a unique distribution of maximum entropy. For almost all sets, we don't know what it is!

New invariants

Definition

Let (X, K) be a symmetric space with similarities.

The **maximum diversity** of X is

$$D_{\max}(X) = \sup_{\mu} D_q(\mu) \text{ for any } q.$$

The **maximum entropy** of X is

$$H_{\max}(X) = \log D_{\max}(X).$$

A distribution attaining the supremum is called **maximising**.

Part IV

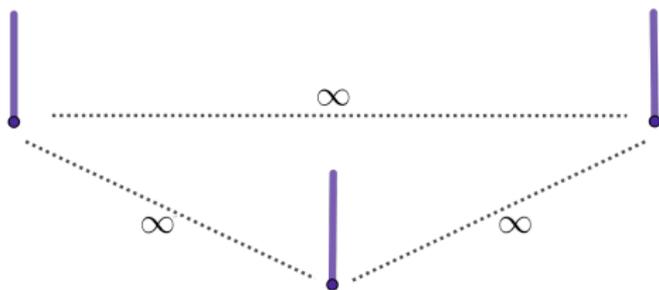
Uniform Distributions

A maximising measure

Take a finite set X , and $K = I$. Then

$$D_{\max}(X) = \sup D_1^I = \sup(\exp(\text{Shannon}))$$

which is uniquely attained by the uniform distribution.

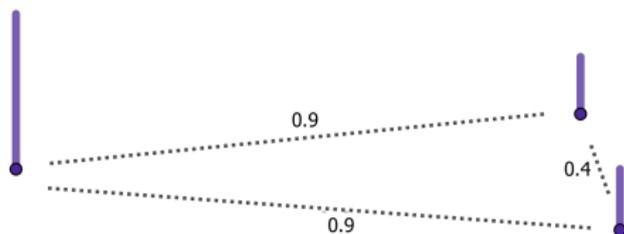


A maximising measure

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This no longer holds when $K \neq I$.

Balance

Maximising distributions possess a different sort of 'evenness', which is responsive to the geometry of the space.

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A distribution μ on X is **balanced** if $K\mu$ is constant on $\text{supp}(\mu)$.

Lemma

Any maximising distribution is balanced.

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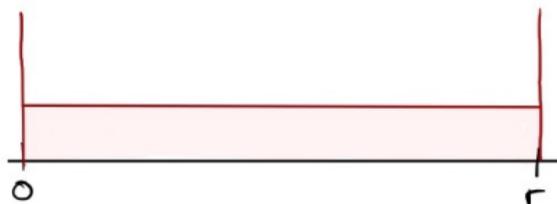
Lemma

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Example

If an ecological community is **maximally diverse**, then all the species present must be **equally typical**.

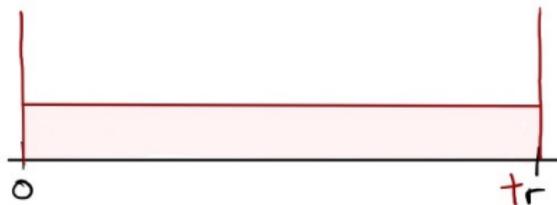
Balance is not uniformity



Consider $[0, r] \subset \mathbb{R}$. Its maximising distribution is

$$\mu = \frac{\delta_0 + \lambda_{[0,r]} + \delta_r}{2 + r}.$$

Balance is not uniformity



Scale the space by $t > 0$. The maximising distribution on $[0, tr]$ is

$$\mu_t = \frac{\delta_0 + t\lambda_{[0, tr]} + \delta_r}{2 + tr}.$$

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Uniform distribution

Given a metric space X and any $t \in [0, \infty)$, write tX for the space X after its distances have been scaled by t .

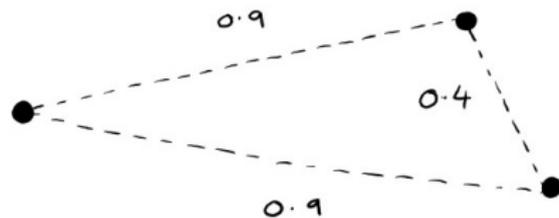
Definition

Let X be a compact metric space. Suppose tX has a unique maximising distribution μ_t for all $t \gg 0$, and that $\lim_{t \rightarrow \infty} \mu_t$ exists in $P(X)$.

Then the **uniform distribution** on X is

$$\mu_X = \lim_{t \rightarrow \infty} \mu_t.$$

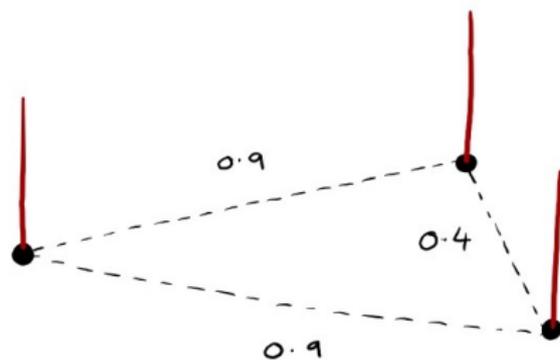
Example



Proposition

On a finite metric space, the uniform measure is the uniform measure.

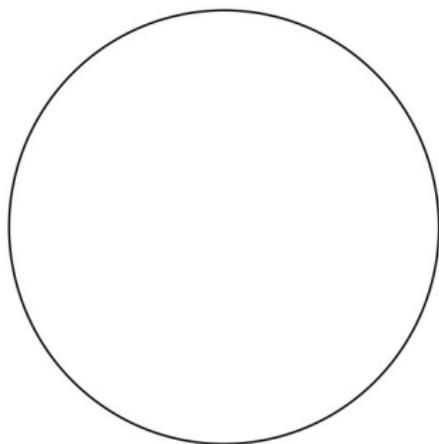
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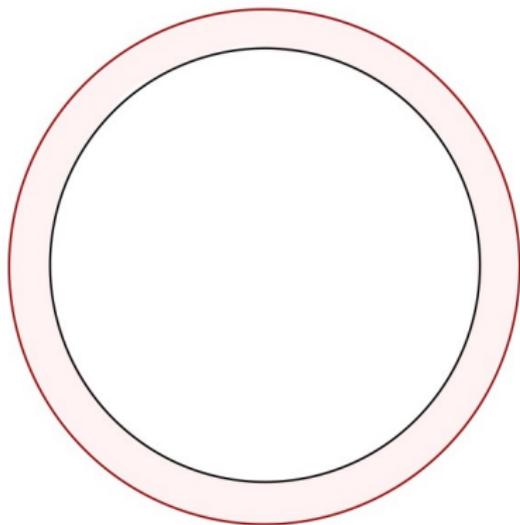
Example



Proposition

On a homogeneous space, the uniform measure is the Haar measure.

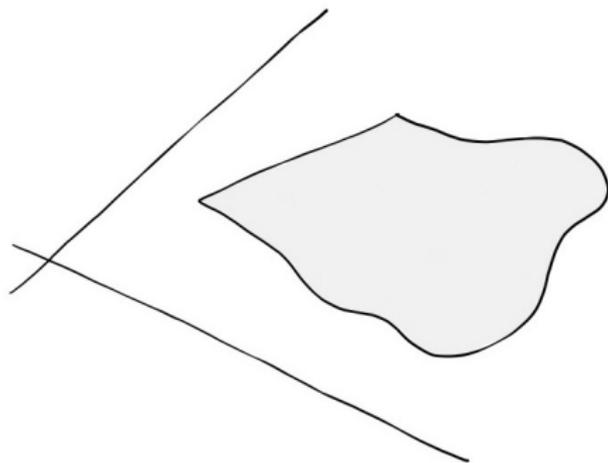
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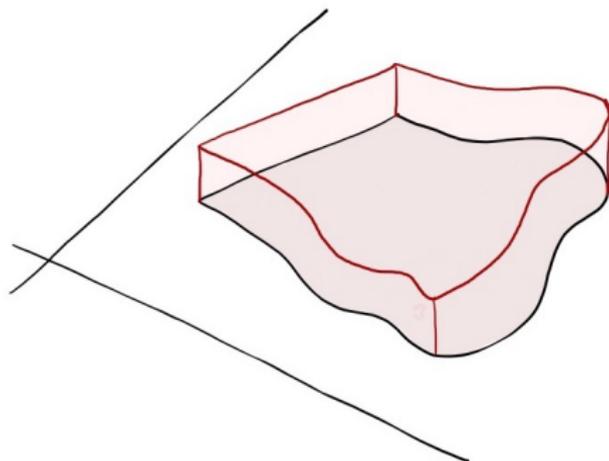
Example



Proposition

On a compact subset of \mathbb{R}^n with nonzero volume, the uniform measure is normalised Lebesgue measure.

Example



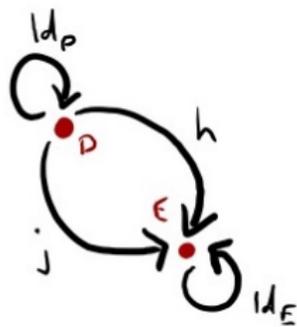
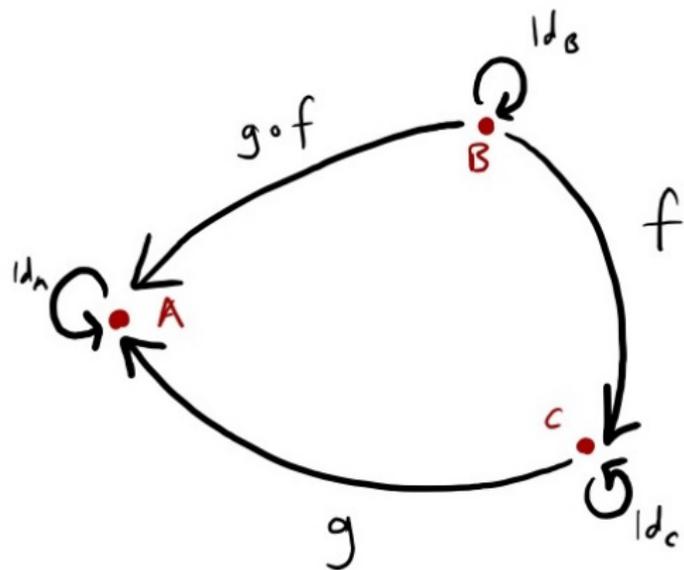
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Part V

Categorical Connections

Ordinary categories



Ordinary categories

A **category** \mathbf{A} consists of

- (Objects) A set $\text{ob}(\mathbf{A})$
- (Morphisms) For each $A, B \in \text{ob}(\mathbf{A})$ a set $\text{Hom}(A, B)$
- (Identities) For each $A \in \text{ob}(\mathbf{A})$ a function $\{*\} \rightarrow \text{Hom}(A, A)$
- (Composition) For each $A, B, C \in \text{ob}(\mathbf{A})$ a function

$$\text{Hom}(A, B) \times \text{Hom}(B, C) \rightarrow \text{Hom}(A, C).$$

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Idea

Why not replace sets and functions with something more interesting?

All we really need is a 'multiplication' like \times with a 'unit' like $\{*\}$.

Enriched categories

Let \mathcal{V} be a category with a monoidal product \otimes and unit I .

A \mathcal{V} -category \mathbf{A} consists of

- (Objects) A set $\text{ob}(\mathbf{A})$
- (Morphisms) For each $A, B \in \text{ob}(\mathbf{A})$ an object of \mathcal{V} , $\text{Hom}(A, B)$
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Examples

- If $\mathcal{V} = (\perp \rightarrow \top, \wedge)$, a \mathcal{V} -category is a preorder.
- If $\mathcal{V} = (\mathbf{Vect}, \otimes)$, a one-object \mathcal{V} -category is an associative algebra.

$[0, \infty)$ -categories

Let $\mathcal{V} = [0, \infty)$. It's a category: there's an arrow $x \rightarrow y$ if and only if $x \geq y$. It has a monoidal product $+$ with unit 0 .

A $[0, \infty)$ -category \mathbf{X} consists of

- (Objects) A set \mathbf{X}
- (Morphisms) For each $x, y \in \mathbf{X}$ a number $d(x, y) \in [0, \infty)$
- (Identities) For each $x \in \mathbf{X}$ an inequality $0 \geq d(x, x)$
- (Composition) For each $x, y, z \in \mathbf{X}$ an inequality,

$$d(x, y) + d(y, z) \geq d(x, z).$$

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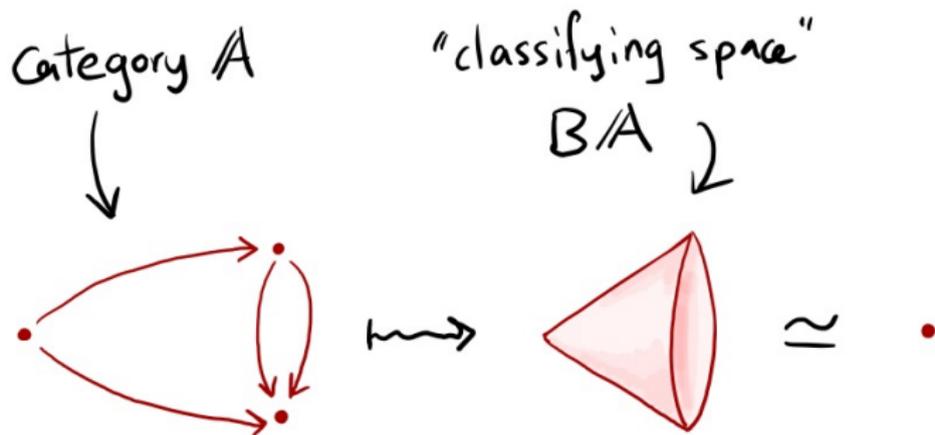
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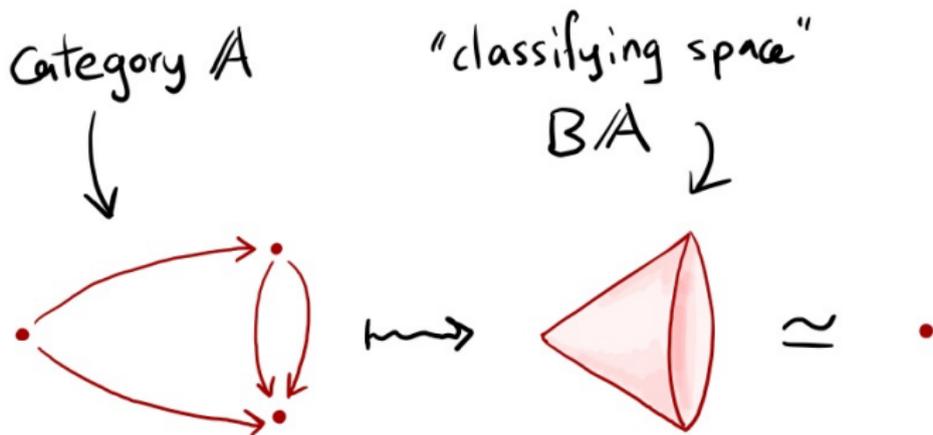
Moral A $[0, \infty)$ -category is a generalized metric space.

The Euler characteristic of a category



$$\chi(A) := \chi(B/A) = 1$$

The Euler characteristic of a category



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Questions

- What is the Euler characteristic of an **enriched category**?
- What is the Euler characteristic of a **metric space**?

The magnitude (or Euler characteristic) of a metric space

Let X be a compact metric space.

Definition

A **weighting** on X is a signed measure ν such that $K\nu \equiv 1$.

If X possesses a weighting ν , the **magnitude** of X is

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The magnitude (or Euler characteristic) of a metric space

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Definition

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If X possesses a weighting ν , the **magnitude** of X is

$$\chi(X) := \nu(X).$$

Now let μ be a **maximum entropy distribution** on X .

We know it's **balanced**: $K\mu|_{\text{supp } \mu} \equiv c$ for some constant c .

So its **restriction to $\text{supp } \mu$** is proportional to a weighting, $\hat{\mu} = \frac{1}{c}\mu$.

Theorem

$D_{\max}(X) = \chi(\text{supp } \mu)$ for any *maximising measure* μ .

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- Leinster and Roff, *The maximum entropy of a metric space*. arXiv:1908.11184 (2019).