



An Introduction to Topological Data Analysis

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- Why Topology?

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- Simplicial Complex
- Nerve, Reeb Graph, and Mapper
- Čech, Vietoris-Rips, and Witness Complexes

3 Persistent Homology

- Betti Number at Different Scales
- Algebraic Theory
- Application: Sensor Network Coverage
- Application: Genetic Recombination
- Application: Biomolecular Structure
- Application: Natural Image Patches

Methods for Summarizing or Visualizing a Geometry

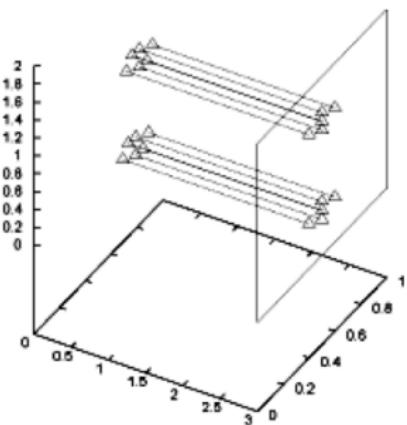


Figure: Linear projection (PCA, MDS, variable selection, etc)

Geometric Data Reduction

- General method of **manifold learning** takes the following **Spectral Kernel Embedding** approach
 - construct a **neighborhood graph** of data, G
 - construct a **positive semi-definite kernel** on graphs, K
 - find global embedding coordinates of data by **eigen-decomposition** of $K = YY^T$
- Sometimes 'distance metric' is just a similarity measure (nonmetric MDS, ordinal embedding)
- Sometimes coordinates are not a good way to organize/visualize the data (e.g. $d > 3$)
- Sometimes all that is required is a **qualitative** view

Why Topology?

Key elements

- Coordinate free representation
- Invariance under deformations
- Compressed qualitative representation

Why Topology?

Topology

- To see points in neighborhood the *same* requires distortion of distances, i.e. stretching and shrinking
- We do not permit *tearing*, i.e. distorting distances in a discontinuous way

Why Topology?

Continuous Topology

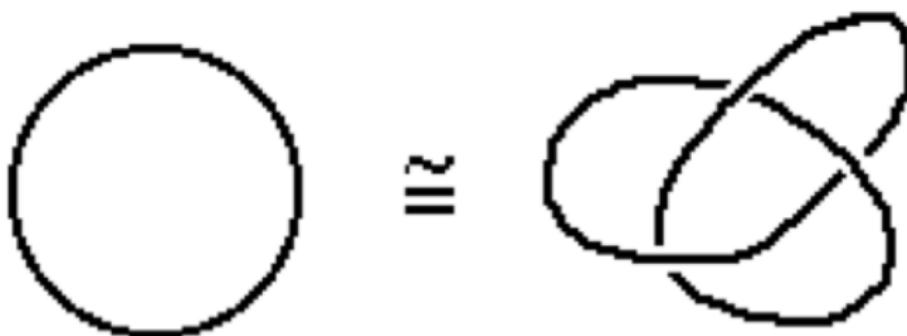


Figure: Homeomorphic

Why Topology?

Properties of Data Geometry

Fact

We Don't Trust Large Distances!

- In life or social sciences, **distance (metric)** are constructed using a notion of **similarity (proximity)**, but have no theoretical backing (e.g. distance between faces, gene expression profiles, Jukes-Cantor distance between sequences)
- Small distances still represent similarity (proximity), but long distance comparisons hardly make sense

Properties of Data Geometry

Fact

We Only Trust Small Distances a Bit!



- Both pairs are regarded as similar, but the strength of the similarity as encoded by the distance may not be so significant
- Similar objects lie in neighborhood of each other, which suffices to define **topology**

Why Topology?

So we need topology for robustness against metric distortions

- Distance measurements are noisy
- Physical device like human eyes may ignore differences in proximity (or as an average effect)
- **Topology** is the crudest way to capture invariants under distortions of distances
- At the presence of **noise**, one need **topology varied with scales**

Why Topology?

What kind of topology?

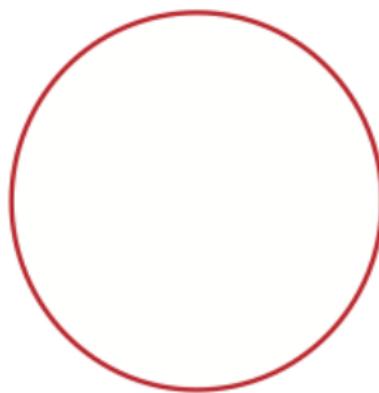
- Topology studies (global) mappings between spaces
- Point-set topology: continuous mappings on open sets
- Differential topology: differentiable mappings on smooth manifolds
 - Morse theory tells us topology of continuous space can be learned by discrete information on critical points
- Algebraic topology: homomorphisms on algebraic structures, the most concise encoder for topology
- Combinatorial topology: mappings on simplicial (cell) complexes
 - simplicial complex may be constructed from data
 - Algebraic, differential structures can be defined here



Topological Data Analysis

- What kind of topological information often useful
 - 0-homology: clustering or connected components
 - 1-homology: coverage of sensor networks; paths in robotic planning
 - 1-homology as obstructions: inconsistency in statistical ranking; harmonic flow games
 - high-order homology: high-order connectivity?
- How to compute homology in a stable way?
 - *simplicial complexes* for data representation
 - *filtration* on simplicial complexes
 - *persistent homology*

Betti Numbers: the number of i -dim holes



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

Betti Numbers and Homology Groups

- Betti numbers are computed as dimensions of Boolean vector spaces (E. Noether, \mathbb{Z}_2 -homology group)

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- $H_i(X)$ is *functorial*, i.e. continuous mapping $f : X \rightarrow Y$ induces linear transformation $H_i(f) : H_i(X) \rightarrow H_i(Y)$, structure preserving

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- computation is simple linear algebra over fields or integers
- data representation by *simplicial complexes*

Simplicial Complexes for Data Representation

Definition (Simplicial Complex)

An abstract simplicial complex is a collection Σ of subsets of V which is closed under inclusion (or deletion), i.e. $\tau \in \Sigma$ and $\sigma \subseteq \tau$, then $\sigma \in \Sigma$.

- Chess-board Complex
- Term-document cooccurrence complex
- Nerve complex
- Point cloud data in metric spaces:
 - Čech, Rips, Witness complex
 - Mayer-Vietoris Blowup
- Clique complex in pairwise comparison graphs
- Strategic complex in game theory

Chess-board Complex

Definition (Chess-board Complex)

Let V be the positions on a Chess board. Σ collects position subsets of V where one can place queens (rooks) without capturing each other.

- Closedness under deletion: if $\sigma \in \Sigma$ is a set of “safe” positions, then any subset $\tau \subseteq \sigma$ is also a set of “safe” positions

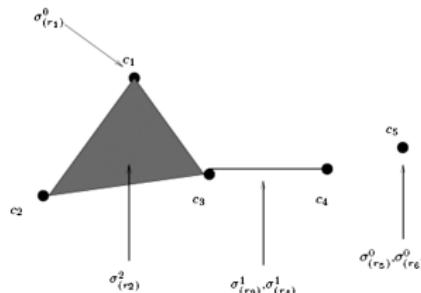


Eight Queens problem



Term-Document Co-occurrence Complex

	c_1	c_2	c_3	c_4	c_5
r_1	1	0	0	0	0
r_2	1	1	1	0	0
r_3	0	0	1	1	0
r_4	0	0	1	1	0
r_5	0	0	0	0	1
r_6	0	0	0	0	1



- Left is a term-document co-occurrence matrix
- Right is a simplicial complex representation of terms
- Connectivity analysis captures more information than Latent Semantic Index (Li & Kwong 2009)

Nerve complex

Definition (Nerve Complex)

Define a cover of X , $X = \cup_{\alpha} U_{\alpha}$. $V = \{U_{\alpha}\}$ and define
 $\Sigma = \{U_I : \cap_{\alpha \in I} U_{\alpha} \neq \emptyset\}$.

- Closedness under deletion
- Can be applied to any topological space X
- **Nerve Theorem:** if every U_I is contractible, then X has the same homotopy type as Σ .

Nerve complex example

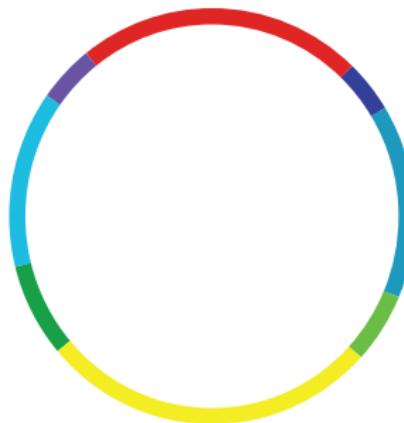


Figure: Covering of circle

Nerve complex example

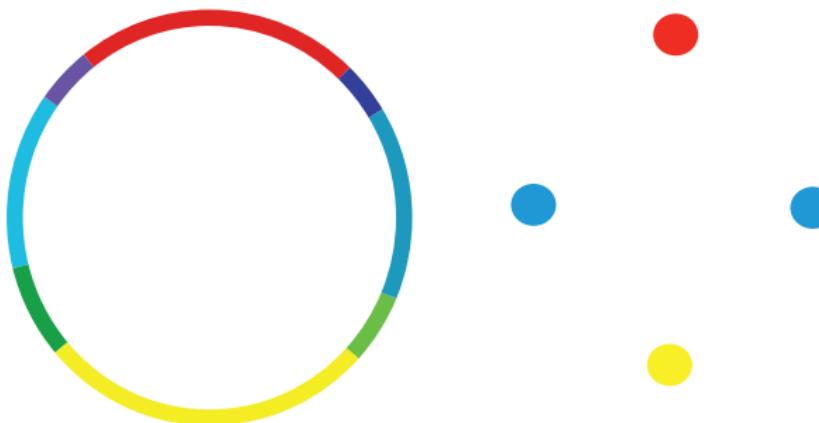


Figure: Create nodes

Nerve complex example

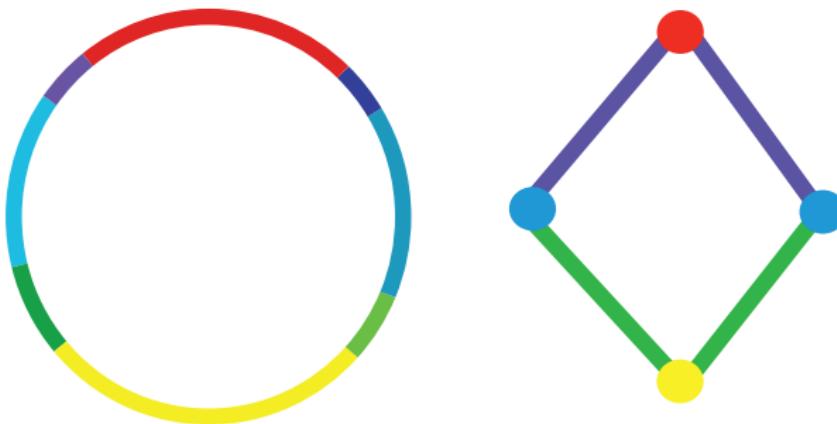


Figure: Create edges, that gives a Nerve complex (graph)

Nerve of Seven Bridges of Königsberg

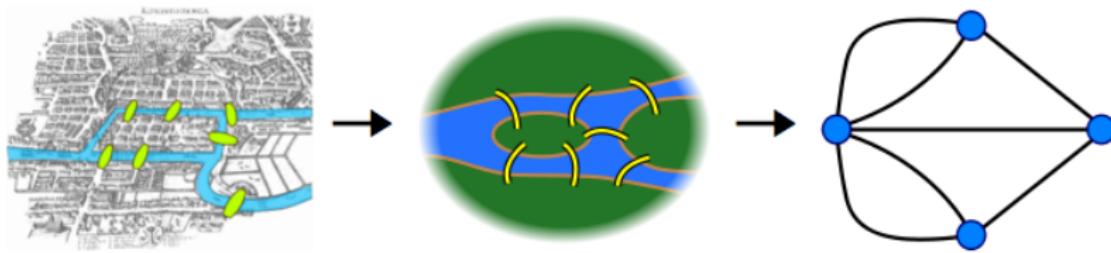


Figure: Nerve graph of Seven Bridges of Königsberg

Point cloud data

- Now given point cloud data $\mathcal{X} = \{x_1, \dots, x_n\}$, and a covering $V = \{U_\alpha\}$, where each U_α is a cluster of data
- Build a simplicial complex (Nerve) in the same way, but components replaced by clusters

Mapping

- How to choose coverings?
- Create a reference map (or filter) $h : \mathcal{X} \rightarrow \mathcal{Z}$, where \mathcal{Z} is a topological space often with interesting metrics (e.g. \mathbb{R} , \mathbb{R}^2 , S^1 etc.), and a covering \mathcal{U} of \mathcal{Z} , then construct the covering of \mathcal{X} using inverse map $\{h^{-1}U_\alpha\}$.

Example: Morse Theory and Reeb graph

- a nice (Morse) function: $h : \mathcal{X} \rightarrow \mathbb{R}$, on a smooth manifold \mathcal{X}
- topology of \mathcal{X} reconstructed from level sets $h^{-1}(t)$
- topological of $h^{-1}(t)$ only changes at '**critical values**'
- **Reeb graph**: a simplified version, contracting into points the connected components in $h^{-1}(t)$

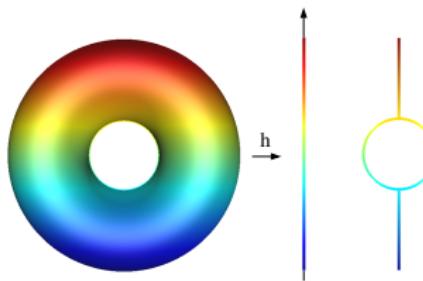


Figure: Construction of Reeb graph; h maps each point on torus to its height.

Mapper: from Continuous to Discrete...

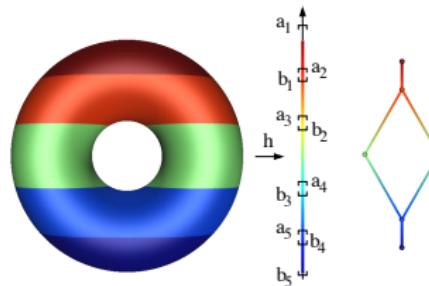


Figure: An illustration of Mapper.

Note:

- degree-one nodes contain local minima/maxima;
- degree-three nodes contain saddle points (critical points);
- degree-two nodes consist of regular points

Mapper algorithm

[Singh-Memoli-Carlsson. Eurograph-PBG, 2007] Given a data set \mathcal{X} ,

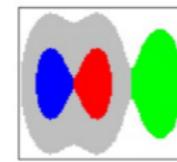
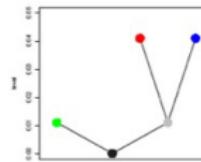
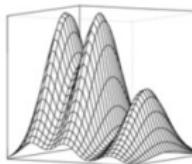
- choose a **filter** map $h : \mathcal{X} \rightarrow \mathcal{Z}$, where \mathcal{Z} is a topological space such as \mathbb{R} , S^1 , \mathbb{R}^d , etc.
- choose a cover $\mathcal{Z} \subseteq \bigcup_{\alpha} U_{\alpha}$
- **cluster/partite** level sets $h^{-1}(U_{\alpha})$ into $V_{\alpha,\beta}$
- **graph** representation: a node for each $V_{\alpha,\beta}$, an edge between $(V_{\alpha_1,\beta_1}, V_{\alpha_2,\beta_2})$ iff $U_{\alpha_1} \cap U_{\alpha_2} \neq \emptyset$ and $V_{\alpha_1,\beta_1} \cap V_{\alpha_2,\beta_2} \neq \emptyset$.
- extendable to **simplicial complex representation**.

Note: it extends **Reeb Graph** from \mathbb{R} to general topological space \mathcal{Z} ; may lead to a particular implementation of **Nerve theorem** through filter map h .

In applications.

Reeb graph has found various applications in computational geometry, statistics under different names.

- computer science: contour trees, Reeb graphs
- statistics: density cluster trees (Hartigan)



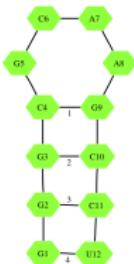
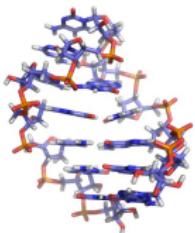
Reference Mapping

Typical one dimensional filters/mappings:

- Density estimators
- Measures of data (ec-)centrality: e.g. $\sum_{x' \in \mathcal{X}} d(x, x')^p$
- Geometric embeddings: PCA/MDS, Manifold learning, Diffusion Maps etc.
- Response variable in statistics: progression stage of disease etc.

Example: RNA Tetraloop

Biological relevance:

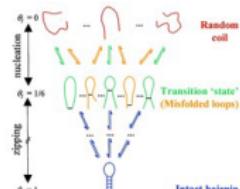


- serve as nucleation site for RNA folding
- form sequence specific tertiary interactions
- protein recognition sites
- certain Tetraloops can pause RNA transcription

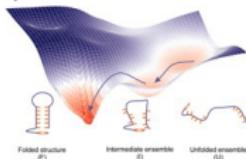
Note: simple, but, **biological debates over intermediate states** on folding pathways

Figure: RNA
GCAA-Tetraloop

Debates: Two-state vs. Multi-state Models



(a) 2-state model



(b) multi-state model

- 2-state: transition state with any one stem base pair, from **thermodynamic** experiments [*Ansari A, et al. PNAS, 2001, 98: 7771-7776*]
- multi-state: there is a stable intermediate state, which contains collapsed structures, from **kinetic** measurements [*Ma H, et al. PNAS, 2007, 104:712-6*]
- experiments: **no** structural information
- computer simulations at full-atom resolution:
 - **exisitence** of intermediate states
 - if yes, what's the **structure?**

Mapper with density filters in biomolecular folding

Reference: Bowman-Huang-Yao et al. J. Am. Chem. Soc. 2008;
Yao, Sun, Huang, et al. J. Chem. Phys. 2009.

- **densest** regions (energy basins) may correspond to **metastates** (e.g. folded, extended)
- **intermediate/transition states** on pathways connecting them are **relatively sparse**

Therefore with Mapper

- **clustering on density level sets** helps separate and identify metastates and intermediate/transition states
- **graph** representation reflects kinetic connectivity between states

A vanilla version

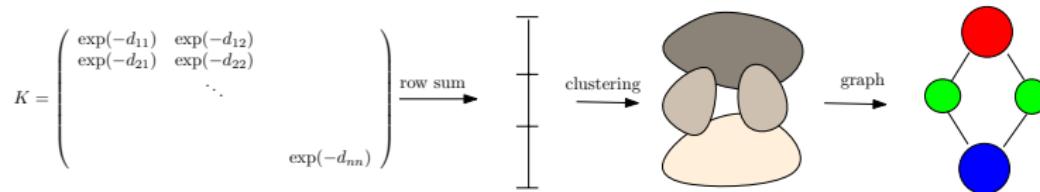


Figure: Mapper Flow Chart

- 1 Kernel density estimation $h(x) = \sum_i K(x, x_i)$ with Hamming distance for contact maps
- 2 Rank the data by h and divide the data into n overlapped sets
- 3 Single-linkage clustering on each level sets
- 4 Graphical representation

Mapper output for Unfolding Pathways

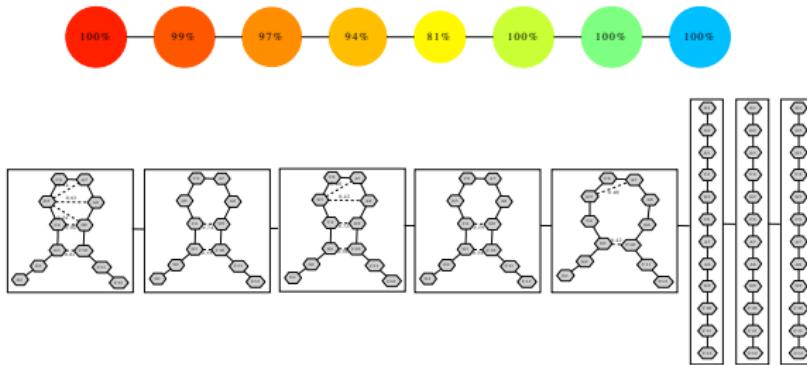


Figure: Unfolding pathway

Mapper output for Refolding Pathways

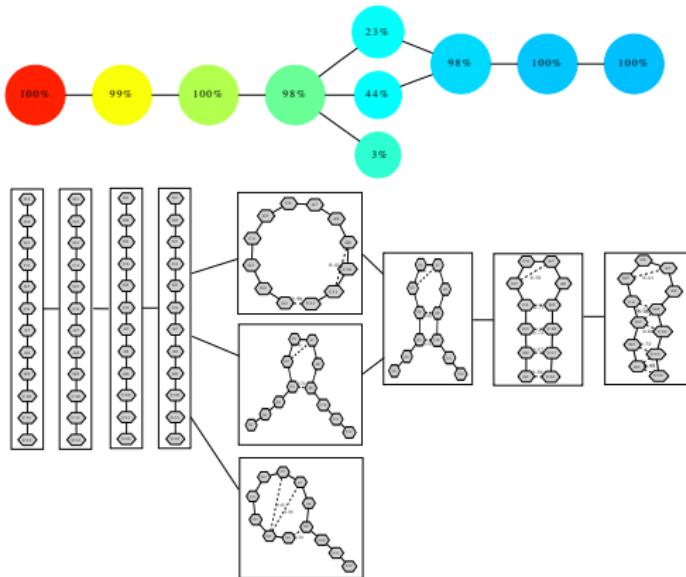


Figure: Refolding pathway

Progression of Breast Cancer: l_2 -eccentricity

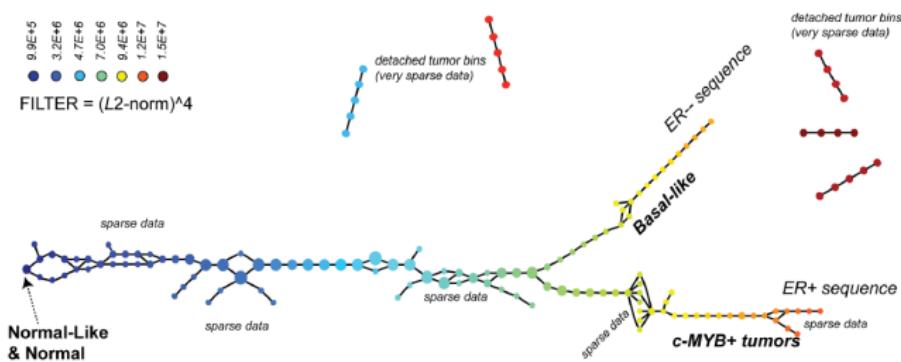


Figure: Monica Nicolau, A. Levine, and Gunnar Carlsson, PNAS'10

Cell Cycles

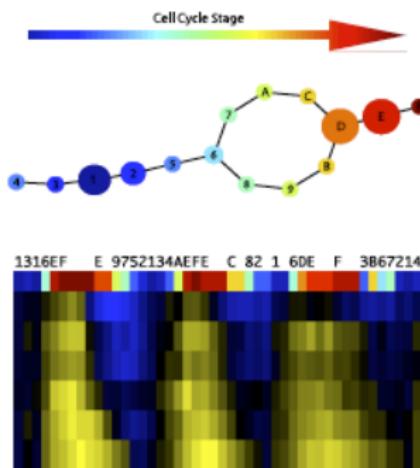


Figure: Cell Cycle Microarray Data, courtesy of M. Nicolau, Nagarajan, G. Singh, Carlsson

Relationships between diabetic, pre-diabetic, and healthy populations

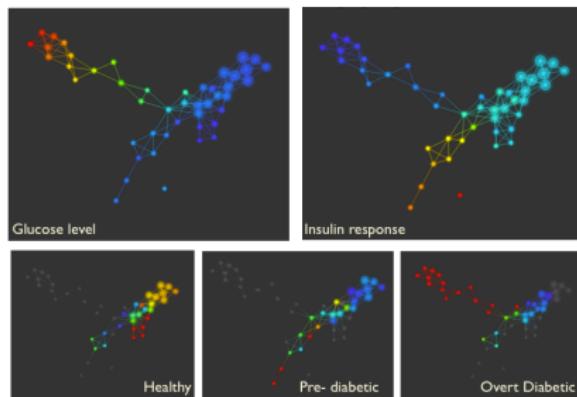
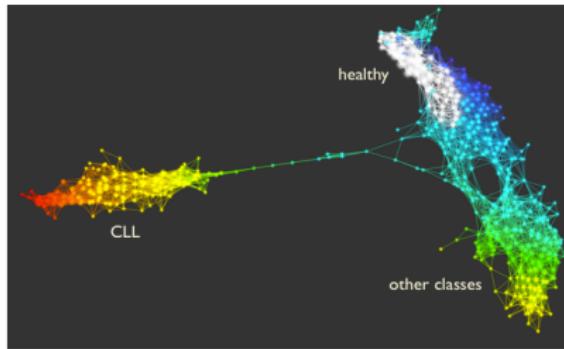


Figure: Miller-Reaven Diabetes Dataset, courtesy of Gunnar Carlsson

Leukemia with gene expression profiles



Data: Gene expression profiles of bone marrow of leukemia patients

Source: PMID 8573112

Columns: 1500 genes

Rows: 1905 patients

Figure: Topological structure of Leukemia: courtesy of Gunnar Carlsson

Čech complex

Definition (Čech Complex C_ϵ)

In a metric space (X, d) , define a cover of X , $X = \cup_{\alpha} U_{\alpha}$ where $U_{\alpha} = B_{\epsilon}(t_{\alpha}) := \{x \in X : d(x - t_{\alpha}) \leq \epsilon\}$. $V = \{U_{\alpha}\}$ and define $\Sigma = \{U_I : \cap_{\alpha \in I} U_{\alpha} \neq \emptyset\}$.

- Closedness under deletion
- Can be applied to any metric space X
- **Nerve Theorem:** if every U_I is contractible, then X has the same homotopy type as Σ .

Example: Čech Complex

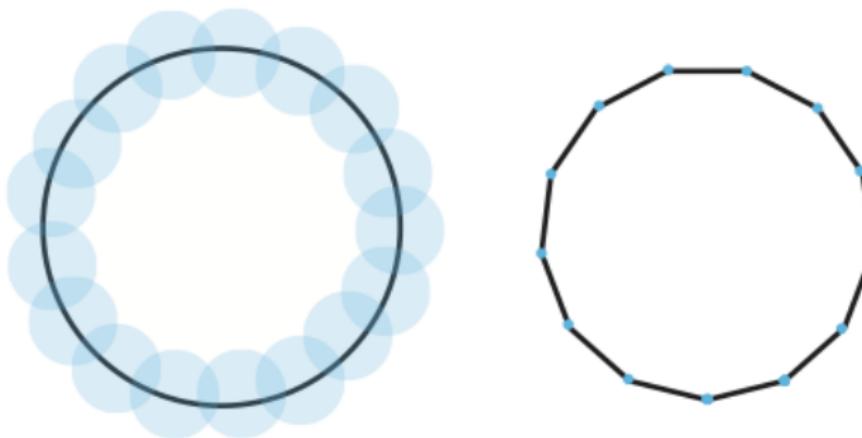


Figure: Čech complex of a circle, C_ϵ , covered by a set of balls.

Vietoris-Rips complex

- Čech complex is hard to compute, even in Euclidean space
- One can easily compute an upper bound for Čech complex
 - Construct a Čech subcomplex of 1-dimension, i.e. a graph with edges connecting point pairs whose distance is no more than ϵ .
 - Find the clique complex, i.e. maximal complex whose 1-skeleton is the graph above, where every k -clique is regarded as a $k - 1$ simplex

Definition (Vietoris-Rips Complex)

Let $V = \{x_\alpha \in X\}$. Define

$$VR_\epsilon = \{U_I \subseteq V : d(x_\alpha, x_\beta) \leq \epsilon, \alpha, \beta \in I\}.$$

Example: Rips Complex

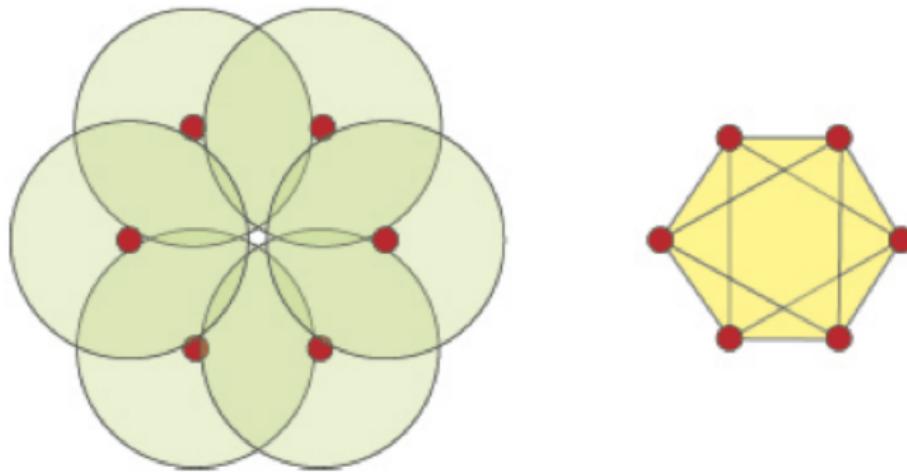


Figure: Left: Čech complex gives a circle; Right: Rips complex gives a sphere S^2 .

Generalized Vietoris-Rips for Symmetric Relations

Definition (Symmetric Relation Complex)

Let V be a set and a symmetric relation $R = \{(u, v)\} \subseteq V^2$ such that $(u, v) \in R \Rightarrow (v, u) \in R$. Σ collects subsets of V which are in pairwise relations.

- Closedness under deletion: if $\sigma \in \Sigma$ is a set of related items, then any subset $\tau \subseteq \sigma$ is a set of related items
- Generalized Vietoris-Rips complex beyond metric spaces
- E.g. Zeeman's tolerance space
- C.H. Dowker defines simplicial complex for unsymmetric relations

Sandwich Theorems

- Rips is easier to compute than Čech
 - even so, Rips is exponential to dimension generally
- However Vietoris-Rips CAN NOT preserve the homotopy type as Čech
- But there is still a hope to find a **lower bound** on homology –

Theorem (“Sandwich”)

$$VR_\epsilon \subseteq C_\epsilon \subseteq VR_{2\epsilon}$$

- If a homology group “persists” through $R_\epsilon \rightarrow R_{2\epsilon}$, then it must exist in C_ϵ ; but not the vice versa.

A further simplification: Witness complex

Definition (Strong Witness Complex)

Let $V = \{t_\alpha \in X\}$. Define

$$W_\epsilon^s = \{U_I \subseteq V : \exists x \in X, \forall \alpha \in I, d(x, t_\alpha) \leq d(x, V) + \epsilon\}.$$

Definition (Weak Witness Complex)

Let $V = \{t_\alpha \in X\}$. Define

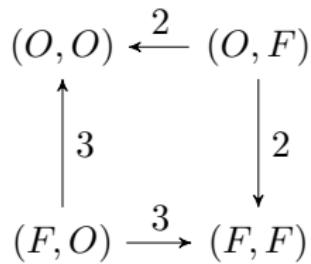
$$W_\epsilon^w = \{U_I \subseteq V : \exists x \in X, \forall \alpha \in I, d(x, t_\alpha) \leq d(x, V_{-I}) + \epsilon\}.$$

- V can be a set of landmarks, much smaller than X
- Monotonicity: $W_\epsilon^* \subseteq W_{\epsilon'}^*$ if $\epsilon \leq \epsilon'$
- But not easy to control homotopy types between W^* and X

Strategic Simplicial Complex for Flow Games

	O	F
O	3, 2	0, 0
F	0, 0	2, 3

(a) Battle of the sexes



- Strategic simplicial complex is the clique complex of pairwise comparison graph above, inspired by ranking
- Every game can be decomposed as the direct sum of potential games and zero-sum games (harmonic games) (Candogan, Menache, Ozdaglar and Parrilo 2010)

Example I: Persistent Homology of Čech Complexes

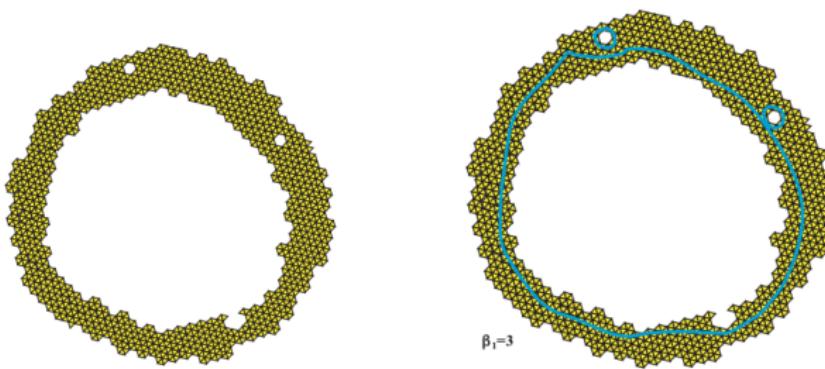


Figure: Scale ϵ_1 : $\beta_0 = 1$, $\beta_1 = 3$

Example I: Persistent Homology of Čech Complexes

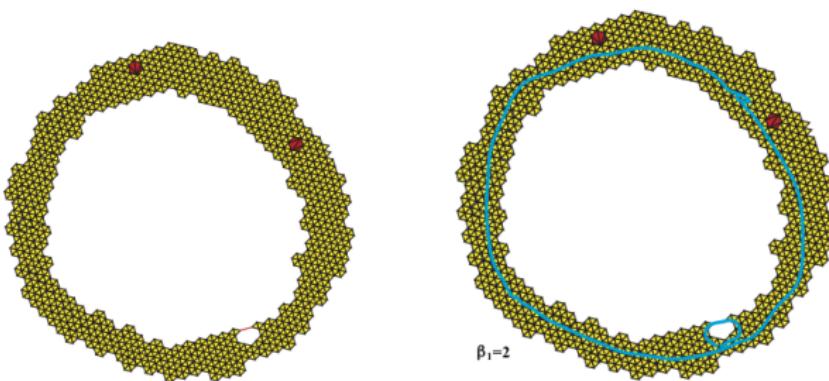


Figure: Scale ϵ_1 : $\beta_0 = 1$, $\beta_1 = 2$

Example II: Persistence 0-Homology induced by Height Function

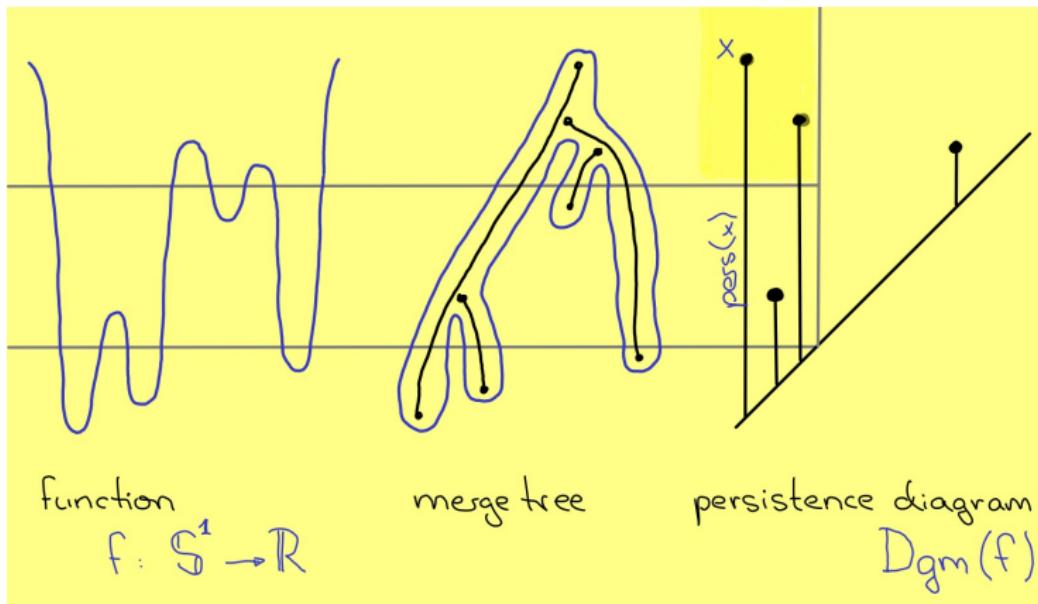
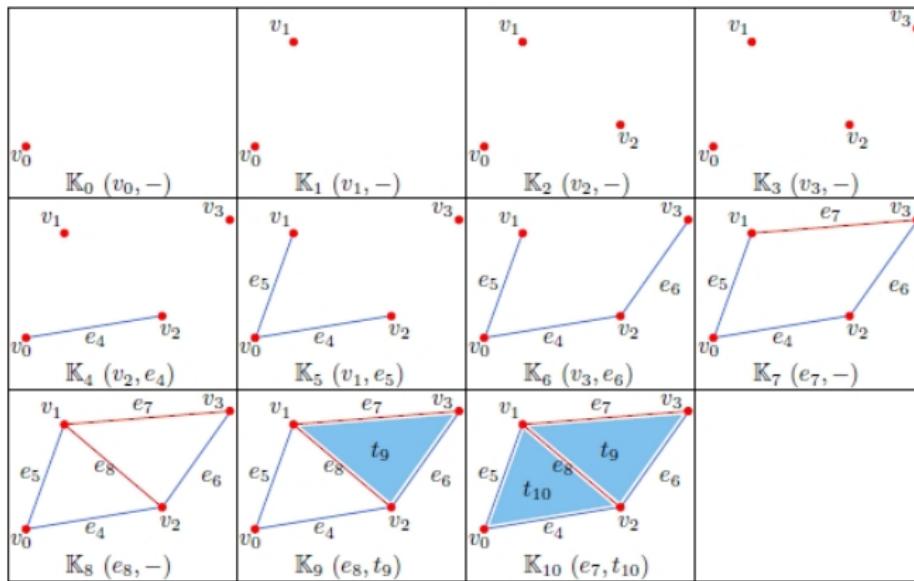
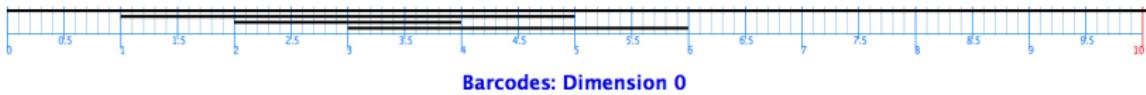


Figure: The birth and death of connected components.

Example III: Persistent Homology as Online Algorithm to Track Topology Changements



Persistent Betti Numbers: Barcodes



- Toolbox: JavaPlex (<https://github.com/appliedtopology/javaplex/wiki/Tutorial>)
 - Java version of Plex, work with matlab
 - Rips, Witness complex, Persistence Homology
- Other Choices: Plex 2.5 for Matlab (not maintained any more), Dionysus (Dmitry Morozov)

Persistent Homology: Algebraic Theory [Zomorodian-Carlsson]

- All above gives rise to a filtration of simplicial complex

$$\emptyset = \Sigma_0 \subseteq \Sigma_1 \subseteq \Sigma_2 \subseteq \dots$$

- Functoriality of inclusion: there are homomorphisms between homology groups

$$0 \rightarrow H_1 \rightarrow H_2 \rightarrow \dots$$

- A persistent homology is the image of H_i in H_j with $j > i$.

Persistent 0-Homology of Rips Complex

- Equivalent to **single-linkage** clustering
- Barcode is the single linkage dendrogram (tree) without labels
- Kleinberg's Impossibility Theorem for clustering: no clustering algorithm satisfies scale invariance, richness, and consistency
- Memoli & Carlsson 2009: single-linkage is the unique **persistent clustering** with scale invariance
- **Open:** but, is persistence the necessity for clustering?
- Notes: try matlab command **linkage** for single-linkage clustering.

Application I: Sensor Network Coverage by Persistent Homology

- V. de Silva and R. Ghrist (2005) Coverage in sensor networks via persistent homology.
- Ideally sensor communication can be modeled by Rips complex
 - two sensors has distance within a short range, then two sensors receive strong signals;
 - two sensors has distance within a middle range, then two sensors receive weak signals;
 - otherwise no signals

Sandwich Theorem

Theorem (de Silva-Ghrist 2005)

Let X be a set of points in \mathbb{R}^d and $C_\epsilon(X)$ the Čech complex of the cover of X by balls of radius $\epsilon/2$. Then there is chain of inclusions

$$R_{\epsilon'}(X) \subset C_\epsilon(X) \subset R_\epsilon(X) \text{ whenever } \frac{\epsilon}{\epsilon'} \geq \sqrt{\frac{2d}{d+1}}.$$

Moreover, this ratio is the smallest for which the inclusions hold in general.

Note: this gives a sufficient condition to detect holes in sensor network coverage

- Čech complex is hard to compute while Rips is easy;
- If a hole persists from $R_{\epsilon'}$ to R_ϵ , then it must exists in C_ϵ .

Persistent 1-Homology in Rips Complexes

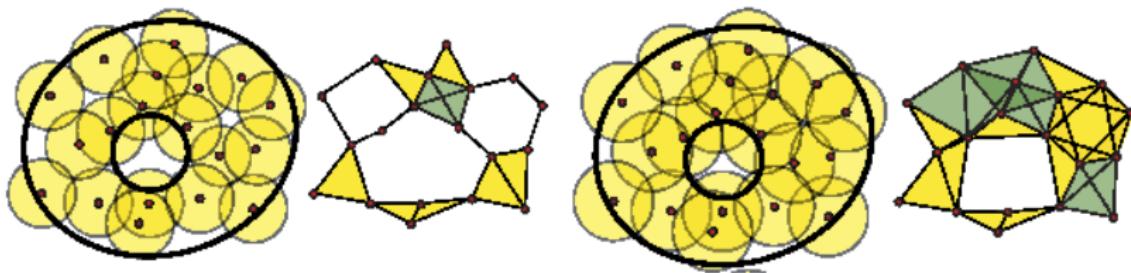


Figure: Left: $R_{\epsilon'}$; Right: R_ϵ . The middle hole persists from $R_{\epsilon'}$ to R_ϵ .

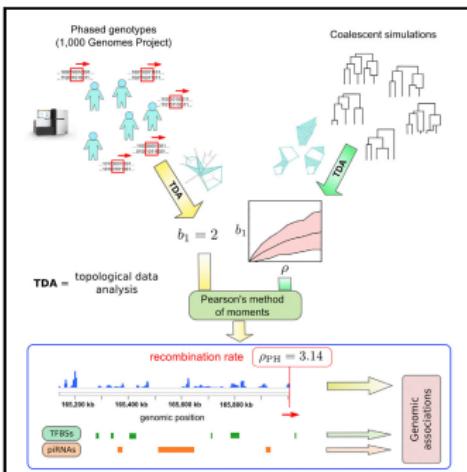
Genome-wide Maps of Human Recombination

Cell Systems

ARTICLE

Topological Data Analysis Generates High-Resolution, Genome-wide Maps of Human Recombination

Graphical Abstract



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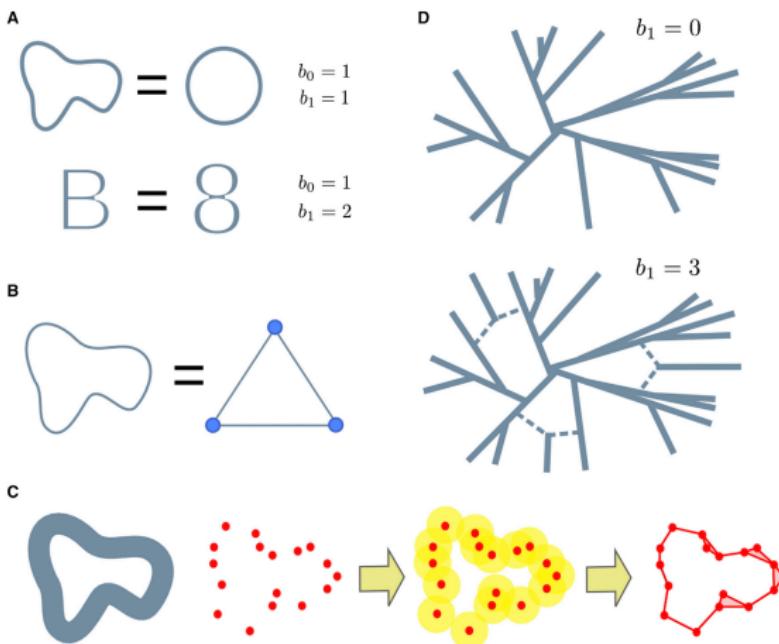
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In Brief

Camara et al. introduce a new method to estimate recombination rates from large genomic samples and present high-resolution recombination maps of seven human populations. Using these maps, they show evidence of previously unreported associations of recombination with binding sites of specific transcription factors and with repeat-derived loci matched by piRNAs.

Persistent β_1 associated with recombination rates



Persistent Homology Analysis of Biomolecular Data

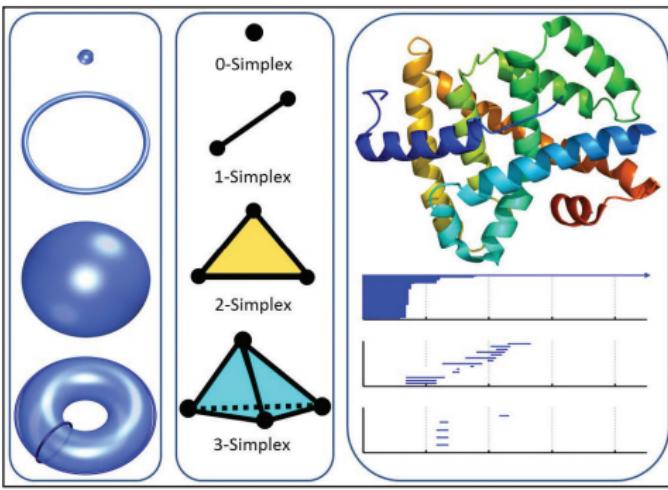


Figure 1. An illustration of topological invariants (left), basic simplices (middle), and protein-persistent barcodes (right). **Left.** A point, a circle, an empty sphere, and a torus are displayed from top to bottom. Betti-0, Betti-1, and Betti-2 numbers are, respectively, 1, 0, and 0 for a point; 0, 1, and 0 for a circle; 0, 0, and 1 for a sphere; and 1, 2, and 1 for a torus. Two auxiliary rings are added to the torus to explain Betti-1=2. **Middle.** Four typical simplices. **Right.** Topological fingerprint (bottom) for a protein (top). Image credit: Zixuan Cang.

Figure: Prof. WEI, Guowei at MSU, SIAM News 2017

Persistent Homology Analysis of Biomolecular Data

- Persistent Homology as Barcodes provides multiscale analysis of protein 3D structure
- Combined with machine learning (deep learning, random forests, boosting), it provides best free energy ranking for Set 1 (Stage 2) in D3R Grand Challenge 2, a worldwide competition in computer-aided drug design
(<http://bit.ly/2h4Vm6q>)

Application II: Natural Image Statistics

- G. Carlsson, V. de Silva, T. Ishkanov, A. Zomorodian (2008)
On the local behavior of spaces of natural images,
International Journal of Computer Vision, 76(1):1-12.
- 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}

Natural Image Statistics

- **D. Mumford:** What can be said about the set of images $\mathcal{I} \subseteq \mathcal{P}$ one obtains when one takes many images with a digital camera?
- **Lee, Mumford, Pedersen:** Useful to study **local** structure of images statistically

Natural Image Statistics

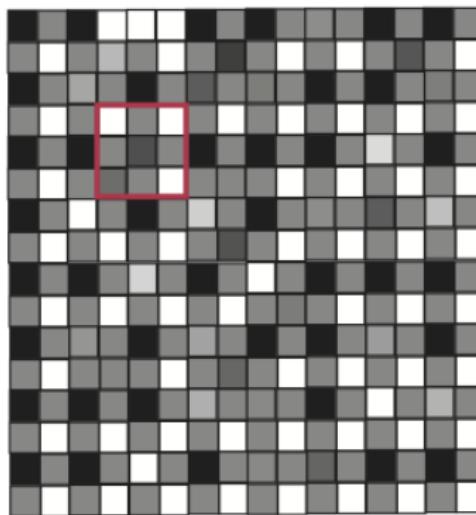


Figure: 3×3 patches in images

Natural Image Statistics

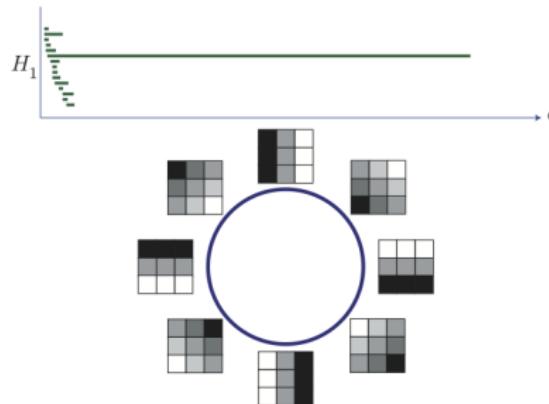
Lee-Mumford-Pedersen [LMP] study only high contrast patches.

- Collect: $4.5M$ 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-D hyperplane, $\approx R^8$
- Furthermore, normalize contrast by dividing by the norm, so obtain patches with norm = 1, whence data lies on a 7-D ellipsoid, $\approx S^7$

Natural Image Statistics: Primary Circle

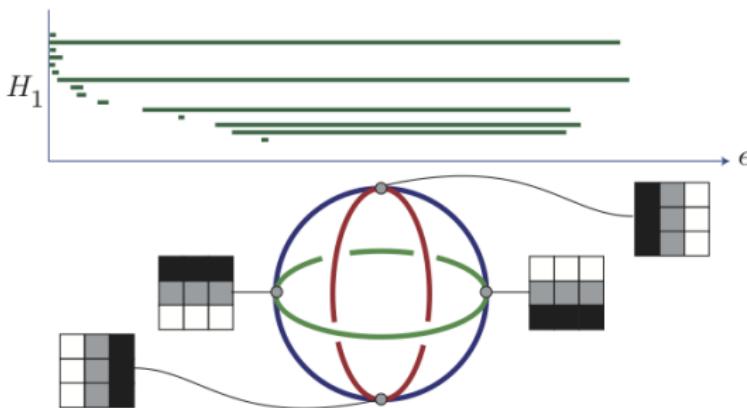
High density subsets $\mathcal{M}(k = 300, t = 0.25)$:

- Codensity filter: $d_k(x)$ be the distance from x to its k -th nearest neighbor
 - the lower $d_k(x)$, the higher density of x
- Take $k = 300$, extract 5,000 top $t = 25\%$ densest points, which concentrate on a **primary circle**



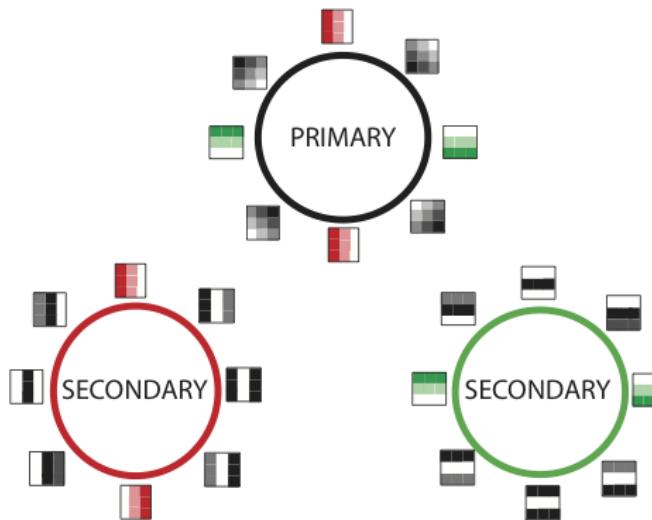
Natural Image Statistics: Three Circles

- Take $k = 15$, extract 5,000 top 25% densest points, which shows persistent $\beta_1 = 5$, 3-circle model

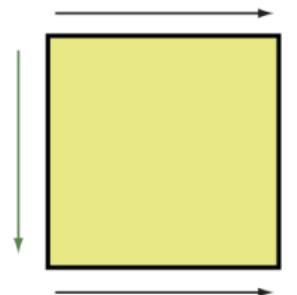


Natural Image Statistics: Three Circles

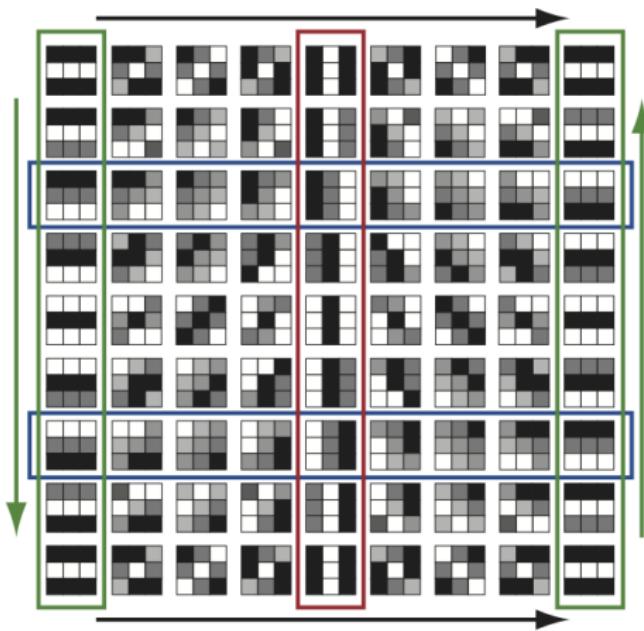
Generators for 3 circles



Natural Image Statistics: Klein Bottle



Natural Image Statistics: Klein Bottle Model



Reference

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