Topological Perspectives On Stratification Learning

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Talk Overview

Stratification learning driven by computation:

- What is stratification learning?
- Stratification in statistics and machine learning
- Stratification learning using geometry
- Stratification learning based on homology and cohomology
- Sheaf-theoretic stratification learning (Brown and Wang (2018))
- Discrete stratified Morse theory (Knudson and Wang (2018))
- Challenges and opportunities

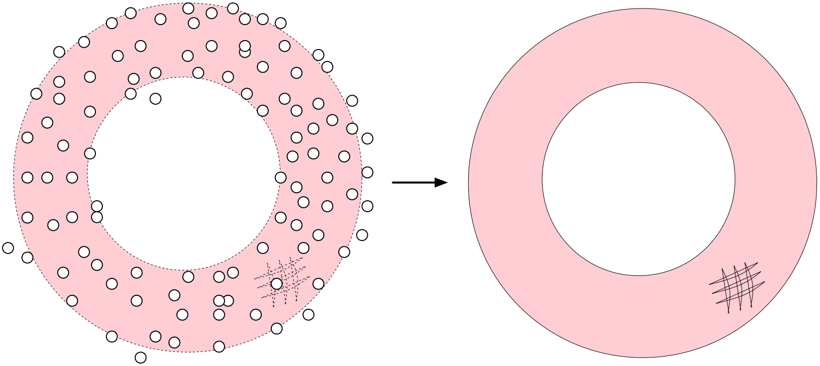
Acknowledgement

- NSF IIS-1513616
- NSF ABI-1661375
- Collaborators: Sayan Mukherjee, Paul Bendich, Adam Brown, Kevin Knudson, Yulong Liang

What is Stratification Learning?

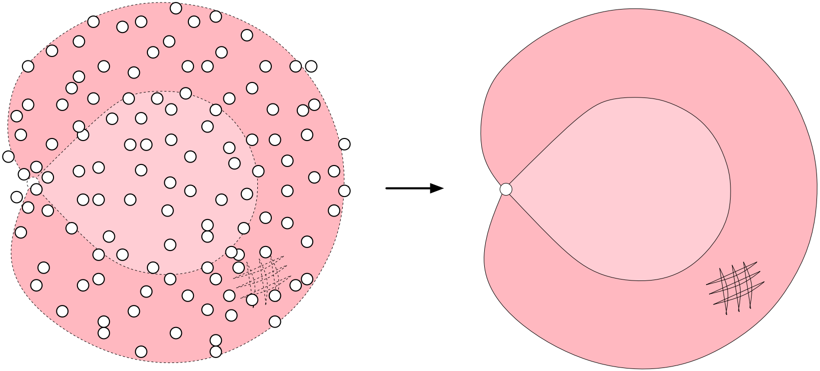
Manifold Learning

Assumption: data is sampled from some unknown manifold



Stratification Learning

Assumption: data is sampled from some unknown underlying space with mixed dimensionality and singularities (beyond manifold)



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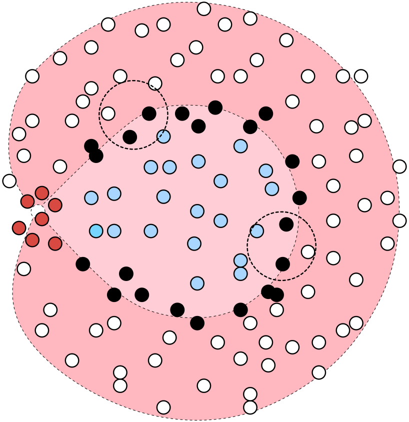
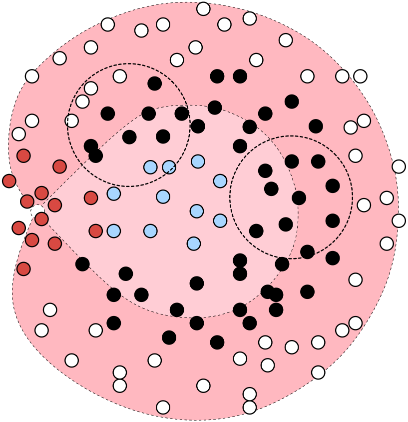

Topological Stratifications

Definition

A topological stratification of a topological space X is a filtration by closed subsets

$$\emptyset = X_{-1} \subset X_0 \subset X_1 \subset \cdots \subset X_n = X$$

such that $X_i - X_{i-1}$ is an i-dimensional (topological) manifold.

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$+$ conditions on how the strata fit together.

Topological Stratification

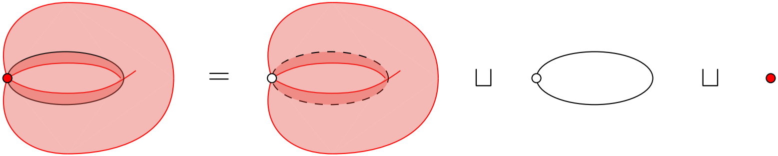

Figure: Example of a topological stratification of a *pinched torus*.

Computing Stratifications

Computing (reasonable) *topological* stratifications of triangulated topological spaces can be difficult.

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Available tools: Statistics, geometry, homology, cohomology.

Stratification Learning

We use the word *stratification learning* loosely to mean:

An *unsupervised*, *exploratory*, *clustering* process that infers a decomposition of data into disjoint subsets that capture recognizable and meaningful structural information.

Goal: better understand the complexity of the data.

Stratification in Statistics and Machine Learning

Statistical Approaches

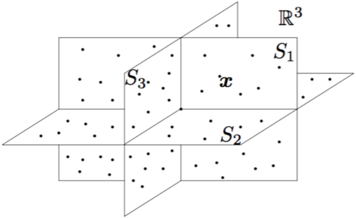
- Inferences of mixture models
- (Local) dimensionality estimation
- With or without linearity assumptions
- Vidal et al. (2005); Haro et al. (2005); Lerman and Zhang (2010)

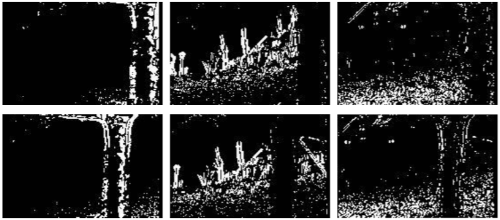
- Challenges: How to handle complex (nonlinear) singularities?
- Opportunities: Can we combine statistical methods with topological ones?

Generalized Principal Component Analysis (GPCA)

Vidal et al. (2005)

- Estimating a mixture of linear subspaces from sample data points.
- A constrained nonlinear least squares problem.
- Minimizes the error between the noisy points and their projections onto the linear subspaces.
- Examples: estimating a mixture of motion models from 2D imagery.



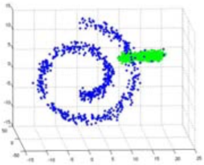


(a) Tree (b) Houses (c) Grass

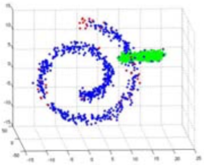
Detecting Mixed Density and Dimensionality

Haro et al. (2005)

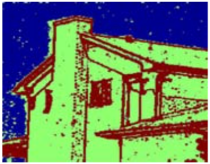
- Simultaneously soft clustering and estimating the mixed dimensionality and density.
- No assumption on linear subspaces.
- Maximum likelihood estimation of a Poisson mixture model (PMM).
- Cluster the data according to the complexity (dimensionality) of the underlying possible multiple manifolds.



(d) PMM ($J = 2$)



(e) PMM ($J = 3$)



Probabilistic Recovery of Multiple Linear Subspaces

Lerman and Zhang (2010)

- l_p energy minimization for modeling data by multiple subspaces.
- Simultaneous recover a number of K fixed subspaces by minimizing the l_p-averaged distances of the sampled data points from any subspace.
- $0 < p \leq 1$: all underlying subspaces can be precisely recovered by l_p minimization with overwhelming probability.
- $K > 1$ and $p > 1$: the underlying subspaces cannot be recovered or even nearly recovered by l_p minimization.

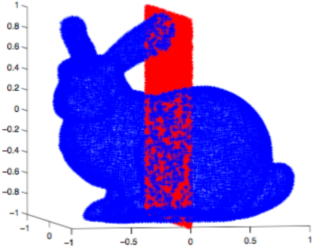
$$e_{l_p}(\mathcal{X}, \mathrm{L}_1, \ldots, \mathrm{L}_K) = \sum_{\mathbf{x} \in \mathcal{X}} \mathrm{dist}^p\left(\mathbf{x}, \bigcup_{i=1}^{K} \mathrm{L}_i\right)$$

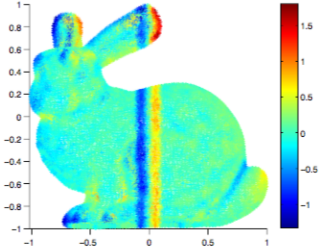
Stratification Learning Using Geometry

Graph Laplacians on Singular Manifolds

Belkin et al. (2012)

- Singularities: *Intersections* (where different manifolds come together) and *sharp edges* (where a manifold sharply changes direction.
- The behavior of graph Laplacian near singularities is quite different from that in the interior of the manifolds.
- In the interior of the manifold: graph Laplacian converges to the Laplace-Beltrami operator.
- Near singularities: graph Laplacian tends to a first-order differential operator.





Stratification Learning based on (Co)Homology

Homological Stratification

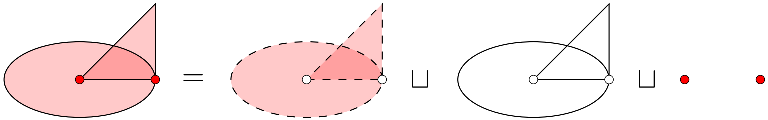


Figure: Example of a homological stratification of a *sundial*.

Homological Stratification: An Incomplete Review

- Rourke and Sanderson (1999): *Homology stratifications and intersection homology*.
- Goresky and MacPherson (1983): *Intersection homology II*.
- Bendich et al. (2007): *Inferring local homology from sampled stratified spaces*.
- Bendich and Harer (2011): *Persistent intersection homology*.
- Bendich et al. (2012): *Local homology transfer and stratification learning*.
- Skraba and Wang (2014): *Approximating Local Homology from Samples*.
- Nanda (2017): *Local cohomology and stratification*.
- Brown and Wang (2018): *Sheaf-theoretic stratification learning*.

- Challenges: One step closer to (certain) topological stratification?
- Opportunities: Beyond (co)homological stratification.

Local Homology

The local homology of a point $x \in X$ is defined as

$$H_\bullet(X, X - x) := \varinjlim_{U \ni x} H_\bullet(X, X - U)$$

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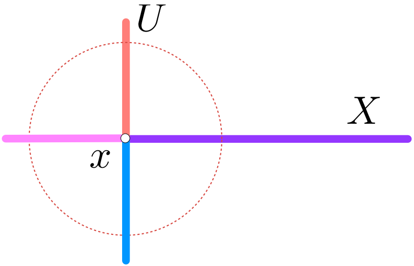
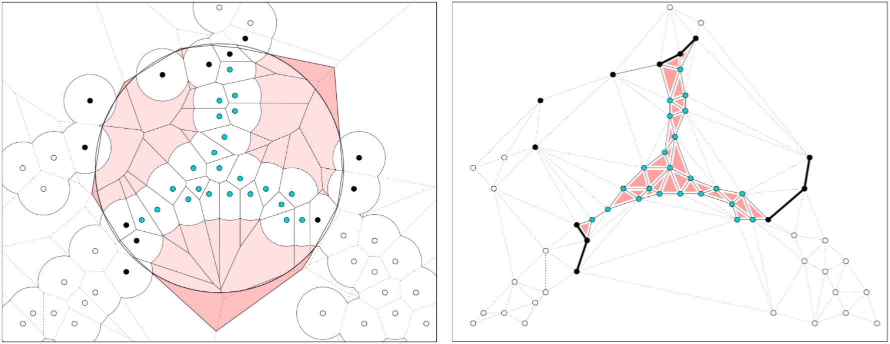


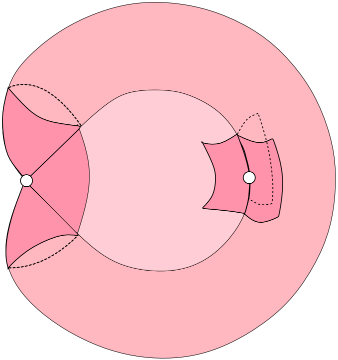
Infer Local Homology from Samples



Bendich et al. (2007)

Local Homology Transfer

Local homology may have the same rank but with different structure.



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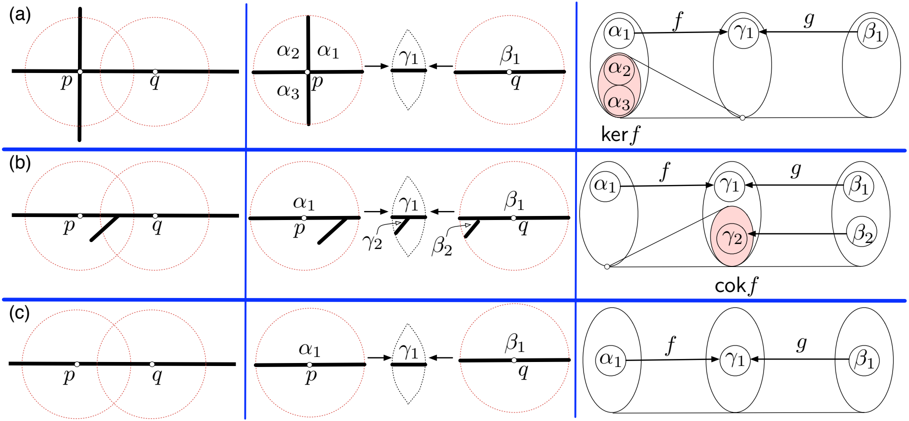

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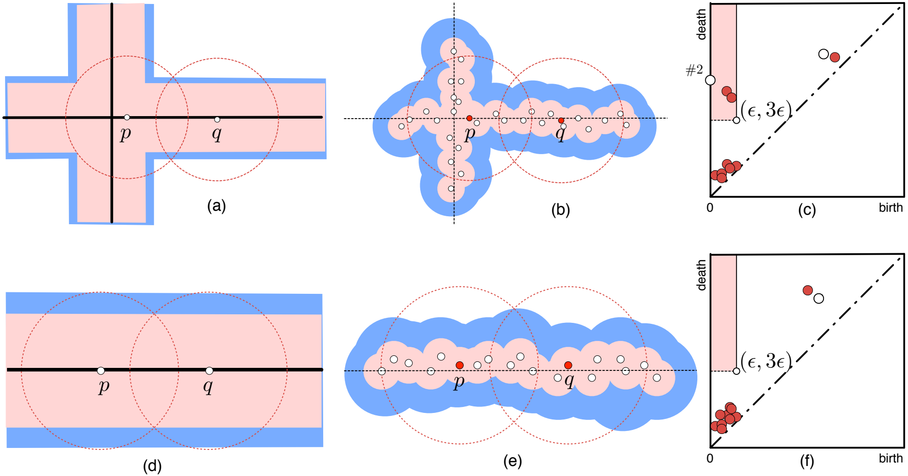

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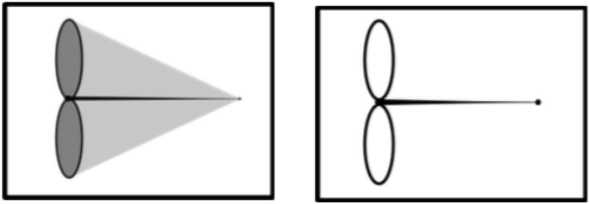
Local Cohomology and Stratification

Nanda (2017)

- Recover the canonical (or, coarsest) stratification of a given regular CW complex into cohomology manifolds, each of which is a union of cells.
- Cosheaves: capture variations in cohomology of cellular neighborhoods across the underlying complex.
- Efficient distributed computation.



Sheaf-Theoretic Stratification Learning

Key Idea

- Use the language of sheaf theory to generalize existing algorithms, e.g. homological stratification.
- Aim to investigate stratifications which can be computed using homological methods and beyond.

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such that there are some nice properties:

1. $\mathcal{F}(\emptyset) = 0$;
2. $\mathcal{F}(U \subset U) = \mathrm{id}_U$.
3. If $U \subset V \subset W$, then $\mathcal{F}(U \subset W) = \mathcal{F}(U \subset V) \circ \mathcal{F}(V \subset W)$.
4. If $\{V_i\}$ is an open cover of U, and $s_i \in \mathcal{F}(V_i)$ has the property that $\forall i, j$, $\mathcal{F}((V_i \cap V_j) \subset V_i)(s_i) = \mathcal{F}((V_j \cap V_i) \subset V_j)(s_j)$, then there exists a unique $s \in \mathcal{F}(U)$ such that $\forall i$, $\mathcal{F}(V_i \subset U)(s) = s_i$.

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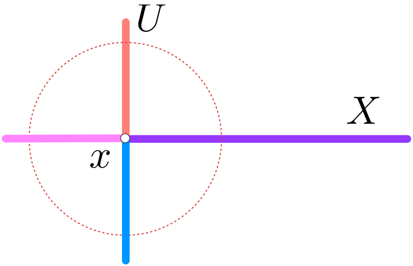
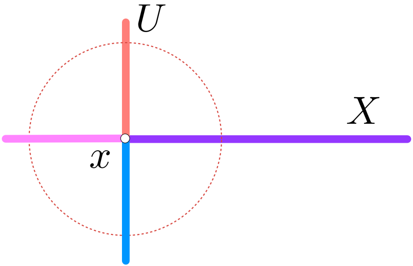


Local Homology Sheaf

Local homology can be viewed as a sheaf on X:

$$\mathcal{L}(U) = H_\bullet(X, X - U)$$



$\mathcal{F}$-Stratifications

Suppose $\mathcal{F}$ is a sheaf on a topological space X.

Definition

An $\mathcal{F}$-stratification of a topological space X is a filtration by closed subsets

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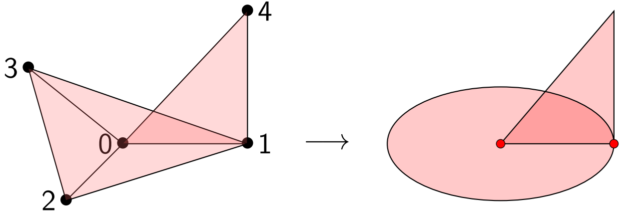
such that $\mathcal{F}$ is locally constant [a] when restricted to $X_i - X_{i-1}$, for each i.

---

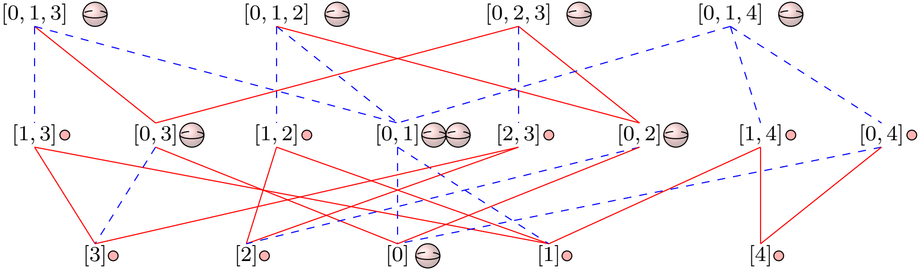
[a] A sheaf $\mathcal{F}$ is a *constant sheaf* if $\mathcal{F}$ is isomorphic to the pull back of a sheaf $\mathcal{G}$ on a single point space $\{x\}$, along the projection map $p : X \to x$. A sheaf $\mathcal{F}$ is *locally constant* if for all $x \in X$, there is a neighborhood U of x such that $\mathcal{F}|_U$ (the restriction of $\mathcal{F}$ to U), is a constant sheaf.

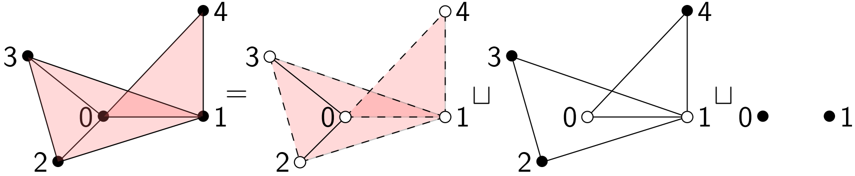
Triangulation of the Sundial



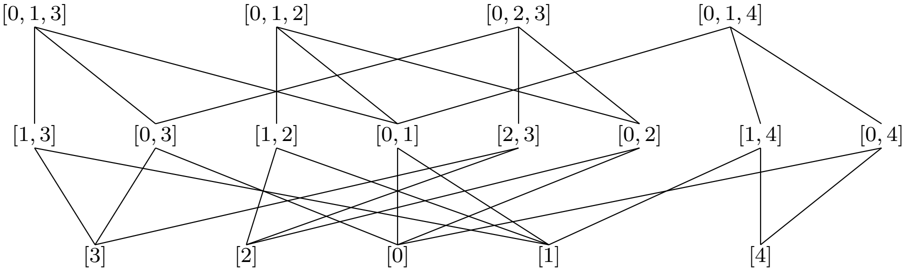
Sheaf-Theoretic Stratifications by Example

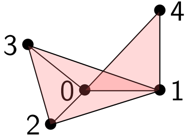
Using labeled Hasse diagram:



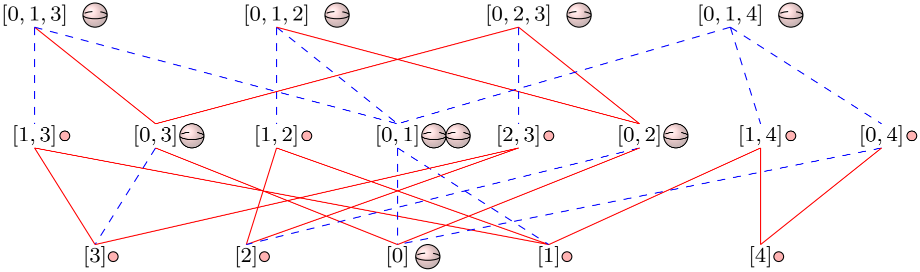


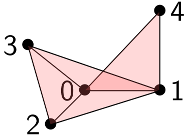
Hasse Diagram





Labeled Hasse Diagram





Inductively defined stratification

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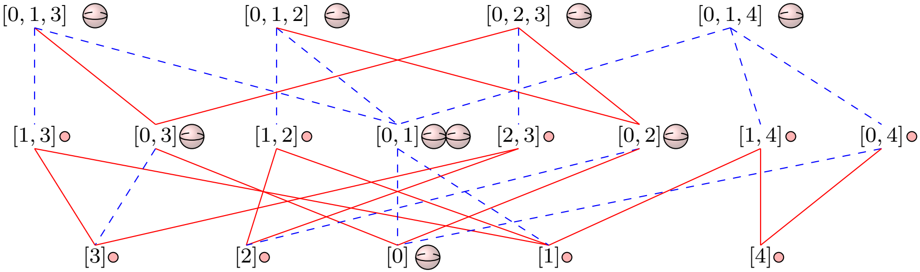
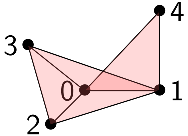
$$S_n = \{\sigma \in X : \mathcal{L}|_{\mathsf{St}\sigma} \text{ is constant}\}$$

Labeled Hasse Diagram, $\mathrm{St}[4]$





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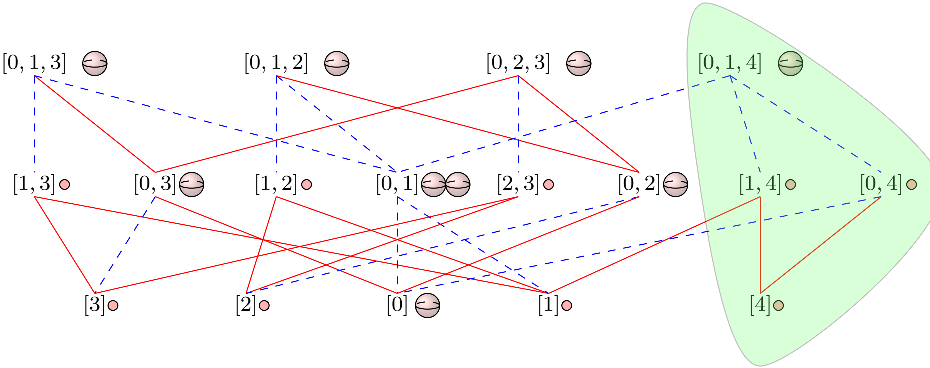
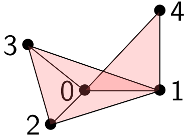
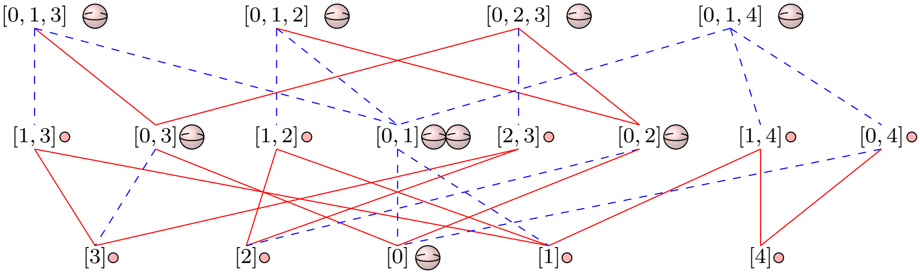
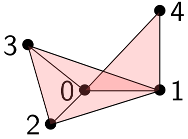




Labeled Hasse Diagram, St[0, 2]





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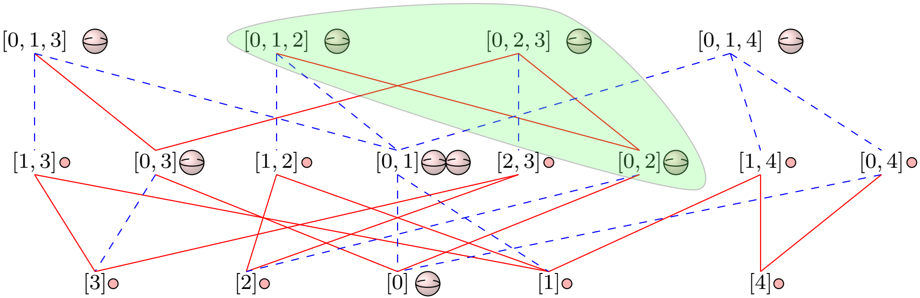
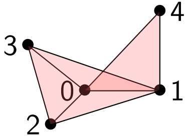
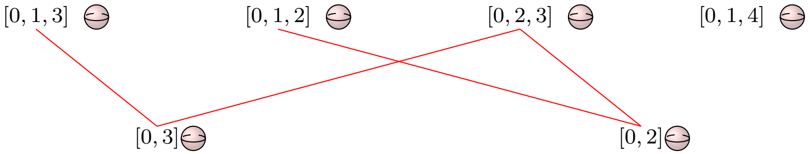
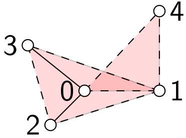




Labeled Hasse Diagram of S_2





Inductively defined stratification

Inductive step: Restrict the local homology sheaf from X to the complement of S_n and repeat:

$$S_{n-1} = \{\sigma \in X - S_n : \mathcal{L}|_{\mathsf{St}_{(X-S_n)}\sigma} \text{ is constant}\}$$

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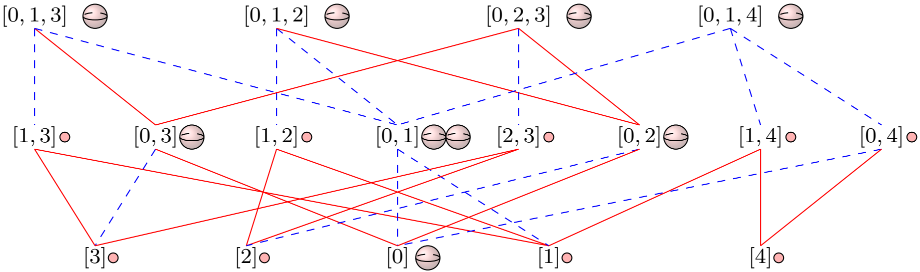

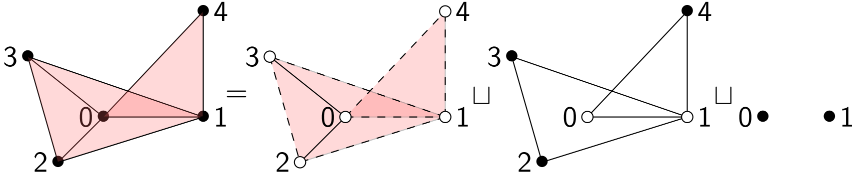

Highlight

computational topology

computational geometry

statistics

Highlight

sheaf theory

computational topology

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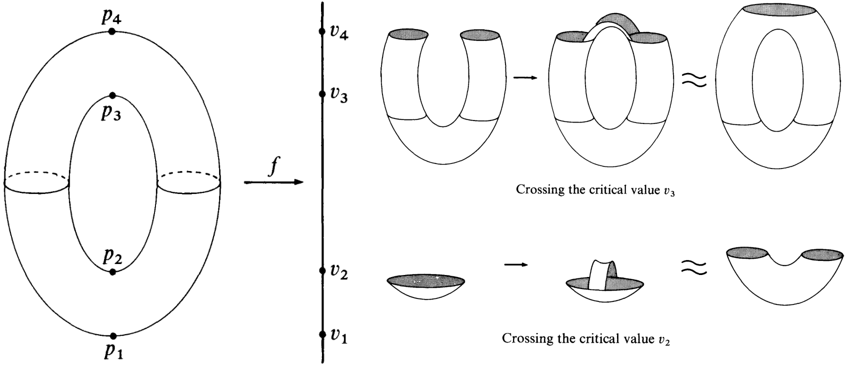
computable stratification theory

Discrete Stratified Morse Theory for Stratification Learning

Key Ideas

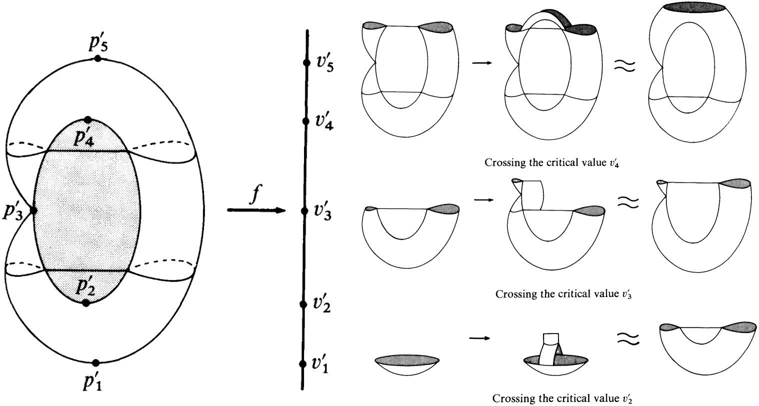
- Data as a simplicial complex equipped with an arbitrary function
- When the function is not a discrete Morse function, we can introduce a *stratification* so that the function restricted to each strata is a discrete Morse function.
- Data simplification and compression

Classic Morse Theory by Picture



Goresky and MacPherson (1988)

Stratified Morse Theory by Picture



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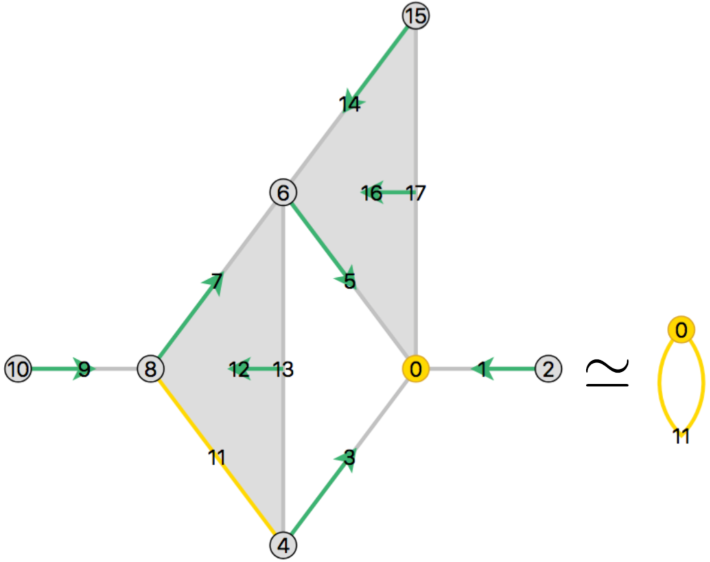
Discrete Morse Theory by Picture



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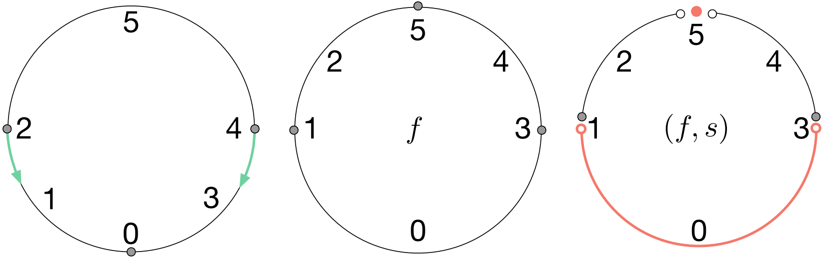
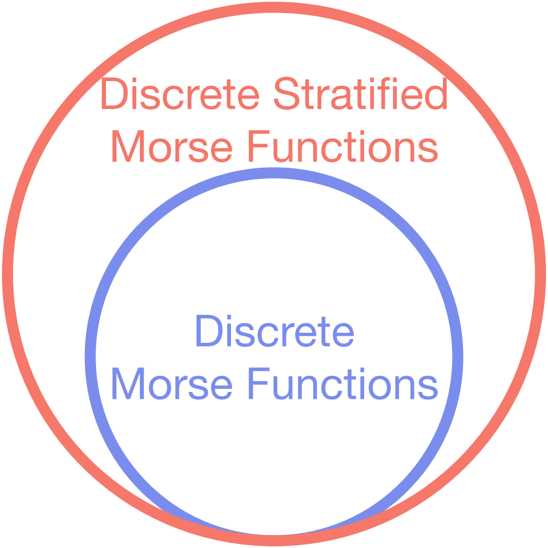


Highlight: Space of Functions



- Data: A simplicial complex K equipped with an arbitrary, real-valued function $f : K \to \mathbb{R}$.

A Combinatorial Adaptation of Stratified Morse Theory

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- Goal: Construct a *discrete stratified Morse function* (DSMF) on the data by introducing a stratification.

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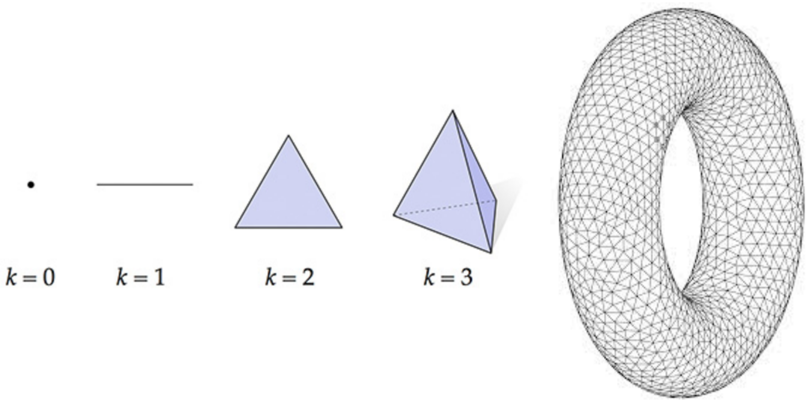
- Applications: data reduction and simplification; parallel computation; imaging and visualization.
- Relevant references: Goresky and MacPherson (1988), Matsumoto (1997), Forman (1998), Forman (2002),...

High-Level Results

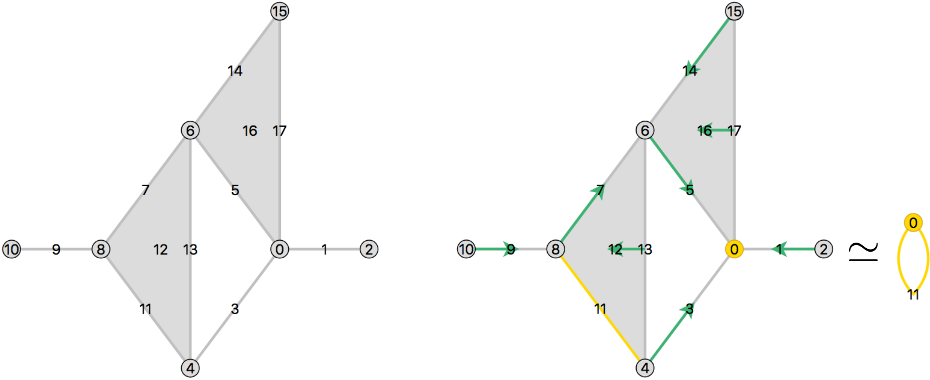
- Relate the *topology* of a finite simplicial complex with the *critical simplices* of a discrete stratified Morse function (DSMF) defined on the complex.
- Provide an algorithm that constructs a DSMF on any finite simplicial complex equipped with a real-valued function.

Discrete Morse Theory (DMT)

Data as a function on a simplicial complex



DMT: an example



Key Definitions

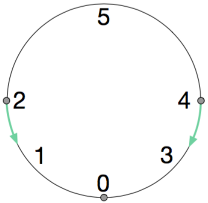
- $U(\alpha) = \{\beta^{(p+1)} > \alpha \mid f(\beta) \leq f(\alpha)\}$
- $L(\alpha) = \{\gamma^{(p-1)} < \alpha \mid f(\gamma) \geq f(\alpha)\}$

Definition

A function $f : K \to \mathbb{R}$ is a *discrete Morse function* if for every $\alpha^{(p)} \in K$, (i) $|U(\alpha)| \leq 1$ and (ii) $|L(\alpha)| \leq 1$.

Definition

A simplex $\alpha^{(p)}$ is *critical* if (i) $|U(\alpha)| = 0$ and (ii) $|L(\alpha)| = 0$.



$$\alpha = f^{-1}(0) : U(\alpha) = L(\alpha) = \emptyset$$
$$\alpha = f^{-1}(1) : U(\alpha) = \emptyset, L(\alpha) = \{f^{-1}(2)\}$$
$$\alpha = f^{-1}(2) : U(\alpha) = \{f^{-1}(1)\}, L(\alpha) = \emptyset$$

Level subcomplex

- Given $c \in \mathbb{R}$, we have the *level subcomplex*

$$K_c = \cup_{f(\alpha) \leq c} \cup_{\beta \leq \alpha} \beta.$$

- K_c contains all simplicies α of K such that $f(\alpha) \leq c$ along with all of their faces.

Two fundamental results of DMT

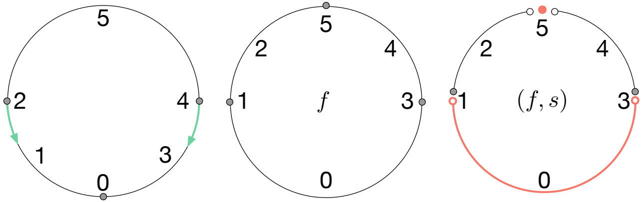
Theorem (DMT-A, Forman (1998))

Suppose the interval $[a, b]$ contains no critical value of f. Then K_b is homotopy equivalent to K_a. In fact, K_a is a deformation retract of K_b and moreover, K_b simplicially collapses onto K_a.

Theorem (DMT-B, Forman (1998))

Suppose $\sigma^{(p)}$ is a critical simplex with $f(\sigma) \in (a, b]$, and there are no other critical simplices with values in $(a, b]$. Then K_b is homotopy equivalent to attaching a p-cell $e^{(p)}$ along its entire boundary; that is,
$K_b = K_a \cup_{\dot{e}^{(p)}} e^{(p)}$.

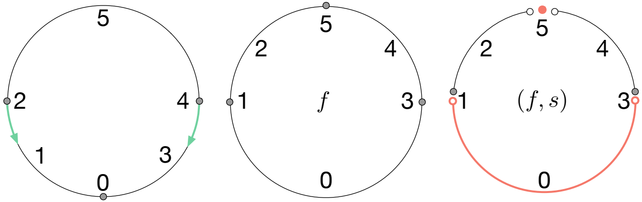
When DMT is not applicable (middle picture)



$$\alpha = f^{-1}(0) : U(\alpha) = \emptyset, L(\alpha) = \{f^{-1}(1), f^{-1}(3)\}$$

- $f : K \to \mathbb{R}$ is not a DMF (not well behaved)

When DMT is not applicable (middle picture)

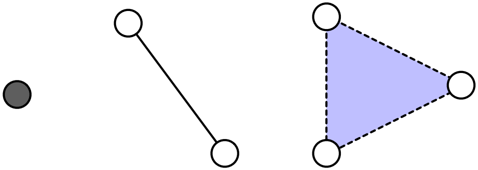


$$\alpha = f^{-1}(0) : U(\alpha) = \emptyset, L(\alpha) = \{f^{-1}(1), f^{-1}(3)\}$$

- $f : K \to \mathbb{R}$ is not a DMF (not well behaved)
- **Solution:** Introduce a stratification s of K such that f restricted to each stratum is a DMF

Discrete Stratified Morse Theory

Open simplices



Stratified simplicial complex

Definition

A *stratification* of a simplicial complex K is a finite filtration

$$\emptyset = K^0 \subset K^1 \subset \cdots \subset K^m = K,$$

such that K^1 is a subcomplex of K, and for each i, $K^i - K^{i-1}$ is a locally closed subset of K [a].

[a] A subset $L \subset K$ is locally closed if it is the intersection of an open and a closed set in K.

- A simplicial complex K equipped with a stratification is referred to as a *stratified simplicial complex*.
- A connected component of the space $K^i - K^{i-1}$ is a *stratum*; and the collection of all strata is denoted by $\mathcal{S} = \{S_j\}$.
- A stratification is an assignment from K to the set $\mathcal{S}$, denoted $s : K \to \mathcal{S}$.

Key Definitions

- Given a simplicial complex K equipped with a stratification $s : K \to \mathcal{S}$, and a function $f : K \to \mathbb{R}$,

$$U_s(\alpha) = \{\beta^{(p+1)} > \alpha \mid s(\beta) = s(\alpha) \text{ and } f(\beta) \leq f(\alpha)\},$$
$$L_s(\alpha) = \{\gamma^{(p-1)} < \alpha \mid s(\gamma) = s(\alpha) \text{ and } f(\gamma) \geq f(\alpha)\}.$$

Definition

A function $f : K \to \mathbb{R}$ (equipped with s) is a *discrete stratified Morse function* if for every $\alpha^{(p)} \in K$, (i) $|U_s(\alpha)| \leq 1$ and (ii) $|L_s(\alpha)| \leq 1$.

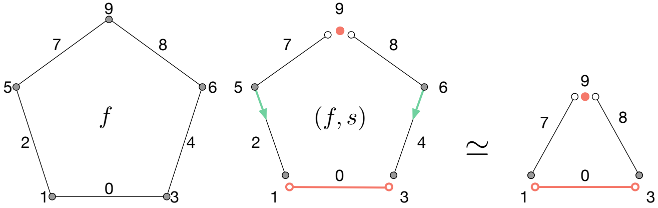
Definition

A simplex $\alpha^{(p)}$ is *critical* if (i) $|U_s(\alpha)| = 0$ and (ii) $|L_s(\alpha)| = 0$.

Violators

Definition

A simplex $\alpha^{(p)}$ is a *violator* (of the conditions associated with a discrete Morse function) if one of these conditions hold: (i) $|U(\alpha)| \geq 2$; (ii) $|L(\alpha)| \geq 2$; (iii) $|U(\alpha)| = 1$ and $|L(\alpha)| = 1$.

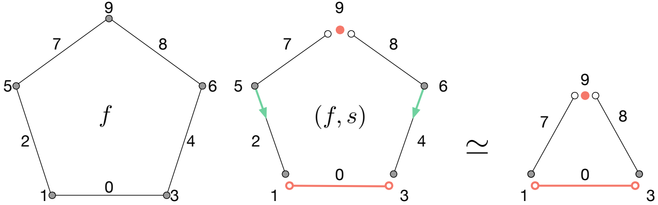


Violator $\alpha = f^{-1}(0), L(\alpha) = \{f^{-1}(1), f^{-1}(3)\}$
Critical $\alpha = f^{-1}(7), L(\alpha) = \{f^{-1}(9)\}, L_s(\alpha) = \emptyset$

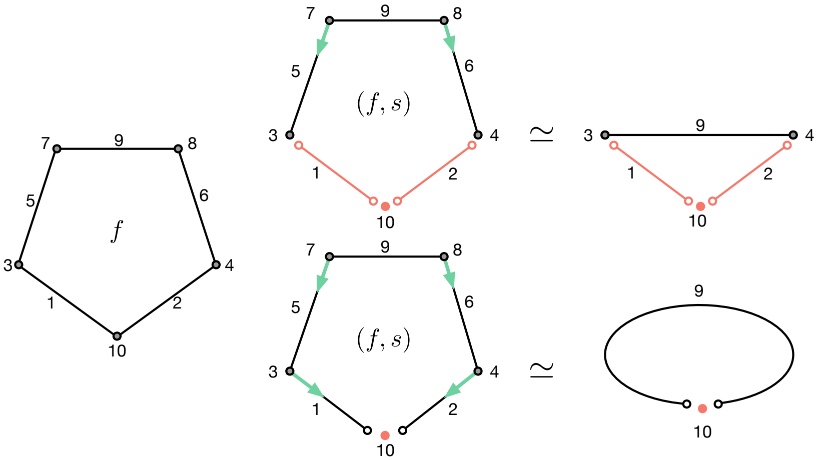
Algorithm

- (Lazy) Make every violator its own stratum; the connected components of the remaining pieces are the other strata.
- (Aggressive) Remove violators one at a time by increasing dimension, and after each removal, check to see if what remains is a discrete Morse function globally.

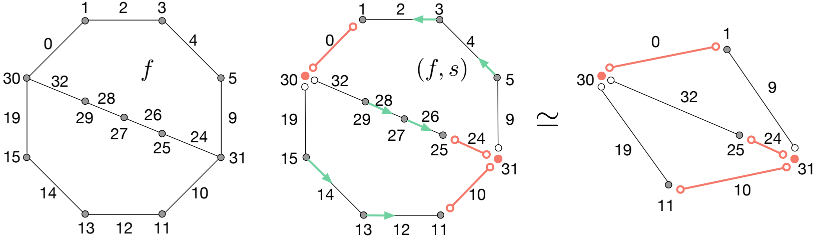
Demo: https://leong1016.github.io/dsmt/



Algorithm: Upside-down pentagon



Algorithm: Split Octagon



Sublevel set

- *Sublevel set* of an open simplicial complex K: $\forall c \in \mathbb{R}$,

$$K_c = \cup_{f(\alpha) \leq c} \alpha.$$

- K_c contains all open simplices α of K such that $f(\alpha) \leq c$.
- Suppose that K is a simplicial complex equipped with a stratification s and a discrete stratified Morse function $f : K \to \mathbb{R}$.

Two fundamental results of DSMT

A map between two stratified sets $f : \mathbb{X} \to \mathbb{Y}$ is strata-preserving if it maps each stratum in $\mathbb{X}$ bijectively onto some stratum in $\mathbb{Y}$.

Theorem (DSMT-A, Knudson and Wang (2018))

Suppose the interval $(a, b]$ contains no critical value of f. Then K_b is strata-preserving homotopy equivalent to K_a.

Theorem (DSMT-B, Knudson and Wang (2018))

Suppose $\sigma^{(p)}$ is a critical simplex with $f(\sigma) \in (a, b]$, and there are no other critical simplices with values in $(a, b]$. Then K_b is homotopy equivalent to attaching a p-cell $e^{(p)}$ along its boundary in K_a; that is,
$K_b = K_a \cup_{\dot{e}^{(p)}|_{K_a}} e^{(p)}$.

Challenges and Opportunities

Stratification Learning with Computational Topology

- Combining statistics with topological methods?
- Combining geometric with topological approaches?
- What are other sheaves that could be used in the sheaf-theoretic framework for stratification learning? We are currently considering geometric ones.
- What about sheaves beyond homology/cohomology?
- Computability?
- Unifying DSTM and sheaf-theoretic framework for stratification learning?

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