Topology and Data

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Introduction / Motivations

- General area of *geometric data analysis* attempts to give insight into data by imposing a geometry on it

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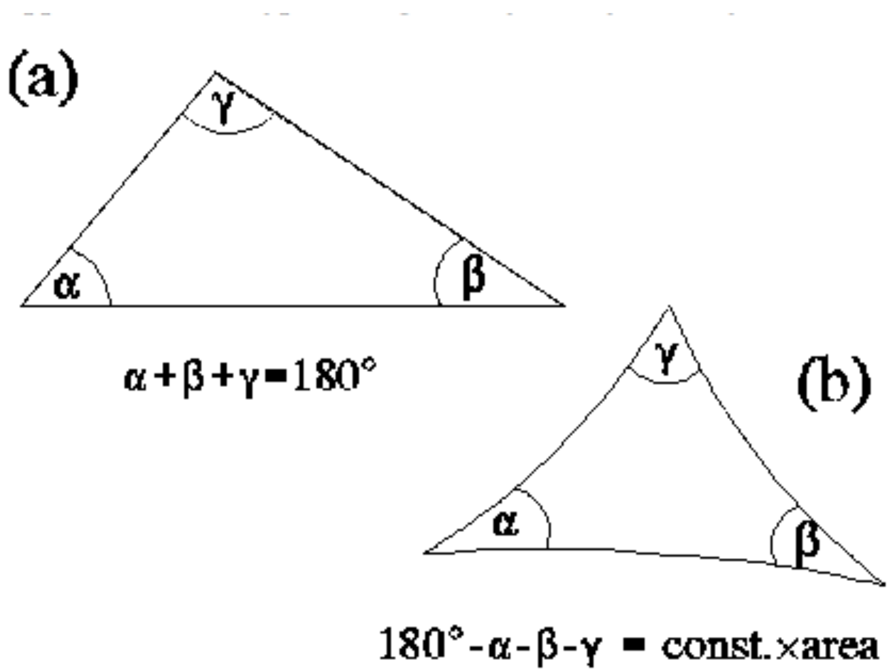
- Value of geometry is that it allows us to organize and view data more effectively, for better understanding
- Can obtain an idea of a reasonable layout or overview of the data
- Sometimes all that is required is a qualitative overview

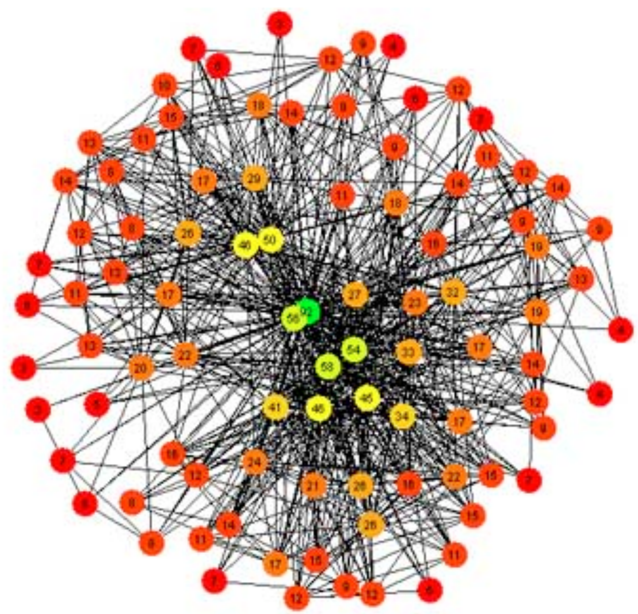
Methods for Imposing a Geometry



hyperbolic metric
(non-Euclidean)

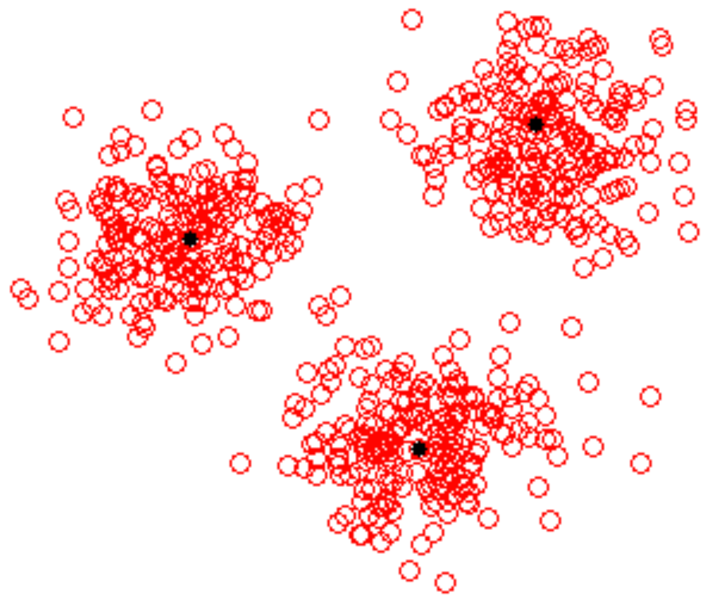
Define a metric

Methods for Imposing a Geometry



Define a graph or network structure

Methods for Imposing a Geometry



Cluster the data

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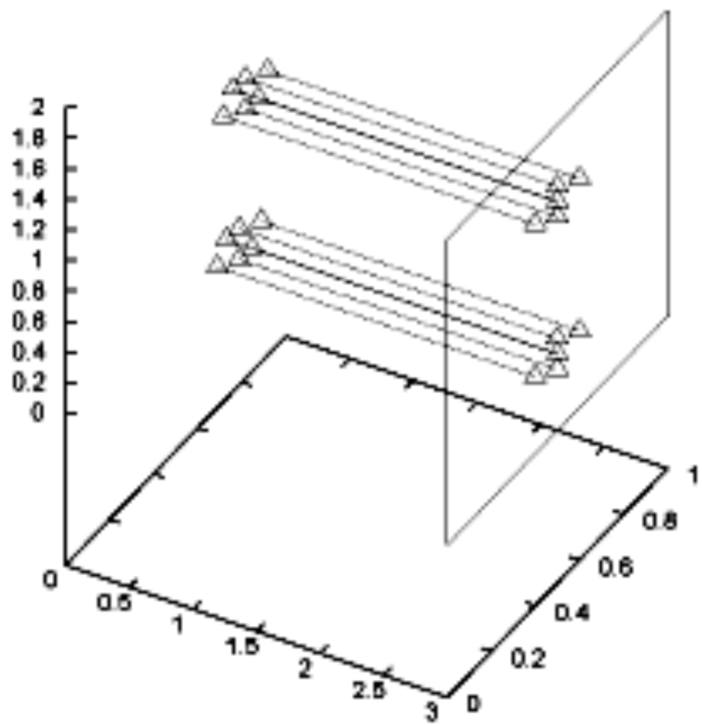
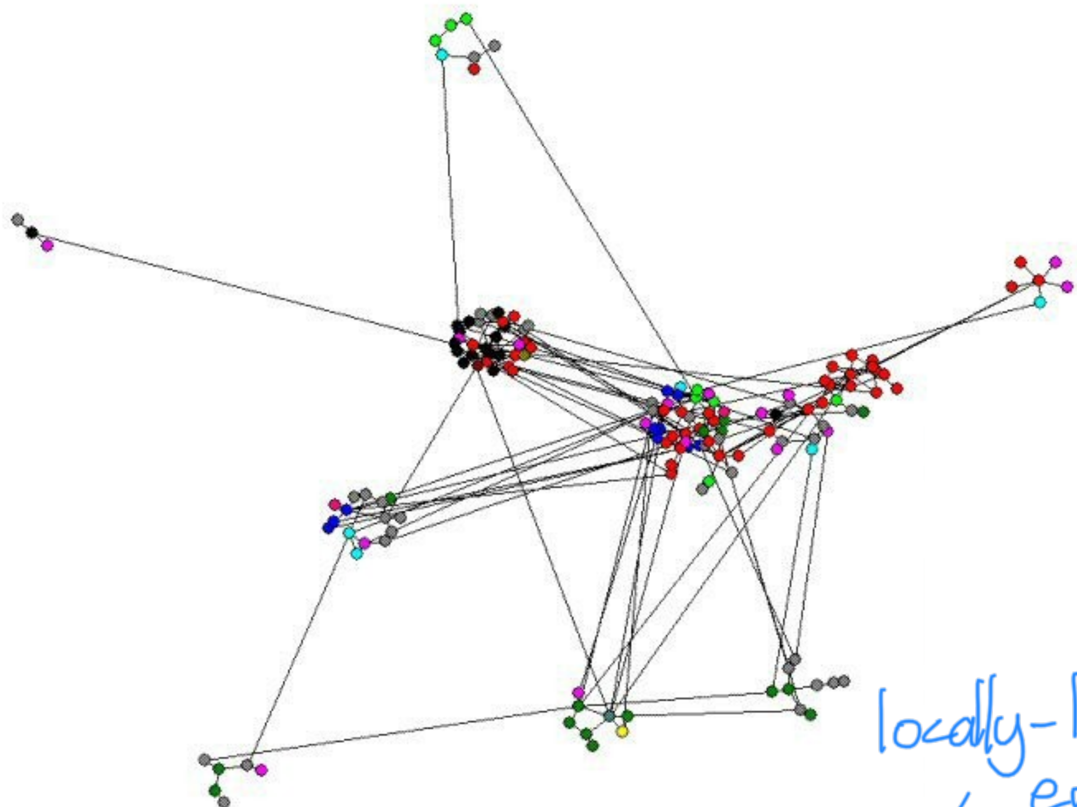
Methods for Summarizing or Visualizing a Geometry



dimensionality reduction

Linear projections

Methods for Summarizing or Visualizing a Geometry



locally-linear embedding

Multidimensional scaling, ISOMAP, LLE

nonlinear dimensionality reduction

Methods for Summarizing or Visualizing a Geometry

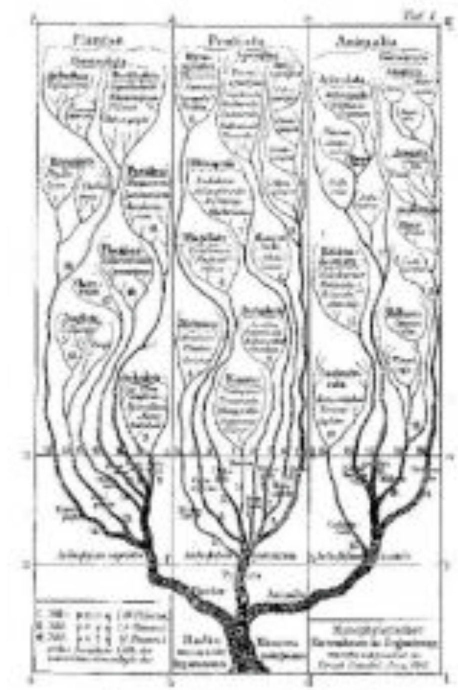


Figure 1: Haeckel's tree with 3 branches

Project to a tree

Properties of Data Geometries

We Don't Trust Large Distances

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models of DNA evolution

evolutionary distance (in terms of the expected number of changes) between two sequences:

$$d = -\frac{3}{4}\ln\left(1-\frac{4}{3}p\right)$$

p: portion of sites that differ between the two sequences

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- In physics, distances have strong theoretical backing, and should be viewed as reliable
- In biology or social sciences, distances are constructed using a notion of similarity, but have no theoretical backing (e.g. Jukes-Cantor distance between sequences)
- Means that small distances still represent similarity, but comparison of long distances makes little sense

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- Similarity more like a 0/1-valued quantity than $\mathbb{R}$-valued

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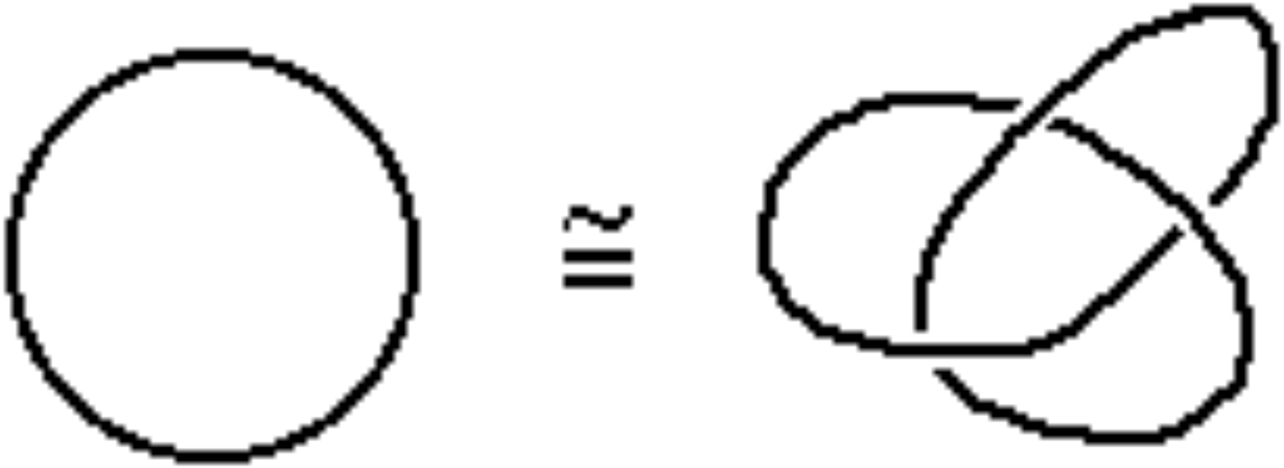
- Distance measurements are noisy, as are the connections in many graph models
- Requires stochastic geometric methods for study
- Methods of Coifman et al and others relevant here

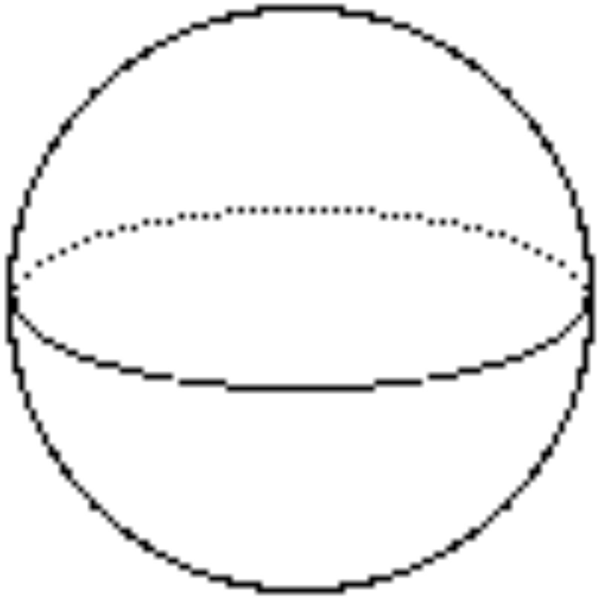
Geometric diffusions as a tool for harmonic analysis and structure definition of data
(Proceedings of the National Academy of Sciences) 2005

Topology

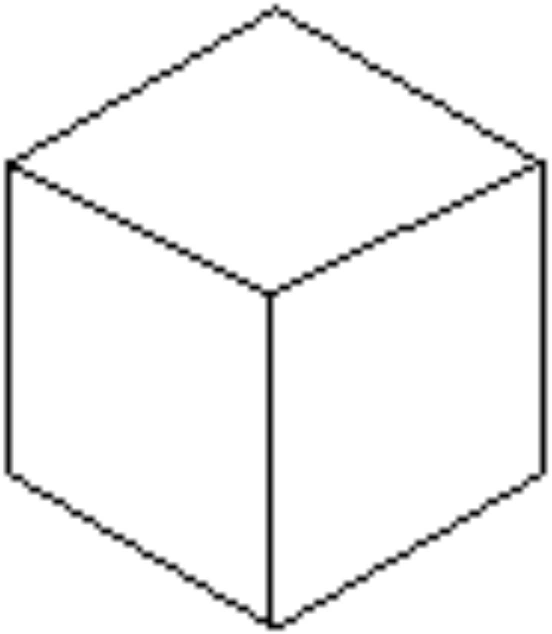


Homeomorphic

Topology



$\cong$



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- We do not permit "tearing", i.e. distorting distances in a discontinuous way
- How to make this precise?

Topology

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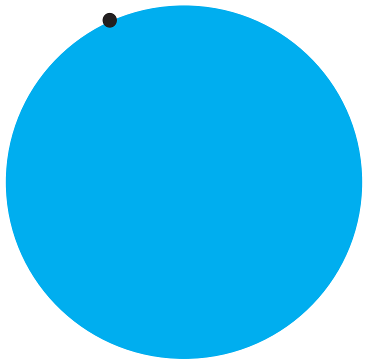
- Idea: consider instead distances from points to subsets. Can be zero.



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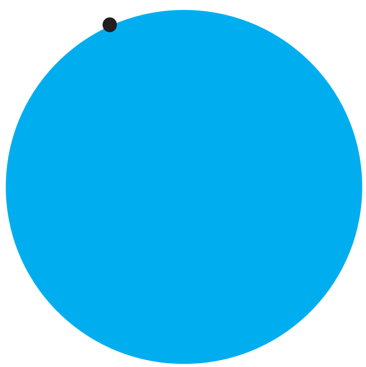

This accomplishes the intuitive idea of permitting arbitrary rescalings of distances while leaving "infinite nearness" intact.

closure

Topology

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- Means in particular finding ways of tracking or summarizing behavior as metrics are deformed or other parameters are changed
- Ultimately means building in noise and uncertainty. This is in the future - "statistical topology".

Outline

1. Homology as signature for shape identification

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4. Signatures for significance of structural invariants

Persistent Homology

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- For every space X and dimension k, constructs a vector space $H_k(X)$ whose dimension (the k-th *Betti number* β_k) is a mathematically precise version of the intuitive notion of counting "k-dimensional holes"

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Gaussian elimination

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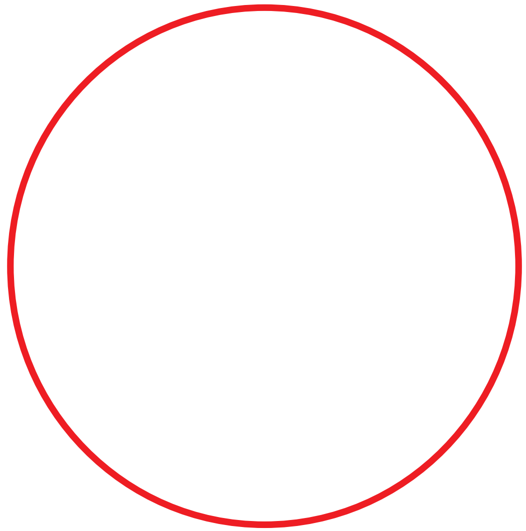
- β_0 is a count of the number of connected components
- β_i's form a signature which encodes topological information about the shape

Persistent Homology



$\beta_0 = 1$, $\beta_1 = 1$, and $\beta_i = 0$ for $i \geq 2$

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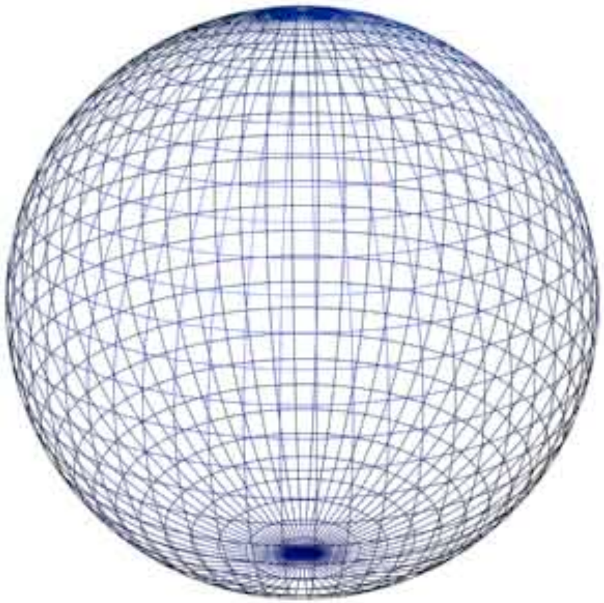

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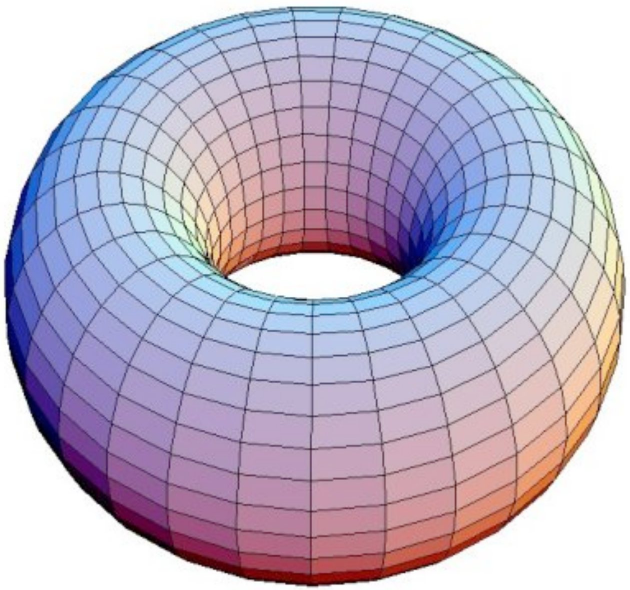

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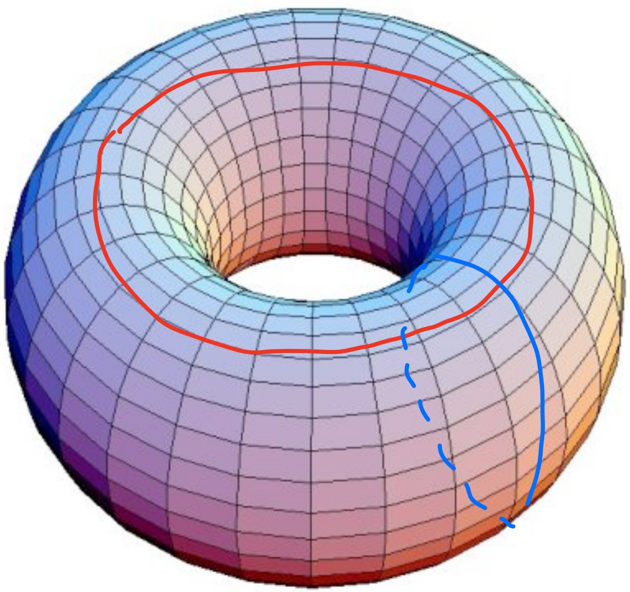

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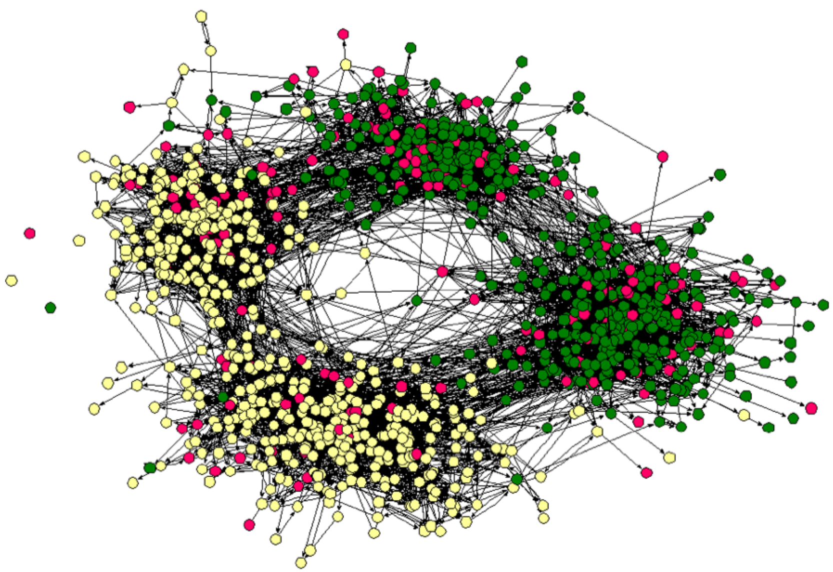
Persistent Homology

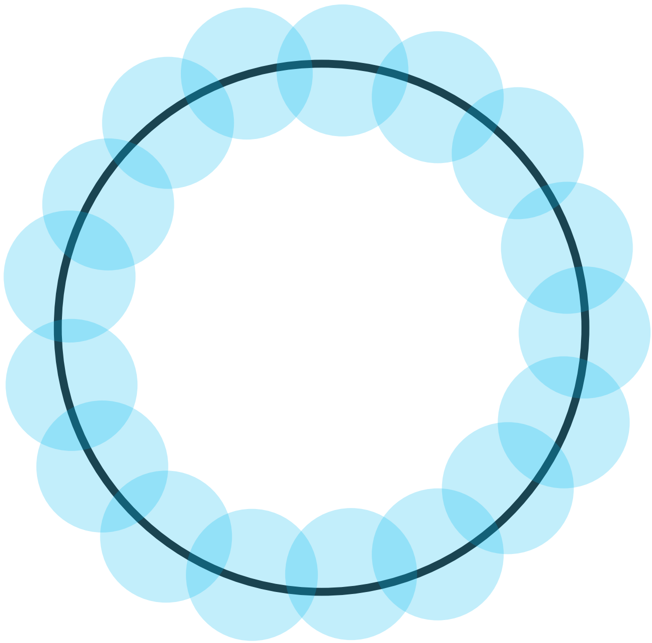
modeling

Question: For a point cloud X , can one infer the Betti numbers of the space $\mathbb{X}$ from which it is sampled?

reality



Persistent Homology - Čech Complex



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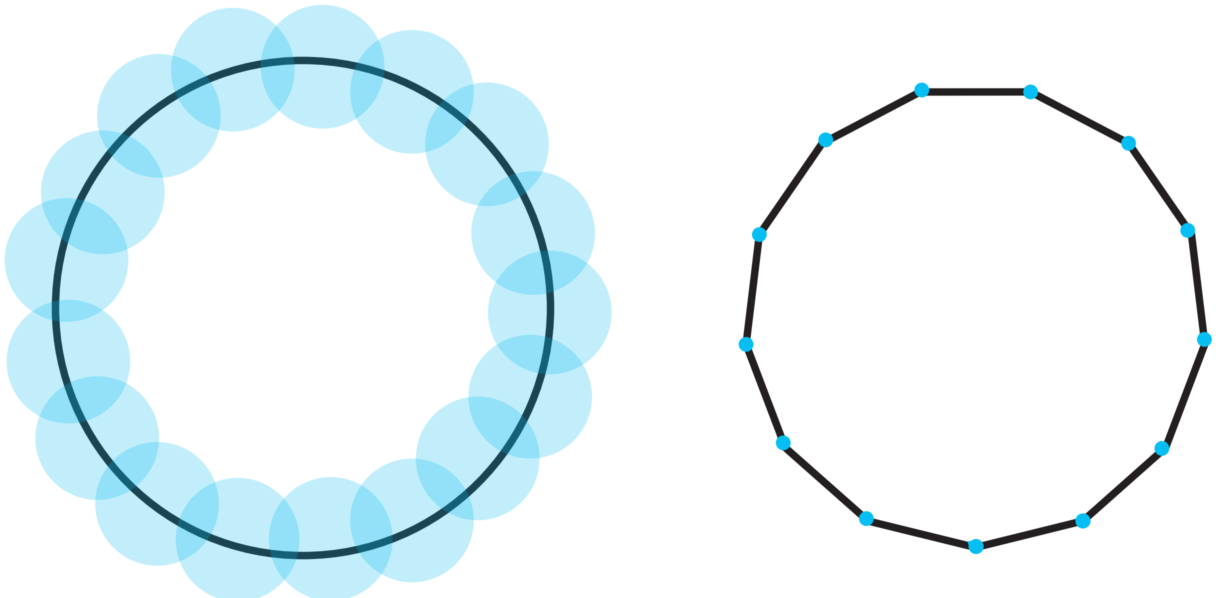

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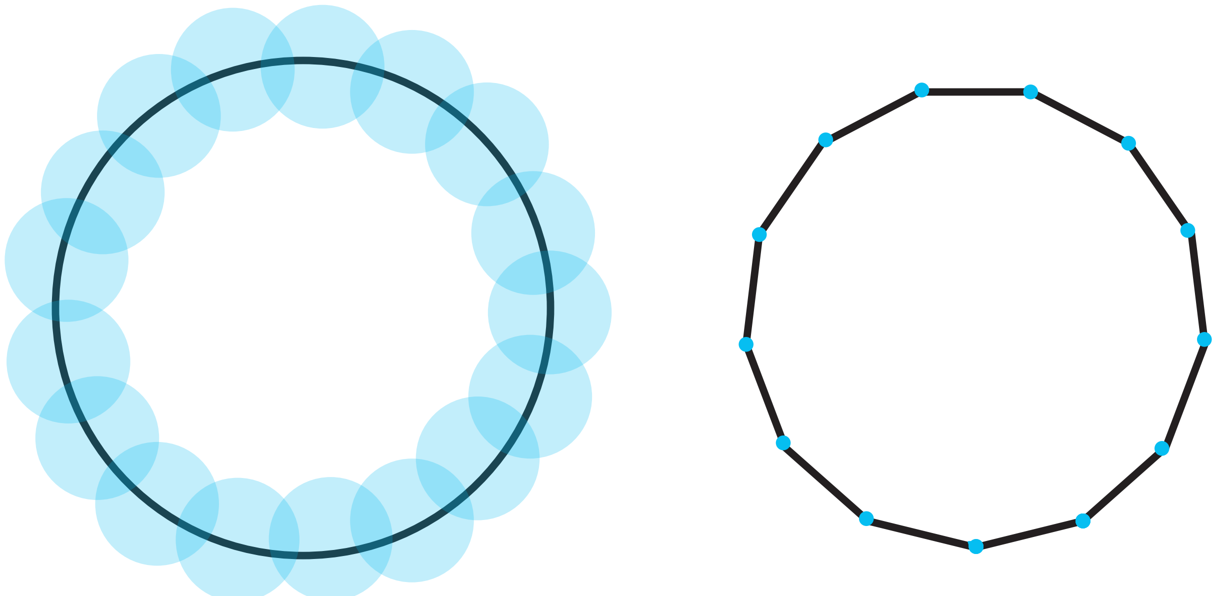

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Points are connected if balls of radius ϵ around them overlap

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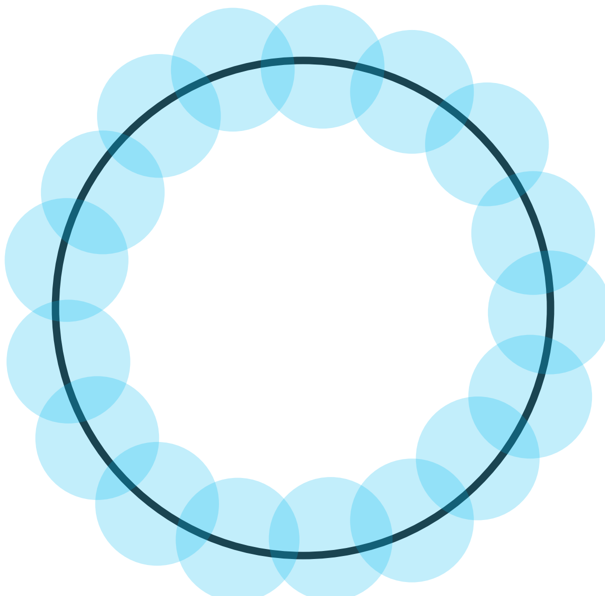

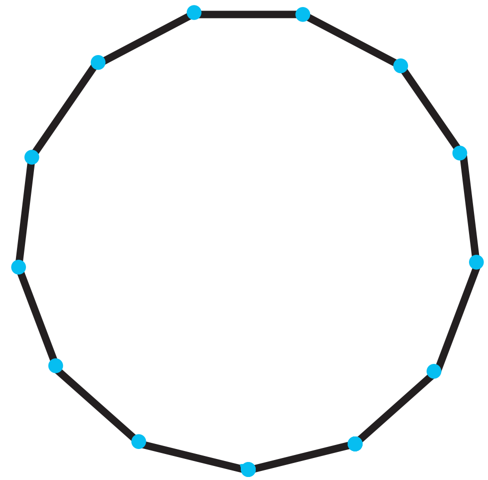

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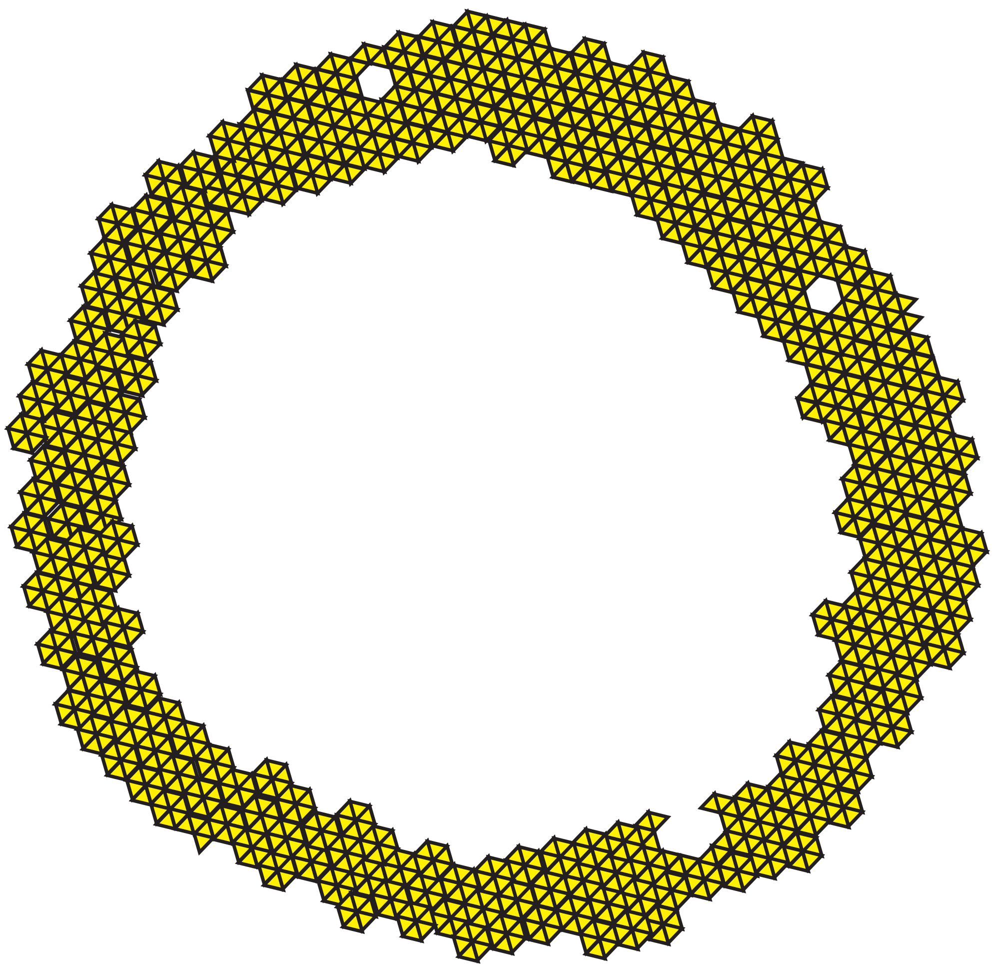
Complex grows with ϵ

Persistent Homology



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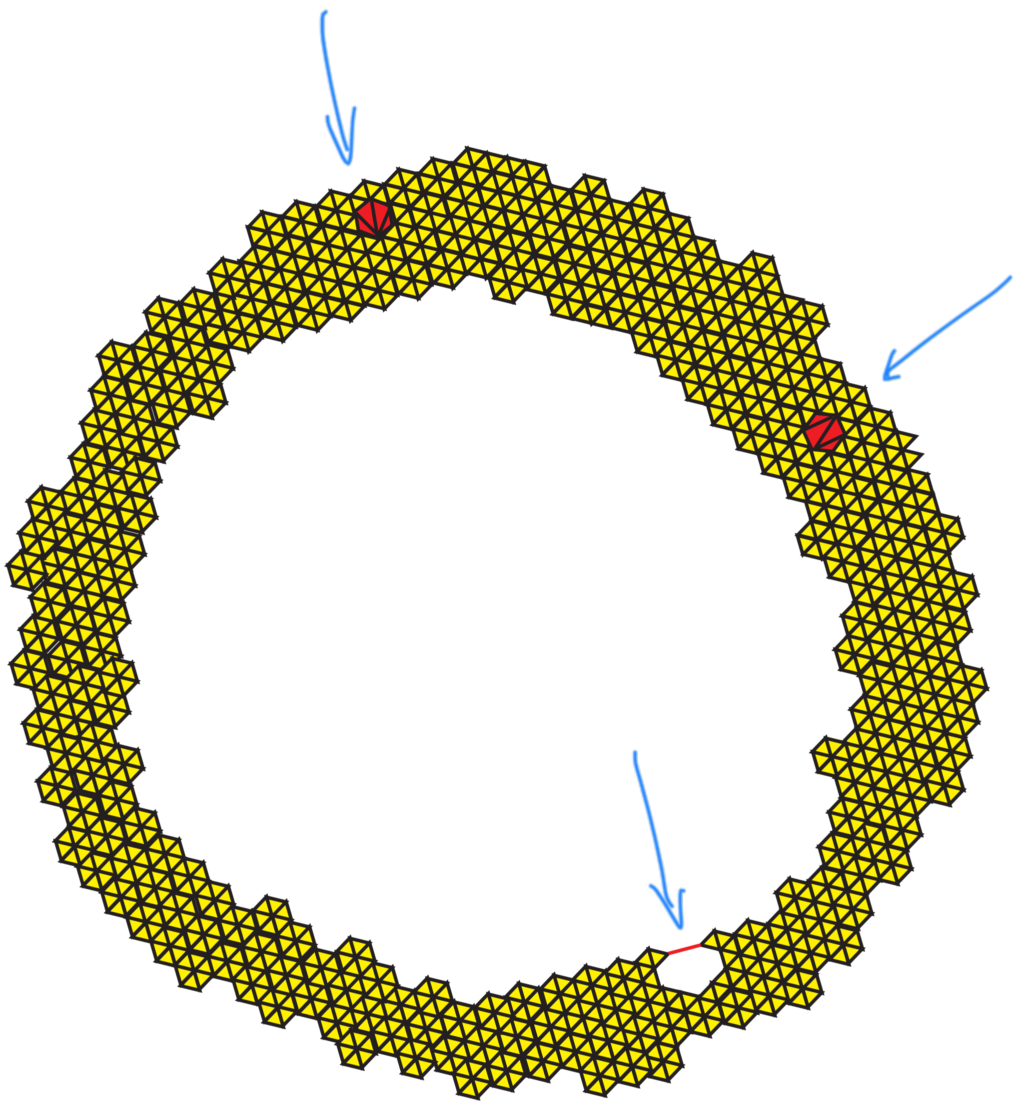

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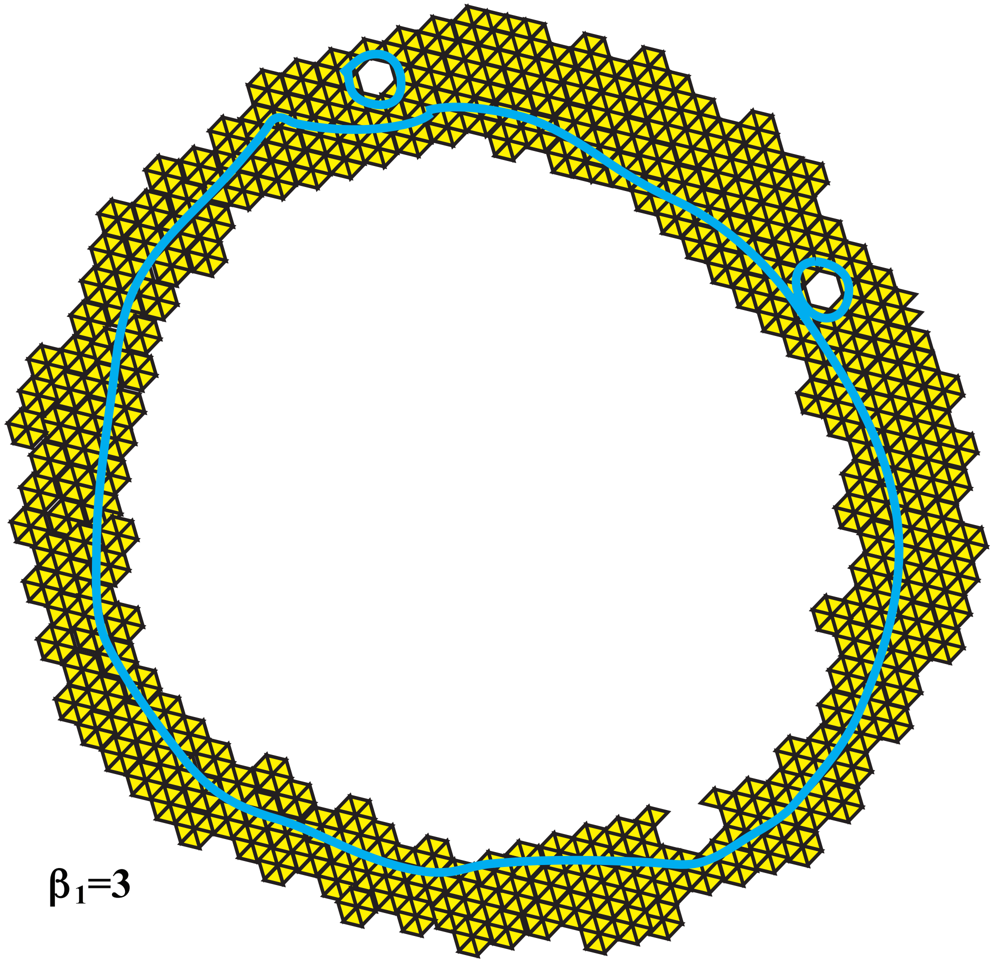

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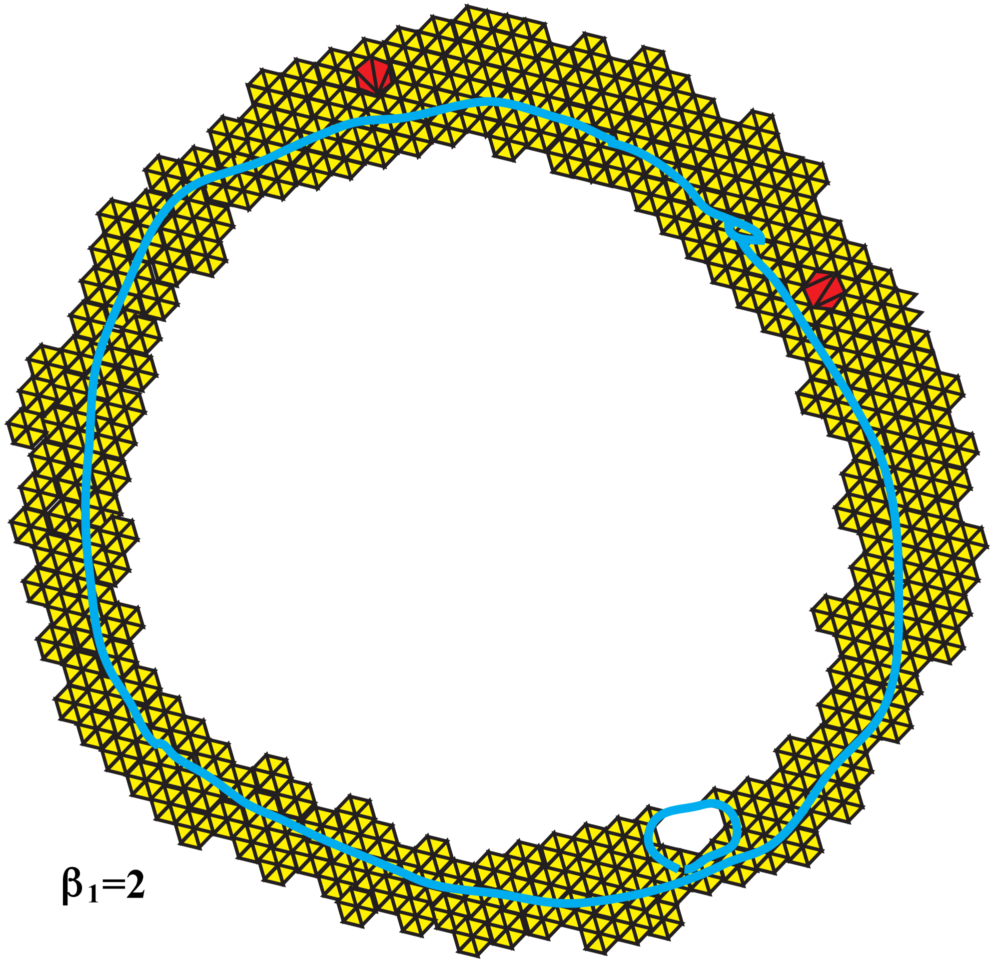

Persistent Homology

- Obtain a diagram of vector spaces

$$\cdots \to H_i(\check{C}(X, \epsilon_1)) \to H_i(\check{C}(X, \epsilon_2)) \to H_i(\check{C}(X, \epsilon_3)) \to \cdots$$

when $\epsilon_1 \leq \epsilon_2 \leq \epsilon_3$ etc.

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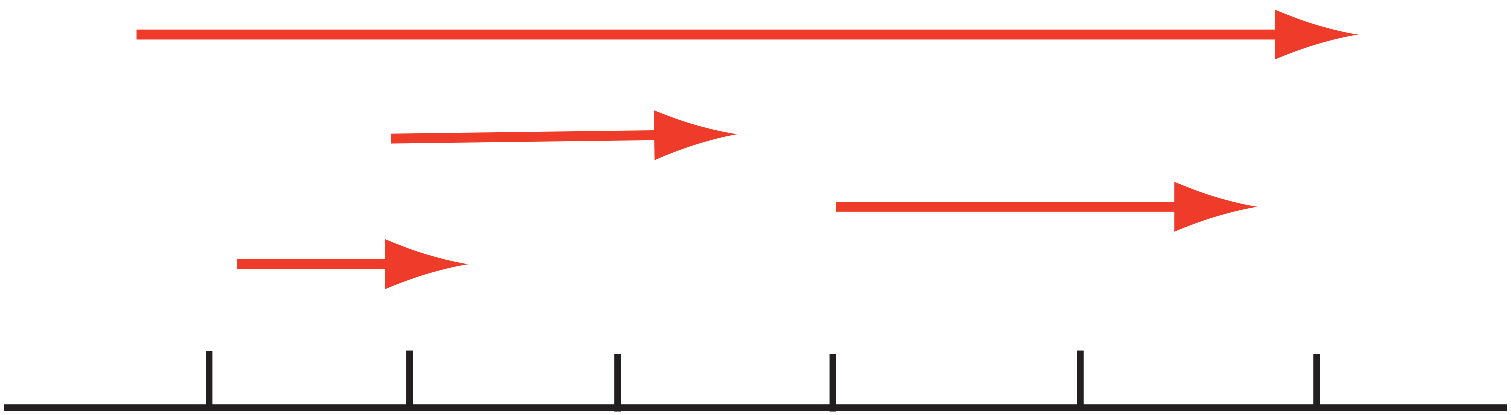
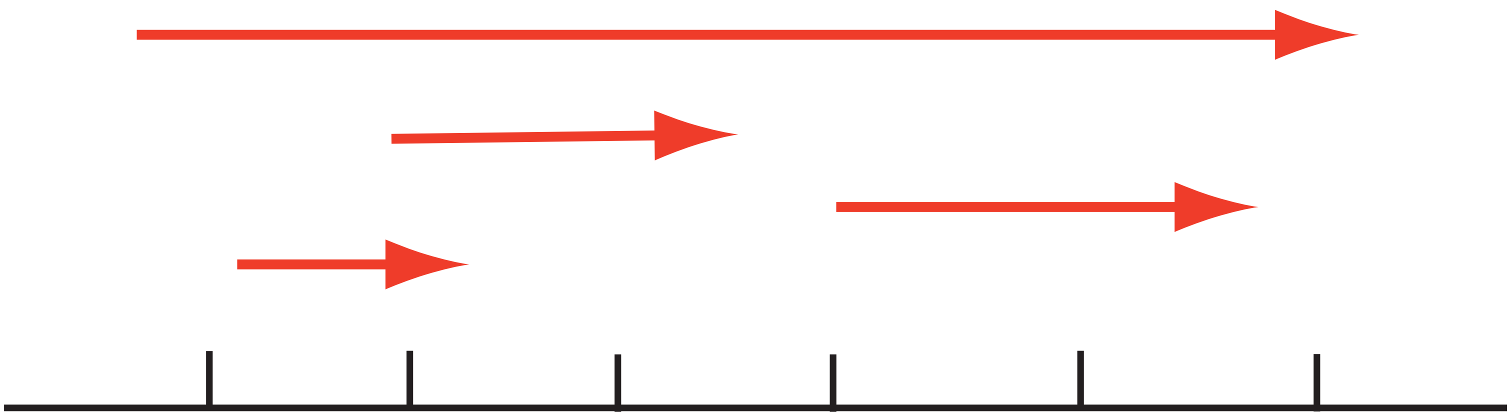
- Analogue of dimension for ordinary vector spaces

Persistent Homology - Bar Codes



A segment indicates a basis element "born" at the left hand endpoint and which dies at the right hand endpoint

Persistent Homology - Bar Codes



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Geometrically, means a loop which begins to exist (i.e. becomes closed) at the left hand point and is filled in at the right hand endpoint.

Persistent Homology - Bar Codes

Interpretation:

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Long segments correspond to “honest” geometric features in the point cloud

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Look at an example.

Example: Natural Image Statistics

- Joint with V. de Silva, T. Ishkanov, A. Zomorodian

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- Joint with V. de Silva, T. Ishkanov, A. Zomorodian
- An image taken by black and white digital camera can be viewed as a vector, with one coordinate for each pixel
- Each pixel has a "gray scale" value, can be thought of as a real number (in reality, takes one of 255 values)
- Typical camera uses tens of thousands of pixels, so images lie in a very high dimensional space, call it *pixel space*, $\mathcal{P}$

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The nonlinear statistics of high-contrast patches in natural images

(International Journal of Computer Vision 2003)

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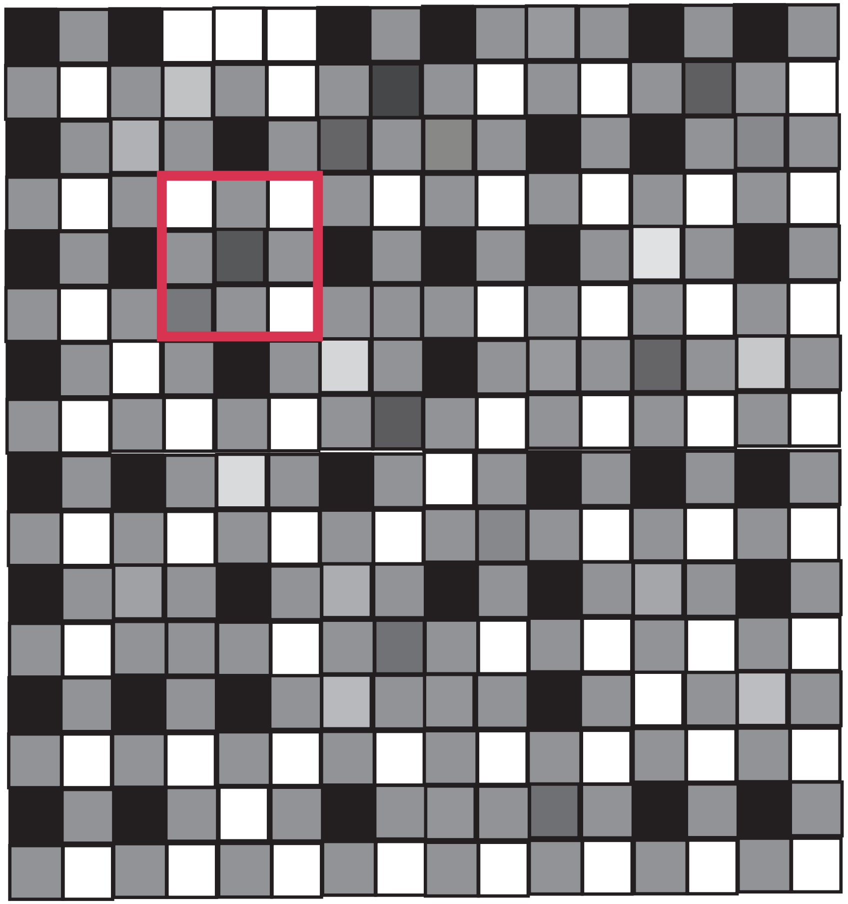

3×3 patches in images

Example: Natural Image Statistics

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1. Each patch gives a vector in $\mathbb{R}^9$
2. Most patches will be nearly constant, or *low contrast*, because of the presence of regions of solid shading in most images
3. Low contrast will dominate statistics, not interesting

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- Collect c:a 4.5×10^6 high contrast patches from a collection of images obtained by van Hateren and van der Schaaf
- Normalize mean intensity by subtracting mean from each pixel value to obtain patches with mean intensity $= 0$
- Puts data on an 8-dimensional hyperplane, $\cong \mathbb{R}^8$

Example: Natural Image Statistics

- Normalize contrast by dividing by the norm, so obtain patches with norm $= 1$

Example: Natural Image Statistics

- Normalize contrast by dividing by the norm, so obtain patches with norm $= 1$
- Means that data now lies on a 7-D ellipsoid, $\cong S^7$

Example: Natural Image Statistics

Result: Point cloud data $\mathcal{M}$ lying on a sphere in $\mathbb{R}^8$

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We wish to analyze it with persistent homology to understand it qualitatively

Example: Natural Image Statistics

First Observation: The points fill out S^7 in the sense that every point in S^7 is “close” to a point in $\mathcal{M}$

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How to analyze?

Example: Natural Image Statistics

Threshholding $\mathcal{M}$

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Define $\mathcal{M}[T] \subseteq \mathcal{M}$ by

$$\mathcal{M}[T] = \{x | x \text{ is in } T\text{-th percentile of densest points}\}$$

Example: Natural Image Statistics

Threshholding $\mathcal{M}$

Define $\mathcal{M}[T] \subseteq \mathcal{M}$ by

$$\mathcal{M}[T] = \{x | x \text{ is in } T\text{-th percentile of densest points}\}$$

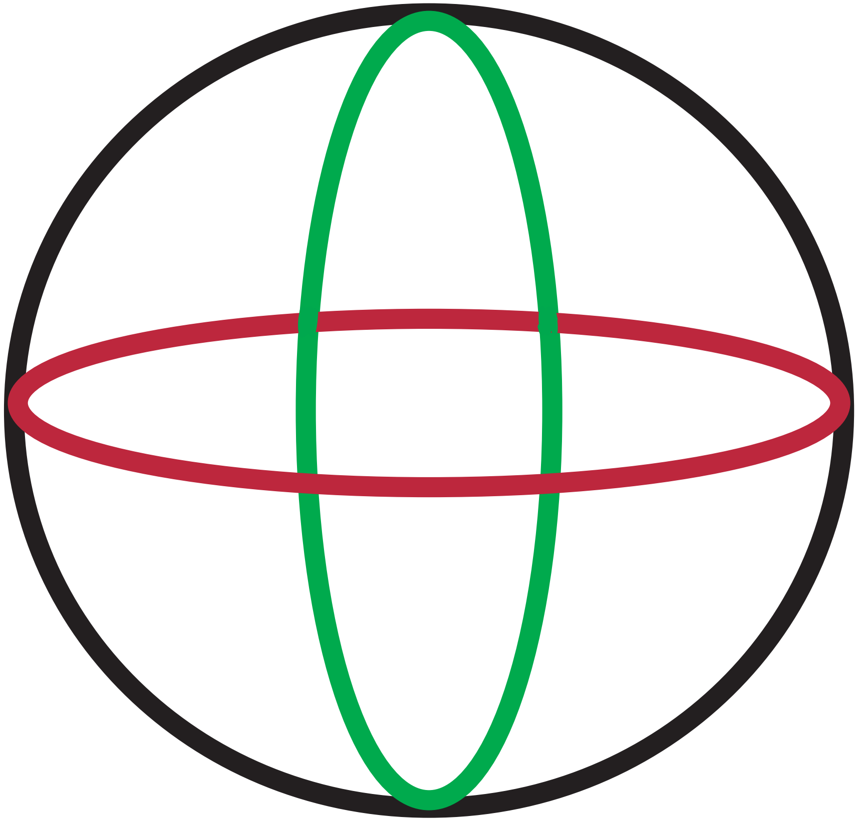
What is the persistent homology of these $\mathcal{M}[T]$'s?

Example: Natural Image Statistics

$$5 \times 10^4 \text{ points, } T = 25$$

One-dimensional barcode, suggests $\beta_1 = 5$

Example: Natural Image Statistics



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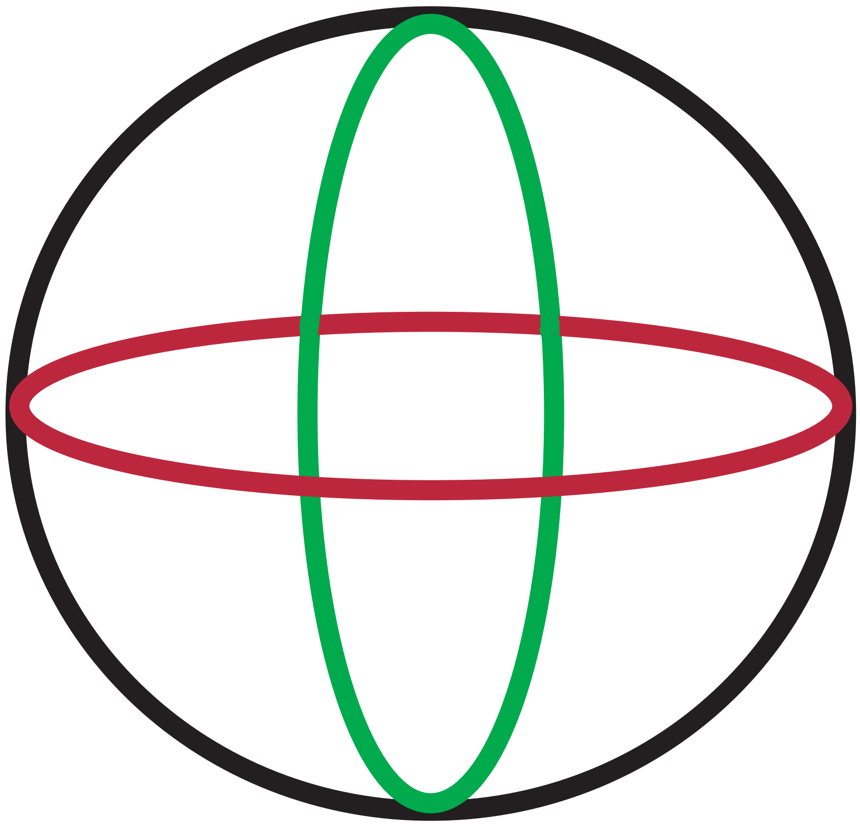
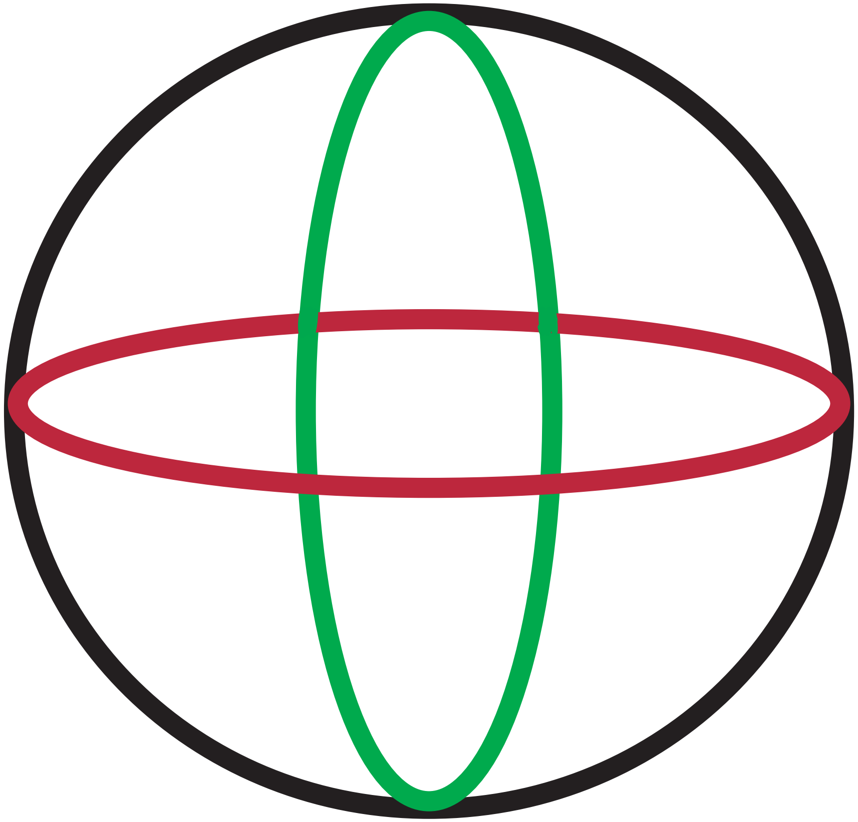


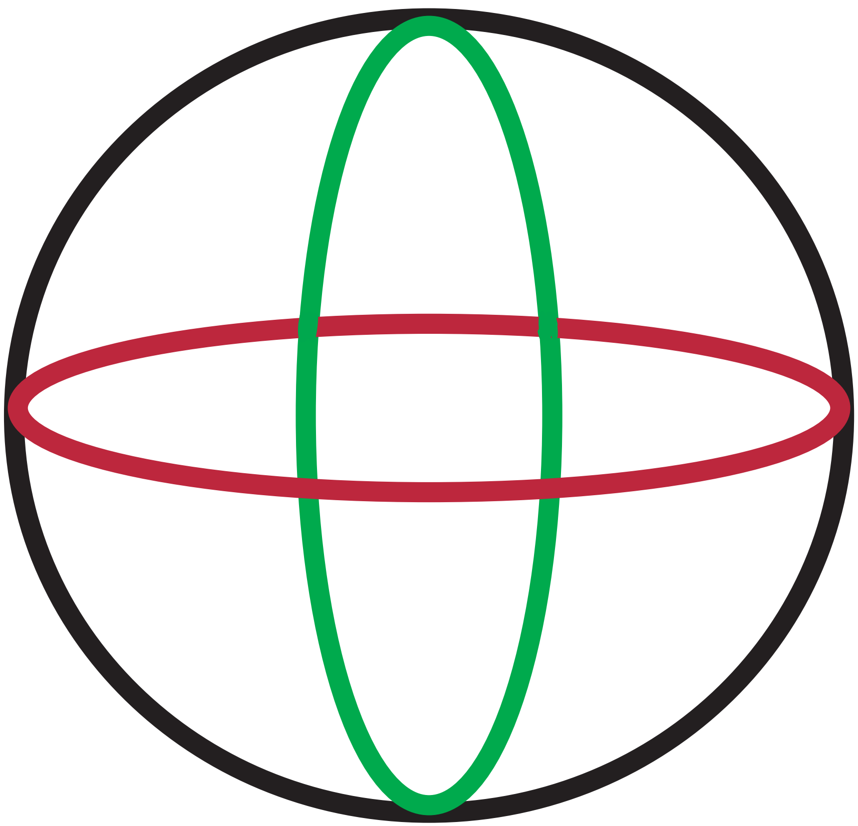
THREE CIRCLE MODEL

Three Circle Model



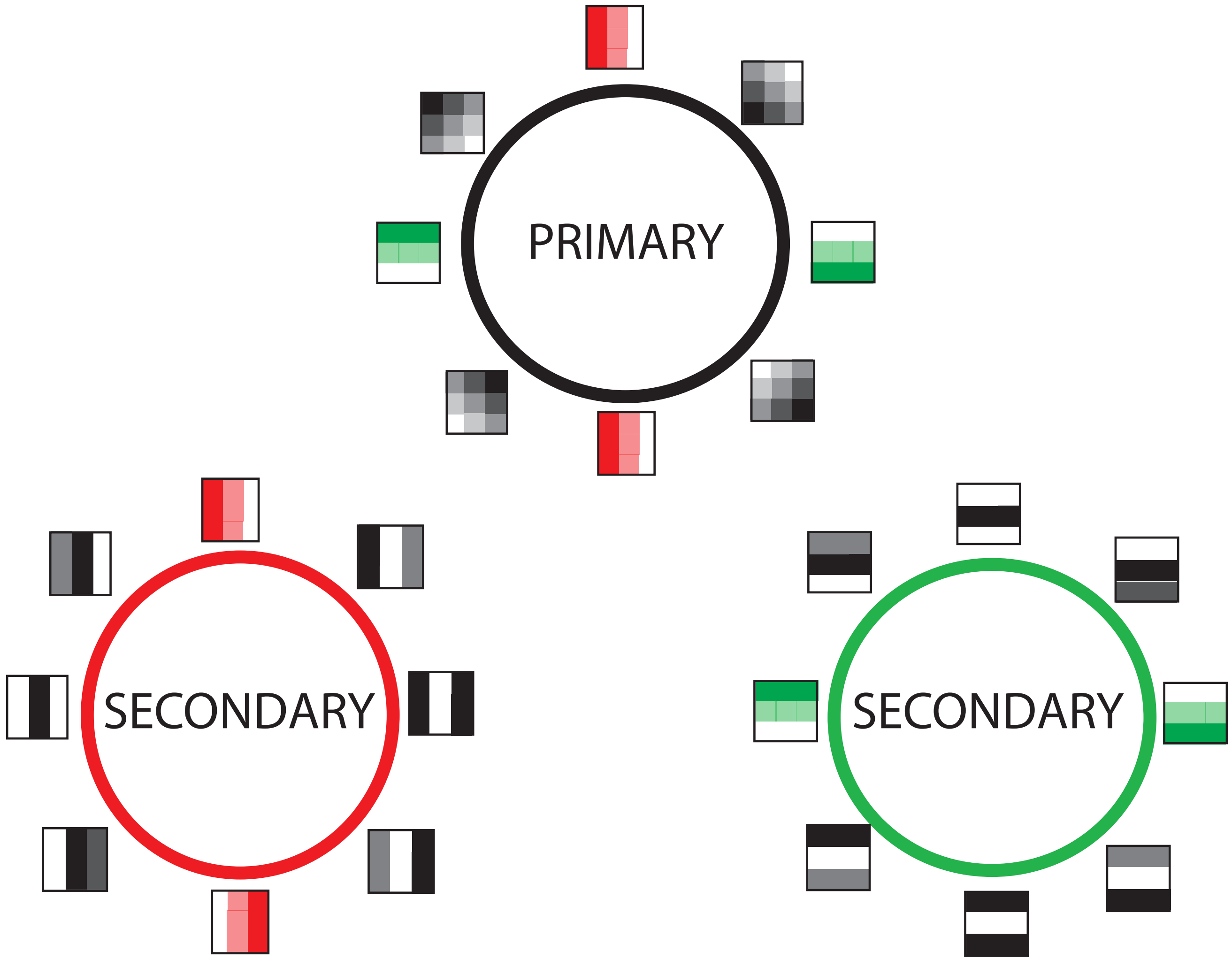
Red and green circles do not touch, each touches black circle

Example: Natural Image Statistics



Does the data fit with this model?

Example: Natural Image Statistics

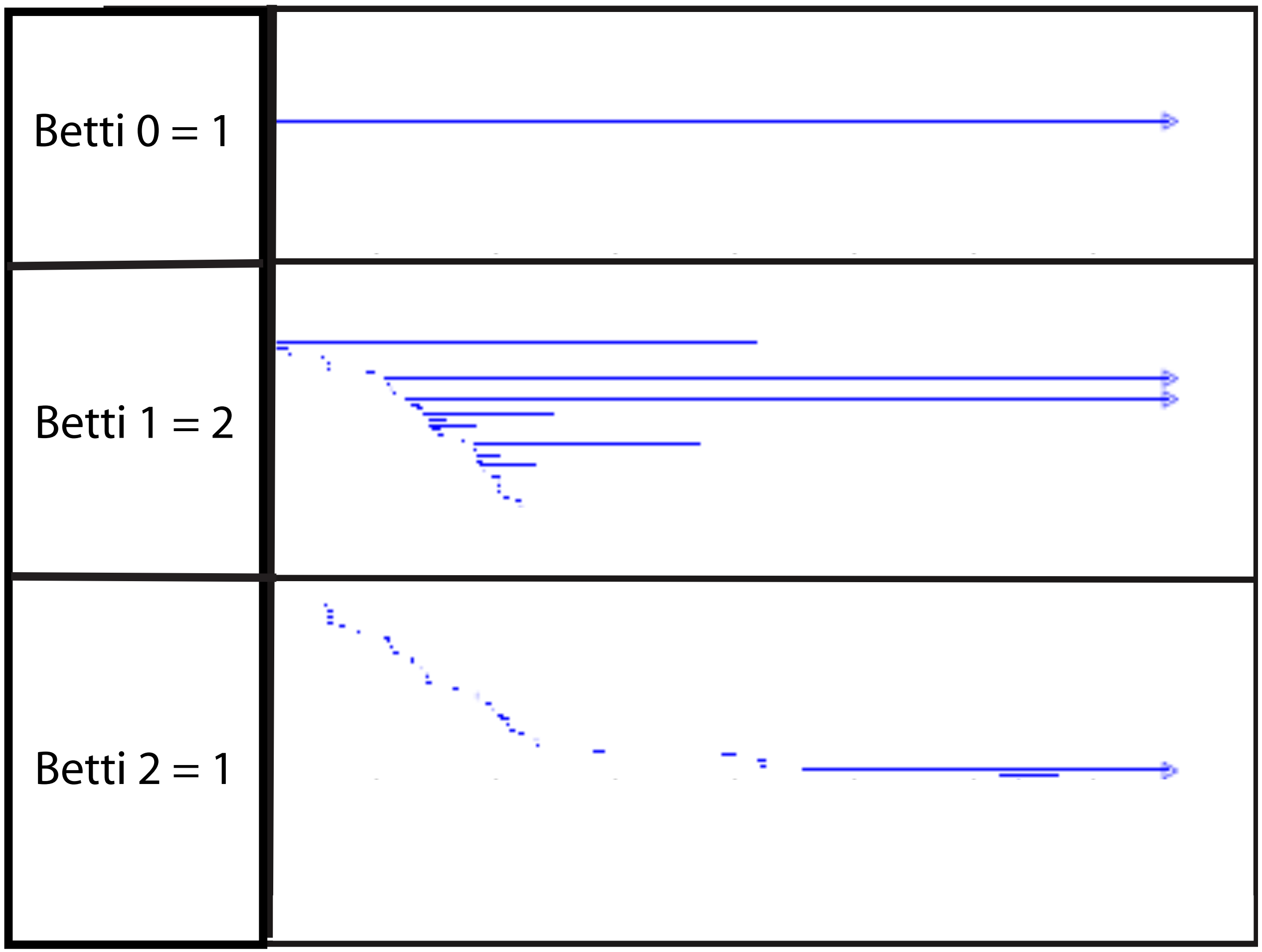


Example: Natural Image Statistics

IS THERE A TWO DIMENSIONAL SURFACE IN WHICH THIS PICTURE FITS?

Example: Natural Image Statistics

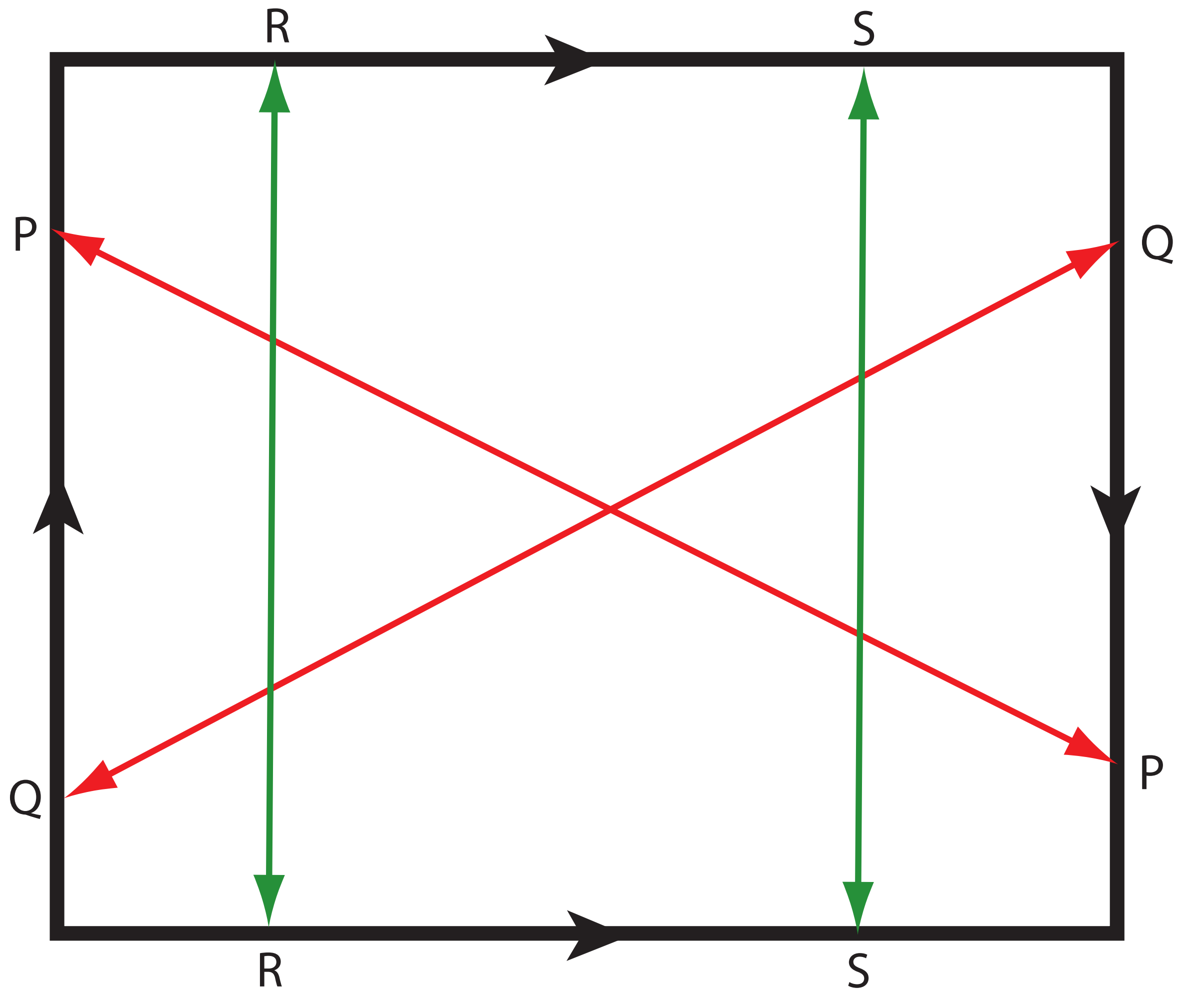
$$4.5 \times 10^6 \text{ points}, \; T = 10$$



Example: Natural Image Statistics

$\mathcal{K}$ - KLEIN BOTTLE

Example: Natural Image Statistics

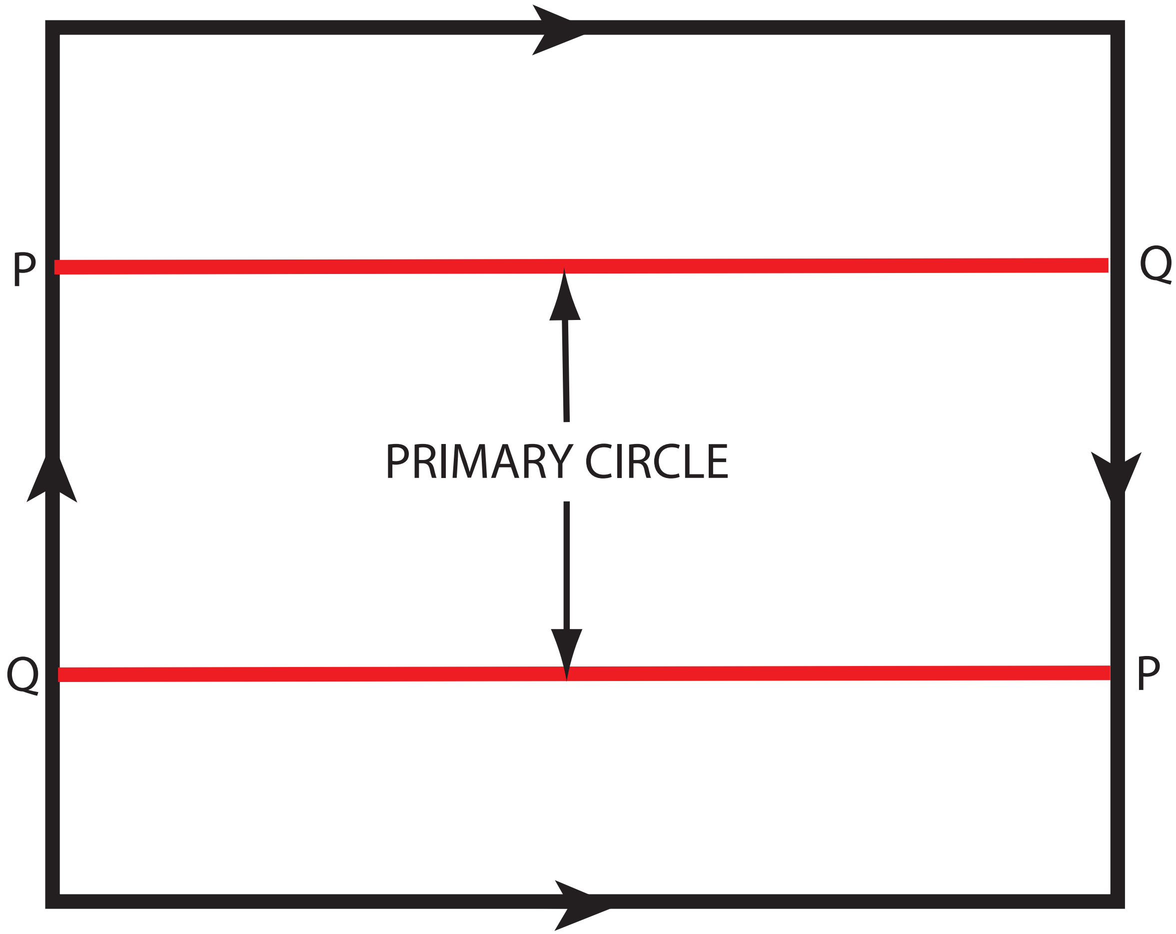


Identification Space Model

Example: Natural Image Statistics

Three circles fit naturally inside $\mathcal{K}$?

Example: Natural Image Statistics



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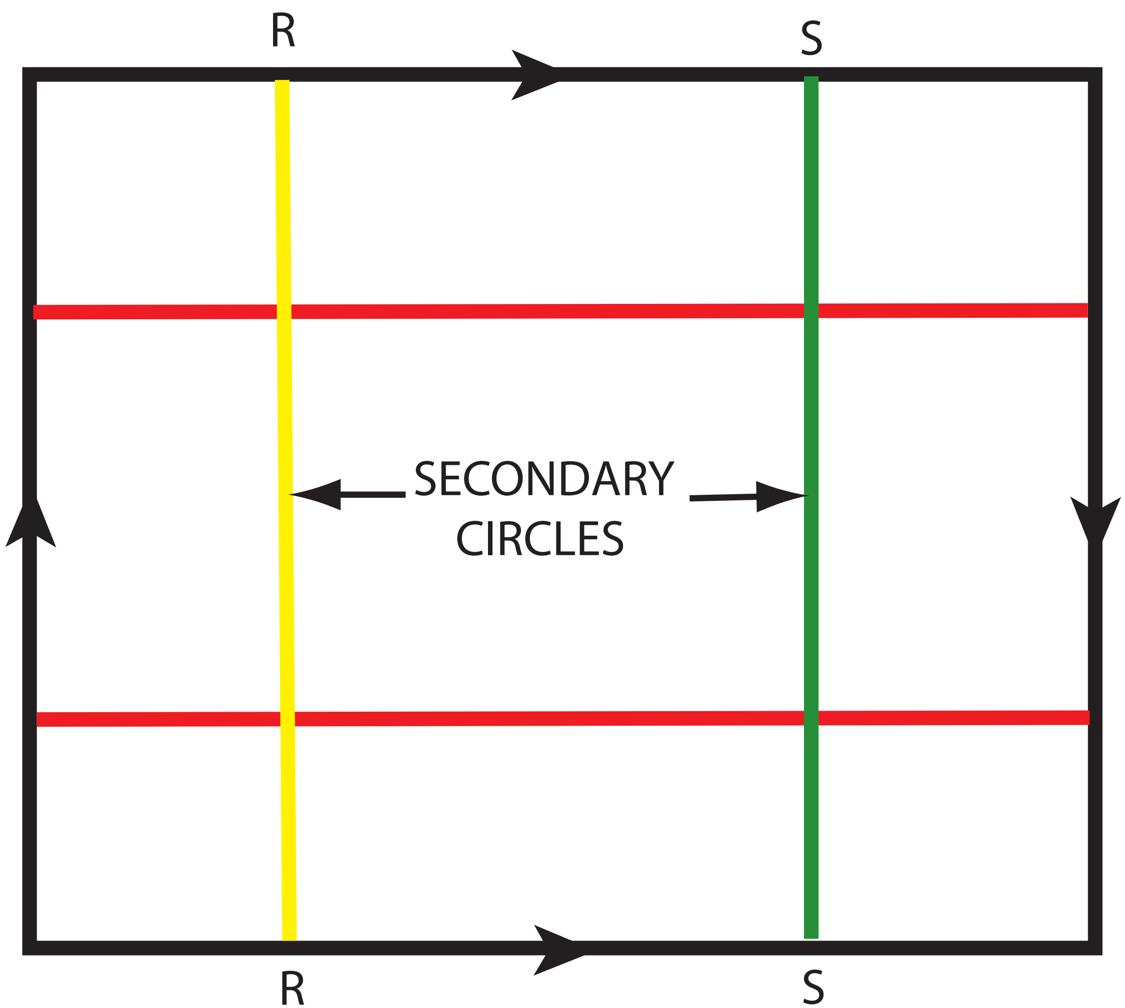

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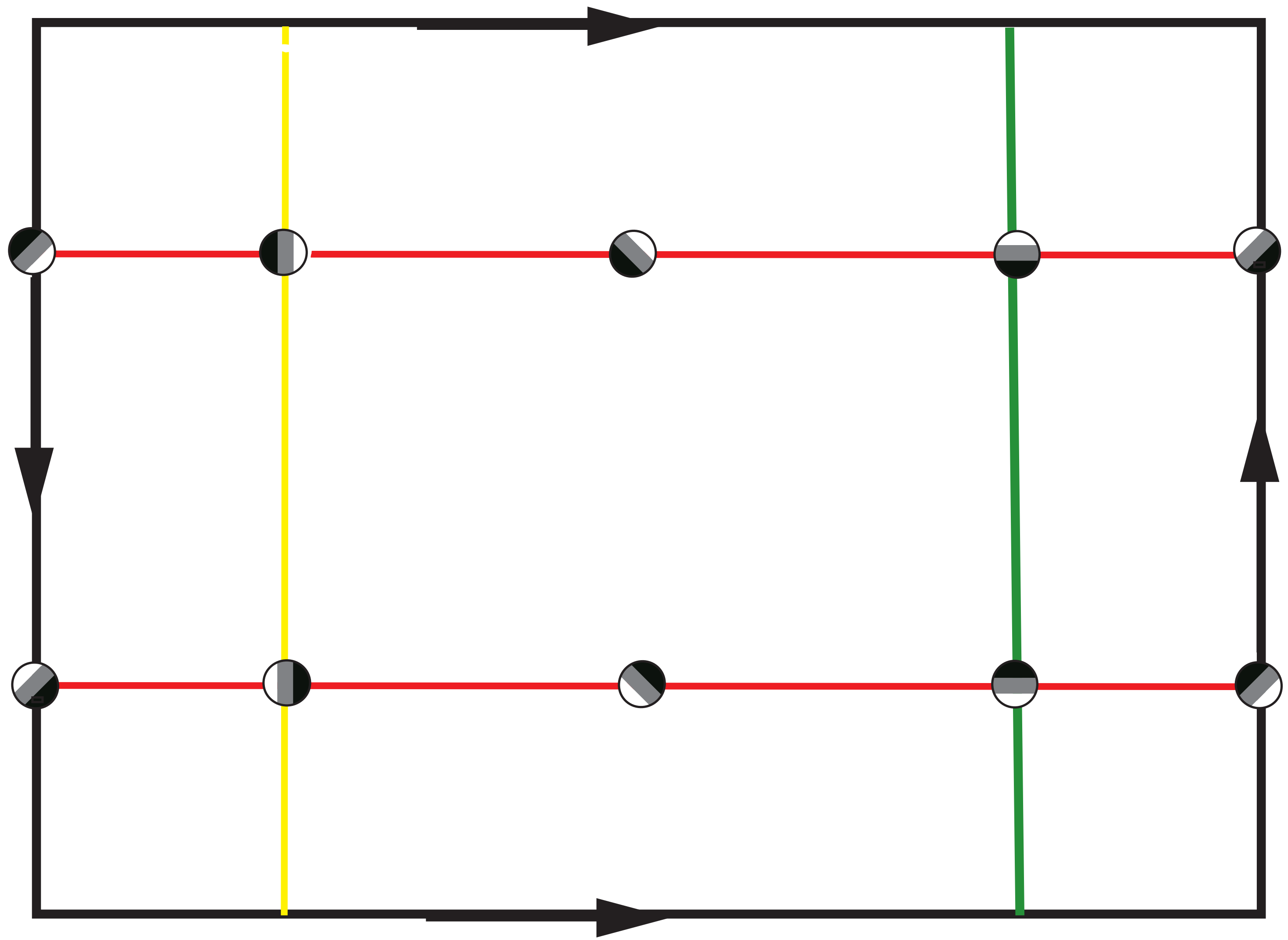

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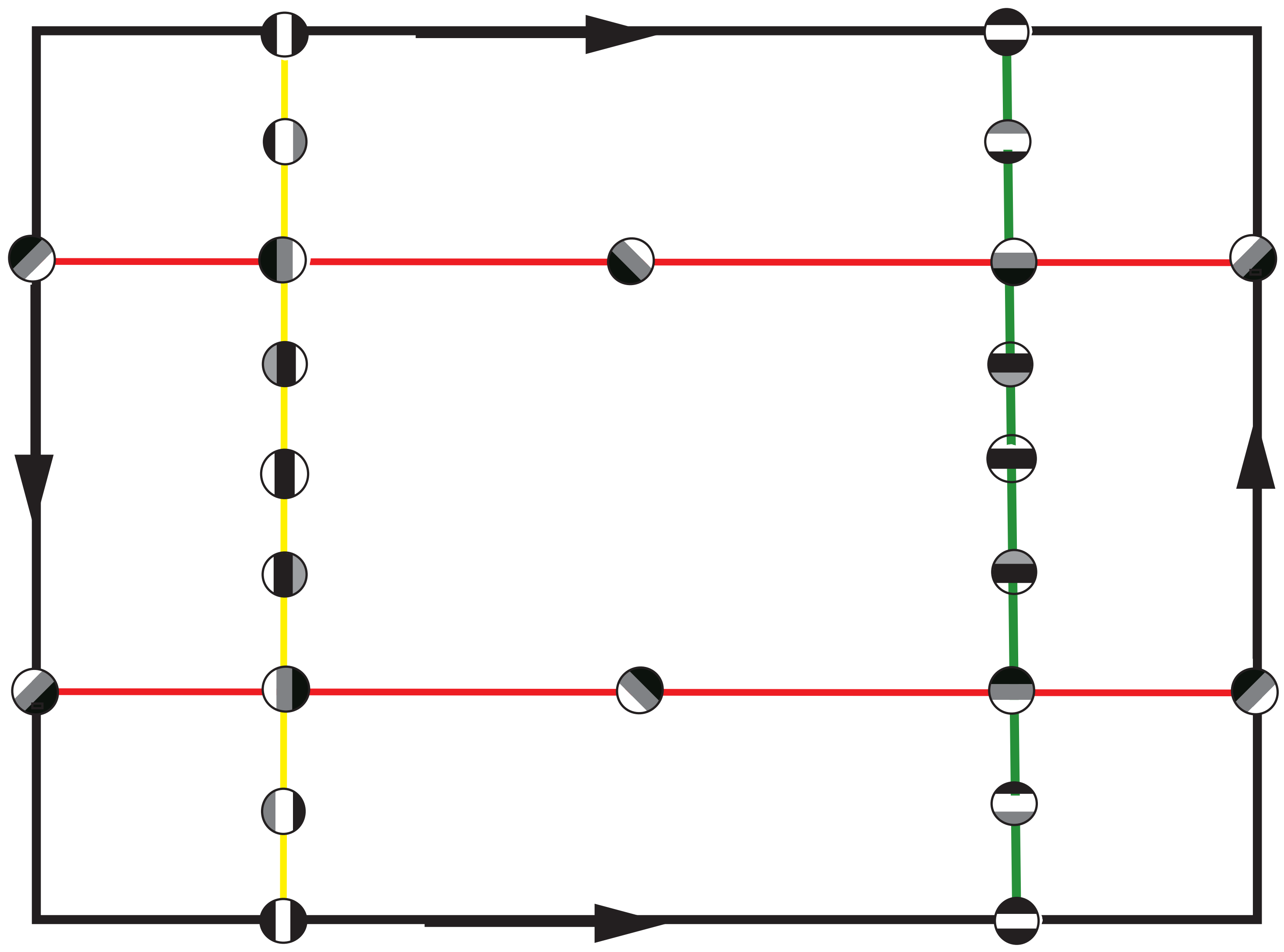

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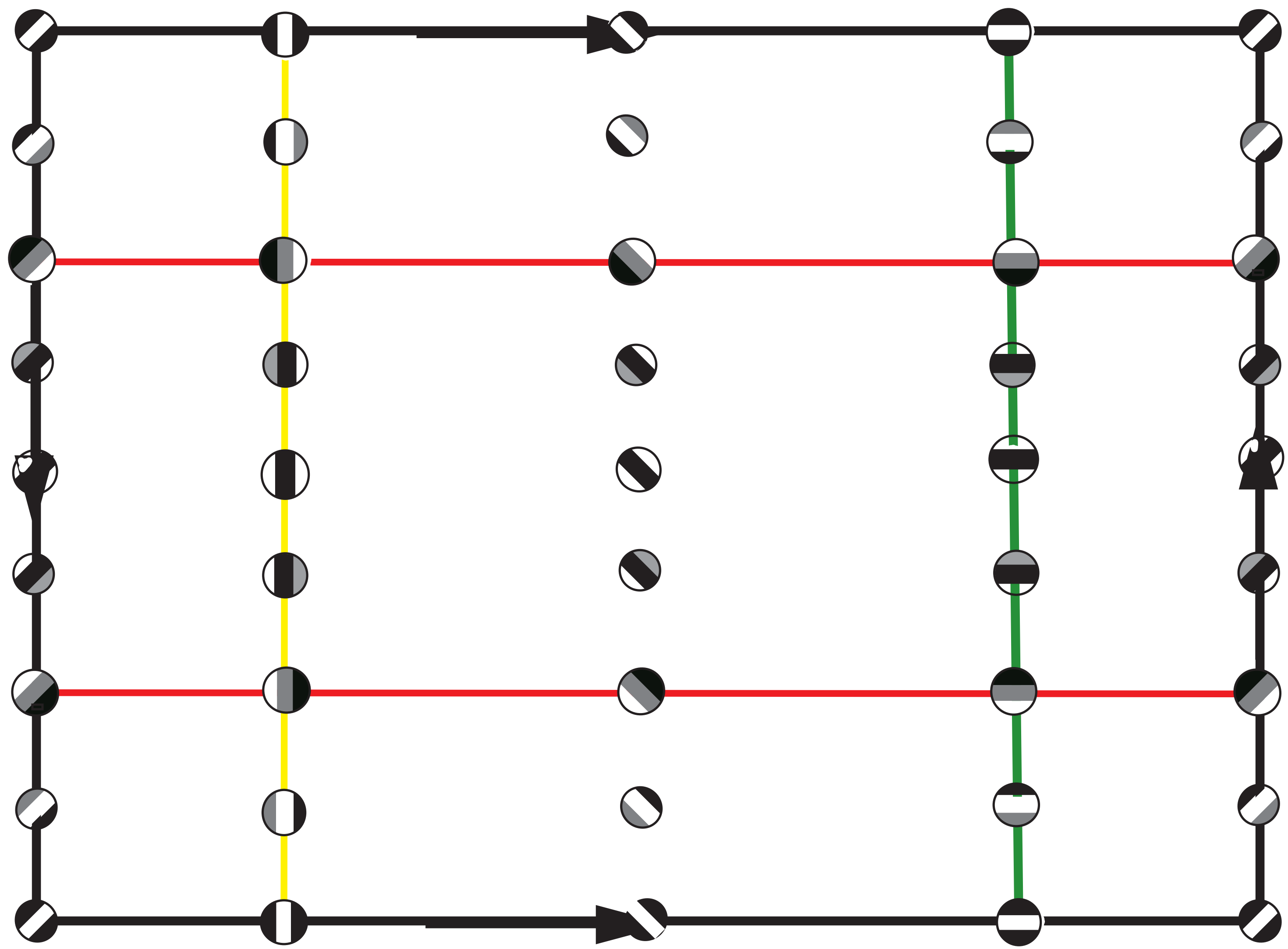


Natural Image Statistics

Klein bottle makes sense in quadratic polynomials in two variables, as polynomials which can be written as

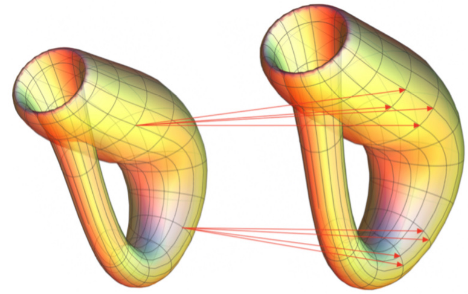
$$f = q(\lambda(x))$$

where

1. q is single variable quadratic
2. λ is a linear functional
3. $\int_D f = 0$
4. $\int_D f^2 = 1$

Carlsson, Ishkhanov, De Silva, Zomorodian
On the local behavior of spaces of natural images.
International Journal of Computer Vision, 2008

A decade later, Love, Filippenko, Maroulas, and Carlsson have made the Klein bottle as a topological input for designing convolutional layers in neural networks that learn image data. Moreover, they have incorporated the tangent bundle of a Klein bottle into TCNNs for learning video data. Both learnings achieved higher accuracies with smaller training sets.

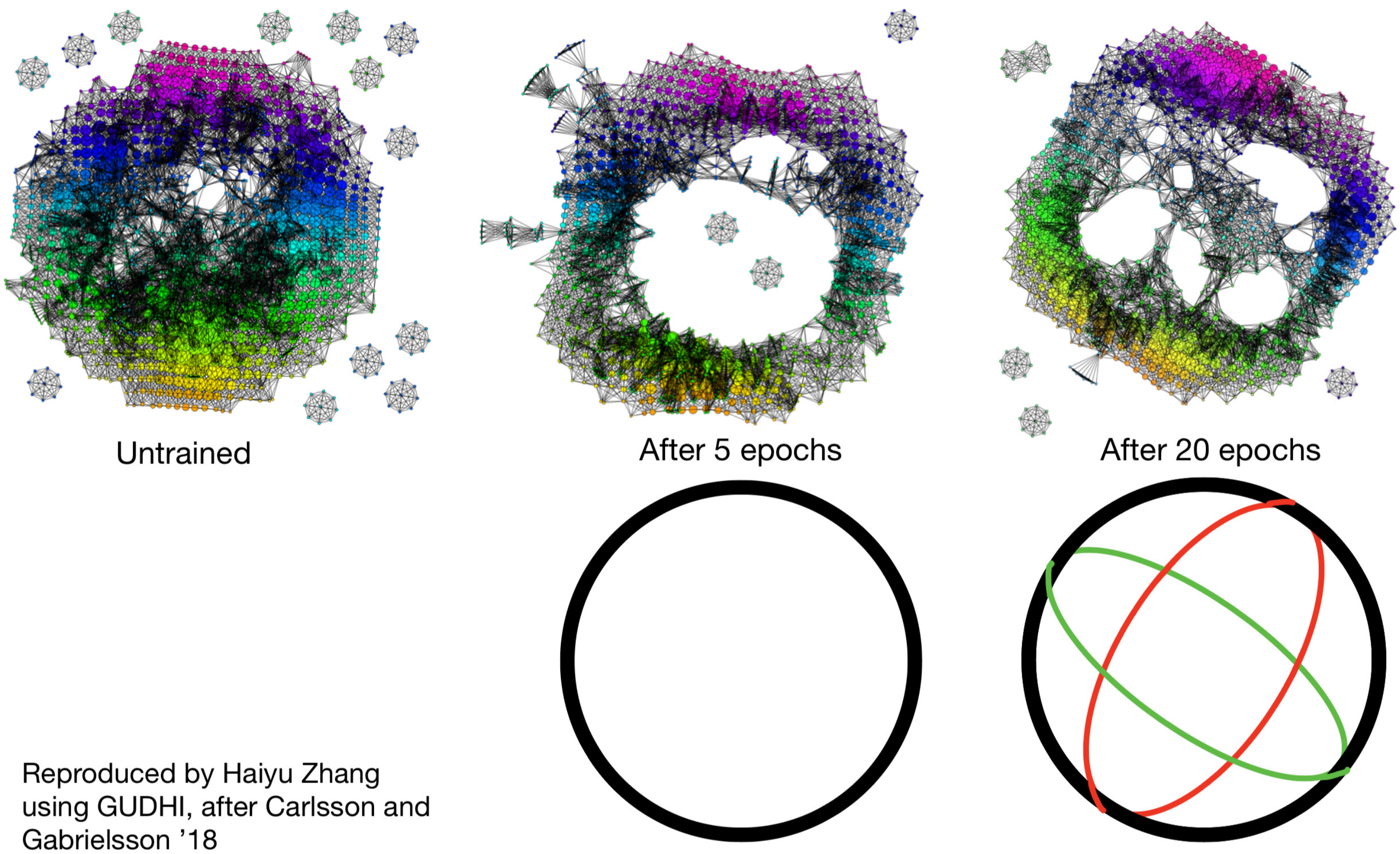


Ephy R. Love et al., Topological convolutional layers for deep learning, ***Journal of Machine Learning Research****, 2023.*

Gunnar Carlsson and Rickard Brüel Gabrielsson, Topological approaches to deep learning, ***Topological Data Analysis: The Abel Symposium****, 2018.*

From topological data analysis to topological deep learning

Topology of convolutional neural networks: Emergence of cycles during a training process



Reproduced by Haiyu Zhang using GUDHI, after Carlsson and Gabrielsson '18

Mapper

Algebraic topology can produce signatures which can help in mapping out a data set.

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Can one obtain flexible topological mapping methods, with combinatorial simplicial complex images?

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Yes, joint work with G. Singh and F. Memoli.

Mapper - Mayer-Vietoris Blowup

X a space, $\mathcal{U} = \{U_\alpha\}_{\alpha \in A}$ a covering of X.

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Let $X^{\mathcal{U}} \subseteq X \times \Delta$, $X^{\mathcal{U}} = \bigcup_S X(S) \times \Delta[S]$

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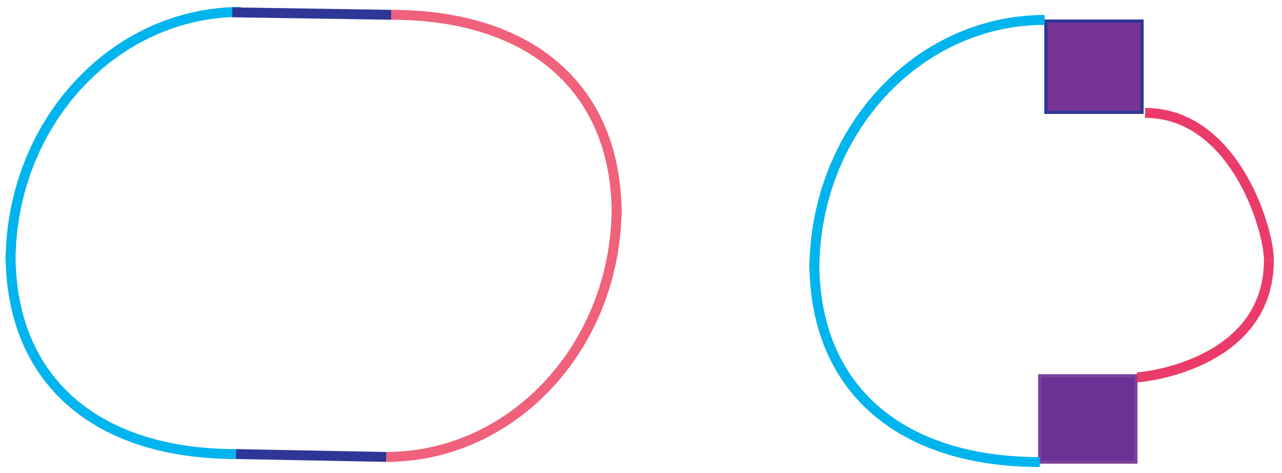

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π_Δ is equivalence if all $X(S)$'s are empty or contractible

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Intermediate construction $\mathcal{M}(X, \mathcal{U})$

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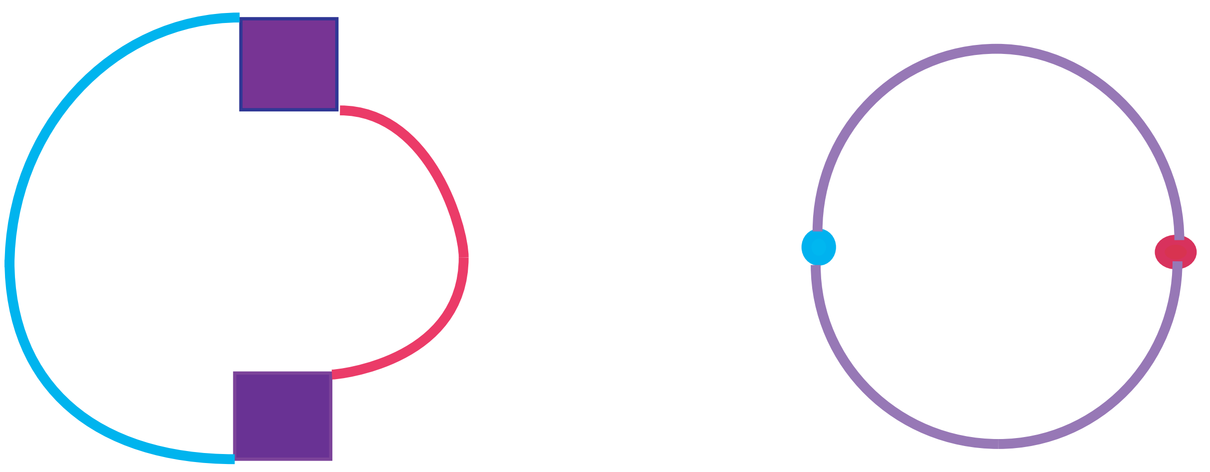
$\phi(x,\zeta) \simeq \psi(x,\zeta)$

Mapper - Mayer-Vietoris Blowup



Mapper - Statistical Version

Now given point cloud data set $\mathbb{X}$, and a covering $\mathcal{U}$.

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Critical that clustering operation be functorial.

Partition of unity subordinate to $\mathcal{U}$ gives map from $\mathbb{X}$ to $\mathcal{M}(\mathbb{X},\mathcal{U})$.

Mapper - Statistical Version

How to choose coverings?

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Given a reference map (or filter) $f : \mathbb{X} \to Z$, where Z is a metric space, and a covering $\mathcal{U}$ of Z, can consider the covering $\{f^{-1}U_\alpha\}_{\alpha \in A}$ of $\mathbb{X}$. Typical choices of Z - $\mathbb{R}$, $\mathbb{R}^2$, S^1.

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Construction gives an image complex of the data set which can reflect interesting properties of $\mathbb{X}$.

Mapper - Statistical Version

Typical one dimensional filters:

- Density estimators

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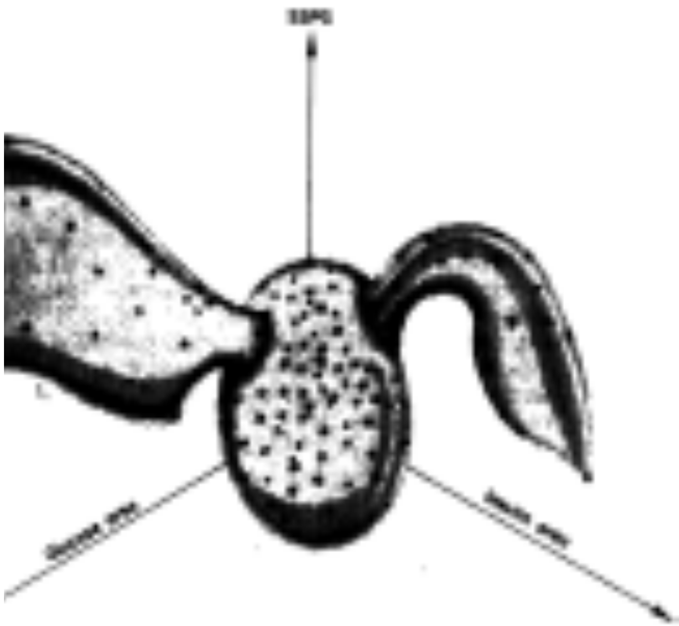
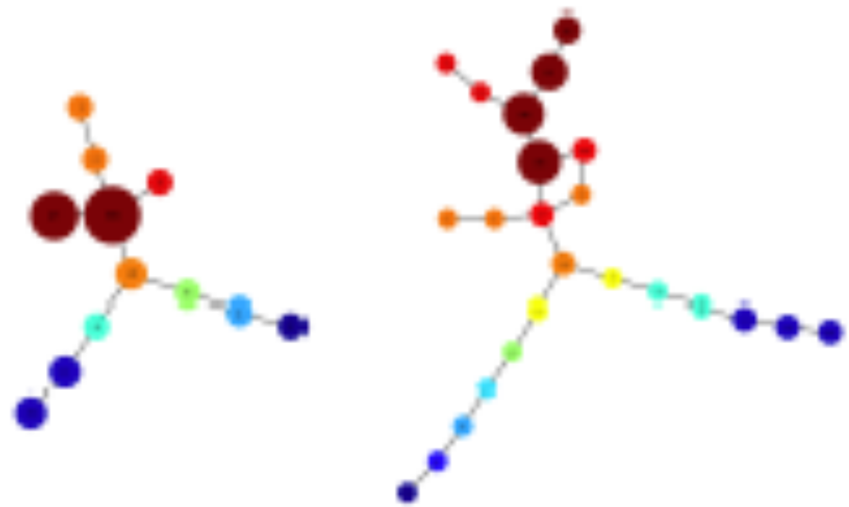
Typical one dimensional filters:

- Density estimators
- "Eccentricity" : $\sum_{x' \in \mathbb{X}} d(x, x')^2$
- Eigenfunctions of graph Laplacian for Vietoris-Rips graph
- User defined, data dependent filter functions

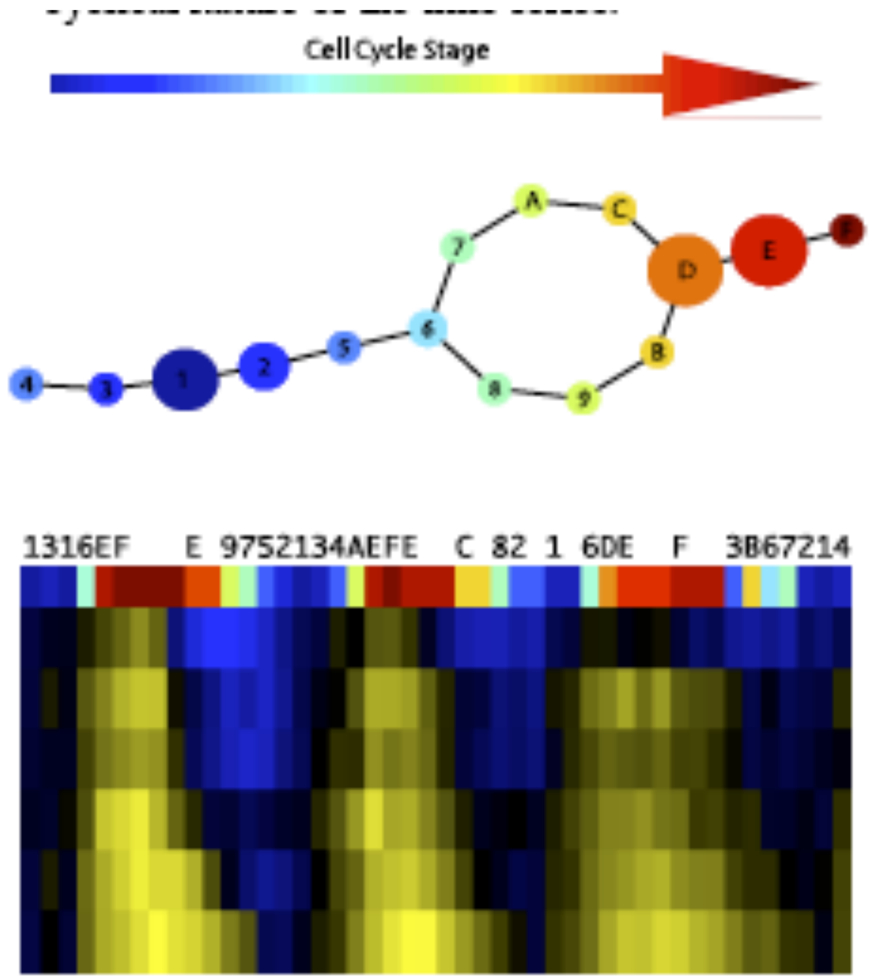
Mapper - Statistical Version





Miller-Reaven Diabetes Study, 1976

Mapper - Statistical Version



Cell Cycle Microarray Data

Joint with M. Nicolau, Nagarajan, G. Singh

Mapper - Scale Space

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Can one allow ε to vary with α?

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Can one allow ε to vary with α?

Important question: too many parameter choices makes tool unusable, and choosing one ε for the entire space is too restrictive.

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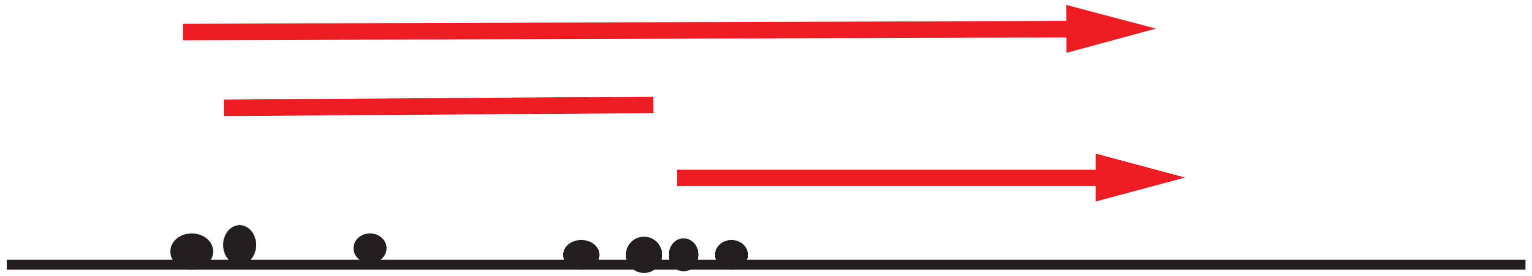
Consider the set of all endpoints of intervals in the persistence diagram. Provides a decomposition of the real line in which ε is varying into intervals. Call these intervals S-intervals.

Mapper - Scale Space



Mapper - Scale Space

- Vertex set of $SS(X, \mathcal{U})$ consists of a pair (α, I), where $\alpha \in A$ and I is an S-interval for the zero dimensional persistence diagram for $f^{-1}(U_\alpha)$.

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- We connect (α, I) and (β, J) with an edge if (a) $U_\alpha \cap U_\beta \neq \emptyset$ and (b) $I \cap J \neq \emptyset$.
- $SS(X)$ is equipped with a reference map $\pi : SS(X, \mathcal{U}) \to N\mathcal{U}$ given on vertices by $(\alpha, I) \to \alpha$

Mapper - Scale Space

A varying choice of scale is now determined by a *section* of π, i.e a map

$$\sigma : N\mathcal{U} \longrightarrow SS(X, \mathcal{U})$$

so that $\pi\sigma = id_{N\mathcal{U}}$.

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Finding the high weight sections in the case of 1-D filters is computationally tractable.

Variants on Persistence: Zig-Zags

Bootstrap - B. Efron

- Studies statistics of measures of central tendency across different samples within a data set

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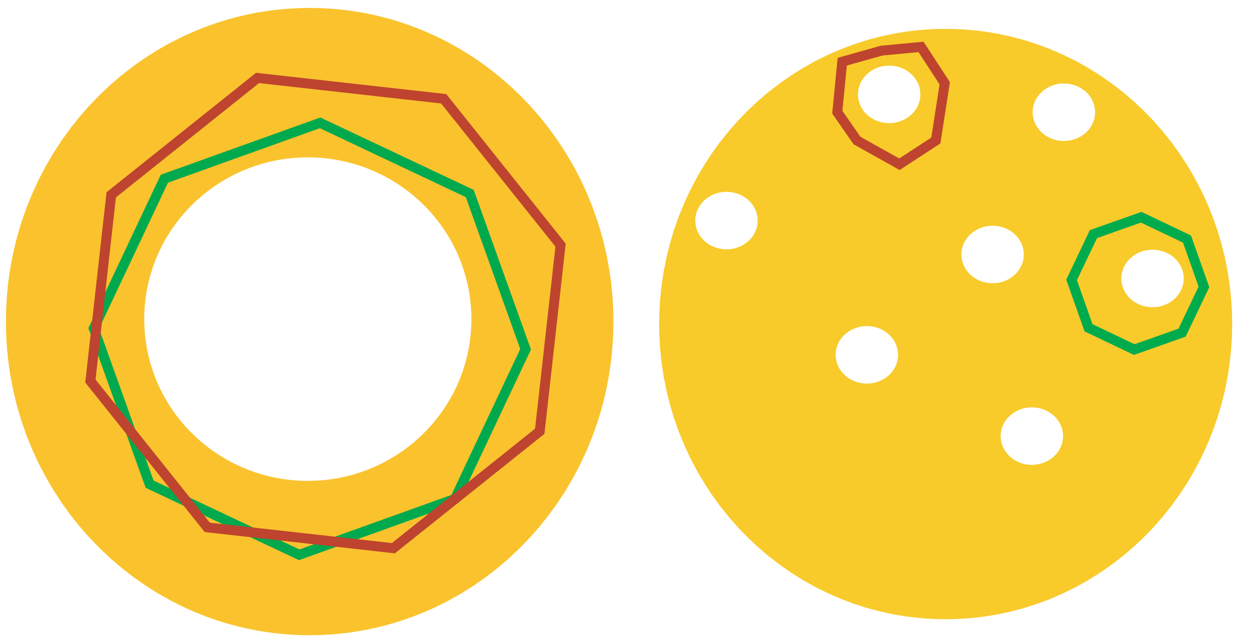
- Can give assessment of reliability of conclusions to be drawn from the statistics of the data set
- How can one adapt the technique to apply to qualitative information, such as presence of loops or decompositions into clusters?

Variants on Persistence: Zig-Zags



How to distinguish?

Variants on Persistence: Zig-Zags

- Family of samples $S_1, S_2, \ldots, S_k$ from point cloud data $\mathbb{X}$

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- Family of samples $S_1, S_2, \ldots, S_k$ from point cloud data $\mathbb{X}$
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- Family of samples $S_1, S_2, \ldots, S_k$ from point cloud data $\mathbb{X}$
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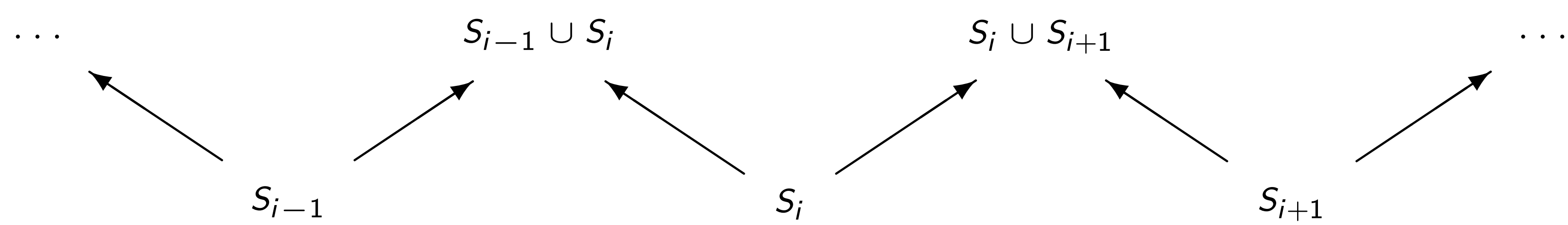

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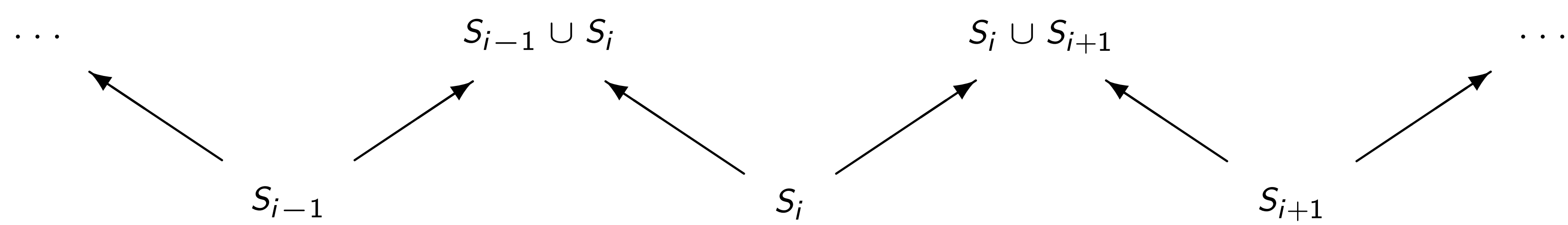

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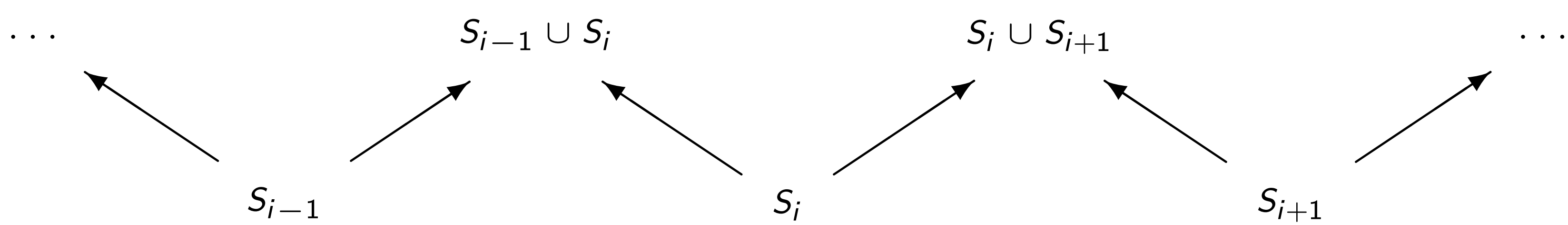
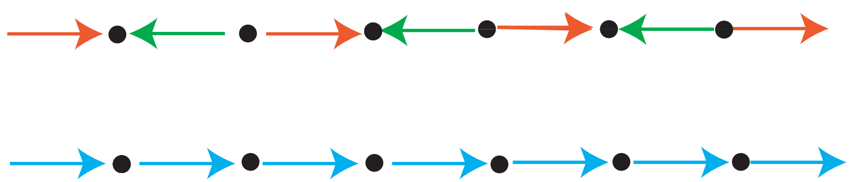


- Apply H_k to VR-complexes on each of these, get a diagram of vector spaces of same shape
- If a family of homology classes "matches up" under induced maps, then they are stable across samples

Variants on Persistence: Zig-Zags

To carry out analysis, one needs a classification of diagrams of vector spaces of shape of upper row. Second row is shape for ordinary persistence.



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Long intervals correspond to elements stable across samples, others are artifacts.

Variants on Persistence: Zig-Zags

Results have value in other situations:

Variants on Persistence: Zig-Zags

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- Analysis of time varying data

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- Analysis of behavior of data under varying choice of density estimators

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- Analysis of time varying data
- Analysis of behavior of data under varying choice of density estimators
- Analysis of behavior of witness complexes under varying choices of landmarks

This analysis is relevant and interesting even in zero dimensional case, i.e. clustering.