Math 412 Topological Data Analysis 08/29/2023

"Basically this room is not actually controlled by Big Trinity"

"Ben-ditch"

Paul Bendich – call him "Paul"

Research prof in math
Runs Duke
Runs Geometry Data Analytics – gov't contracts company

TDA formed at Stanford & Duke

Mixture of Algebraic Topology & Data Science

Applied Math = adapting new math, not necessarily apply old math

Course = 2/3 whiteboard, 1/3 slides

Topology doesn't make sense in the real world: ◯ is more topologically similar to —— than ◯

How we combat this is via point sampling & persistent homology

Sidenote: linalg is important is because it is the last reasonably computable math area

With TDA you can do "applied Math"

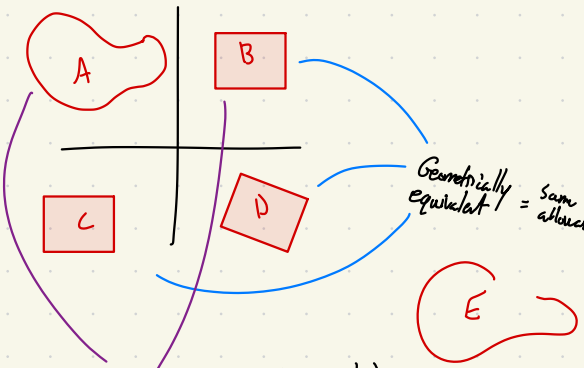
Ask prof ab slide w/ Ezra Miller after class

TDA and Deep Learning are becoming friends
↳ you can use TDA to improve loss function – persistent homology helps w/ image segmentation
↳ Also helps w/ dimension reduction

Now let's put some rigor to this.

Topology vs. Geometry

"What do we mean by things being the same?"



Geometrically equivalent = same modulo some allowable transformations

Topologically equivalent (homeomorphic)
= two shapes can be turned into each other without ripping or gluing

B, C, and D are geometrically equivalent
A, B, C, and D are homeomorphic

Proving post "is", we use constructs.
Proving "impossible," we consider all possibilities

How does undecidability work with AI?

Can we think about homeomorphism algorithmically?

Some inputs cannot return outputs

As it turns out, Markov (father of the chain guy, ~1950s) found that the homeomorphy problem is undecidable

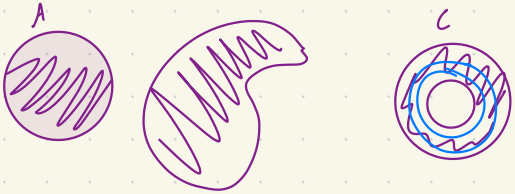
Homology (Noether, ~1920):



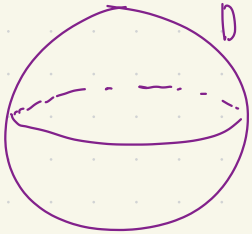
0th-degree homology of a shape
= Number of connected components in a shape
G is topologically invariant

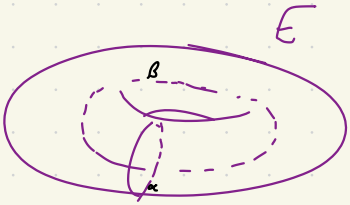
1st degree homology
= Number of linearly independent non-bounding holes/loops in the shape

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"Any time you can turn something geometric into something algebraic, you are doing deep, deep magic"





D & E are not homeomorphic but they both have the same number of voids — a notion of having an inside

2 non-bounding loops = any loop is either ≥ 0, α, or β

Persistent Homology
(2000s) (1920s)

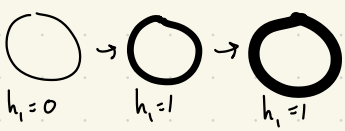




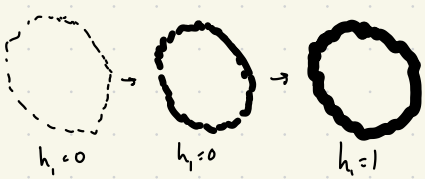


A & C homeomorphic but this doesn't really make much sense because B & C are much more similar than A & C.

With persistent homology, we look at homology dynamically over time as we make shapes fuzzy



This works well with point clouds



Recall: Connected Components



A & B have different # of connected components
$\Rightarrow$ cannot be homeomorphic

How can we turn this from hand-wavey to algorithmic and computational?

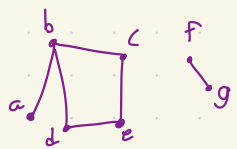
The answer: simplicial complexes/graphs

Def (simple, undirected) A graph (network) G consists of a set of vertices V and a set of edges E which are unordered pairs of elements of V

$$G = (V, E)$$

Example:

This is a drawing of a graph, not a graph itself.



$V = \{a, b, c, d, e, f, g\}$

$E = \{(a,b), (b,c), (c,e), \ldots\}$

Suppose $x, y \in V$ are two vertices in a graph G.
A **path** in G from x to y is a sequence of vertices

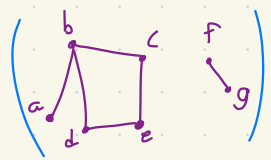
$$x = v_0, v_1, v_2, v_3, \ldots, v_n = y \quad \text{s.t} \quad \forall i, \{v_i, v_{i+1}\} \in E$$

Def G is **connected** if $\forall x, y \in V, \exists$ a path in G from x to y

Def A **connected component** of G is a subgraph H of G which

1) is connected as its own graph
2) if we add one more vertex to H, it is not connected

Def $\beta_0(G) = \#$ of connected components in a graph G
(0th degree homology)

$$\beta_0 \left(\text{} \right) = 2$$

Motivation for filtered graphs:



This point cloud could have 1, 2, or 3 "connected components"

β_0: 3, 2 more points than β_0: 1

→ we can use the persistent homology thing from above (overlapping disks)

So start with $r = 0$ and watch what happens with the connected components

The length of the list of connected components provides interesting significance

Let G be a graph. A filtration of G is a nested sequence of subgraphs of G.

$$\emptyset = G_0 \subseteq G_1 \subseteq G_2 \subseteq \dots \subseteq G_{m-1} \subseteq G_m = G$$

Linear Algebra Review

Def A vector space is a set V along with two operations: addition and scaling, satisfying:

$\forall u, w \in V,\ u+w \in V$

$u+w = w+u$

$x \in V,\ u+(w+x) = (u+w)+x$

addition group: $\exists\, 0 \in V$ s.t. $v+0 = v$.

$\forall v \in V,\ \exists\, -v \in V$ s.t. $v+(-v) = 0$

$\forall v \in V$, $\forall$ scalars r, $rv \in V$

$1v = v$

Examples:
- $(\mathbb{R}^2, +)$, $(\mathbb{R}^3, +)$, $(\mathbb{R}^n, +)$
- Span of functions

Def The Binary Scalar field $\mathbb{Z}/2\mathbb{Z}$ is the set $\{0, 1\}$ with the addition rule $1+1 = 0$.

$0+1 = 1$, $0+0 = 0$

Def Suppose V and W are 2 vector spaces. A linear transformation $T: V \to W$ is a function from V to W which satisfies:

$$\forall v, v' \in V,\quad T(v+v') = T(v)+T(v')$$
$$\forall v \in V,\ \forall \text{ scalars } r,\quad T(rv) = rT(v)$$

Category of Vector Spaces consists of objects called vector spaces and morphisms which are linear transformations

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Def Let V be a vector space. Let W be a subset of V. W is a subspace of V if:

- $\forall w, w' \in W,\ w+w' \in W$
- $\forall w \in W,\ \forall$ scalars $r,\ rw \in W$

Examples Space is $\mathbb{R}^3$, subspaces are any plane or line through the origin, the origin itself, and $\mathbb{R}^3$ itself.

Let $T: V \to V'$ be a linear transformation.

Def: the kernel of T is $\ker(T) = \{v \in V \mid T(v) = 0\}$ ⟲ Nullspace of matrix describing T

Claim: [HW] $\ker(T)$ is a subspace of V

Def: The image of T is $\mathrm{Im}(T) = \{v' \in V' \mid \exists v \in V, v' = T(v)\} = \{T(v) \mid v \in V\}$

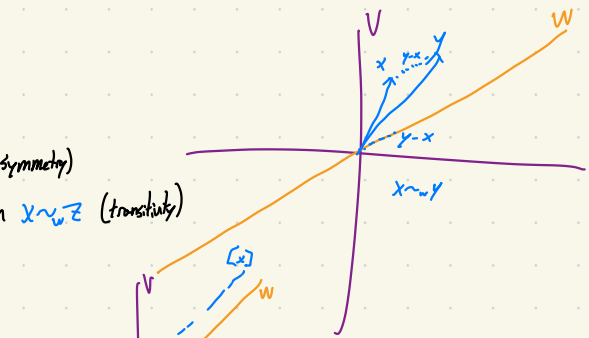
Claim: $\mathrm{Im}(T)$ is a subspace of V'.

Quotient Spaces

"It's a pretty fundamental concept but it's not that deep"

"x equals y mod W" ⇔

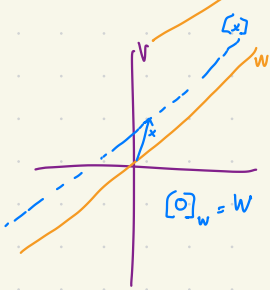
Let V be a vector space, W be a subspace. Suppose $x, y \in V$. We say $x \sim_W y$ if $x - y \in W$



Claim: [HW] (Criteria for an equivalence relation)

- $\forall x \in V$, $x \sim_W x$ (reflexivity)
- $\forall x, y \in V$, if $x \sim_W y$ then $y \sim_W x$ (symmetry)
- $\forall x, y, z \in V$, if $x \sim_W y$ and $y \sim_W z$ then $x \sim_W z$ (transitivity)

Def Suppose $x \in V$ and W is a subspace. The equivalence class of x (mod W) is $[x]_W = \{y \in V \mid y \sim_W x\}$



Claim: [HW] If $x, x' \in W$ then either $[x]_W = [x']_W$ or $[x]_W \cap [x']_W = \emptyset$

Def: Let V/W be the set of equivalence classes mod W. We give it a vector space structure as follows:

if $[x], [y] \in V/W$, define $[x] + [y] := [x+y]$

also, if r is a scalar, $r[x] = [rx]$

Claim if $x \sim_W x'$ and $y \sim_W y'$ then $x+y \sim_W x'+y'$

Proof: since $x \sim_W x'$, $\exists w \in W$ s.t. $x - x' = w$.
$y \sim_W y'$, $\exists z \in W$ s.t. $y - y' = z$.

Now we compute $(x+y) - (x'+y')$
$= (x-x') + (y-y')$
$= w + z \in W$ because W is a subspace.

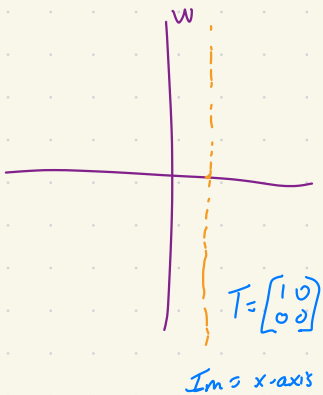
"It's an english paragraph"

So $x+y \sim_W x'+y'$ ∎

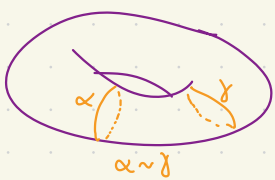
Note: we should prove the same for scaling ($rx \sim_W rx'$)

Claim [HW]: $\dim(V/W) = \dim(V) - \dim(W)$

Claim [HW]: If $T: V \to V'$ is a linear transformation
Then $V/\ker T \cong \text{Im } T$ (first isomorphism theorem)



Motivation:



Def: Let $V = \{v_1, v_2, \dots, v_n\}$ be a finite set called "Vertices."
An (abstract) simplicial complex on V is a set K of subsets of V satisfying

- every element in V is in K
- if $\tau \in K$ and $\sigma \subseteq \tau$ then $\sigma \in K$.

drawing of an abstract simplicial complex



"If I have the triangle I must have the three edges that make up the triangle

Vocab: if $\sigma \in K$, σ is a simplex ($\dim(\phi) = -1$)
The dimension of σ or $\dim(\sigma) = |\sigma| - 1$
If $\dim(\sigma) = k$, σ is a k-simplex

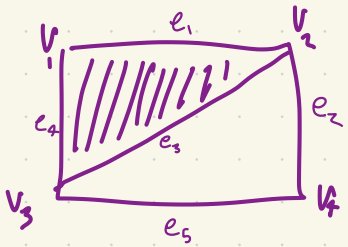
- 0-simplex = vertex
- 1-simplex = edge
- 2-simplex = triangle
- 3-simplex = tetrahedron

$\dim(K) = \max_{\sigma \in K} \dim(\sigma)$



If $\sigma \in K$ and $\tau \subseteq \sigma$ then τ is a face of σ
and σ is a coface of τ.
If τ is a face of σ and $\dim(\tau) = \dim(\sigma) - 1$, then
τ is a boundary face of σ.

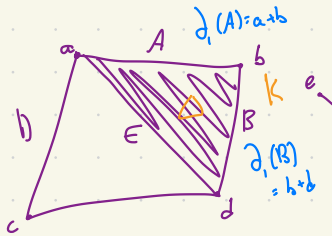
Def Let K be an abstract simplicial complex.
For each nonnegative integer i, define
$C_i(K)$ to be the vector space (over the binary field)
with basis corresponding to the i-simplicies in K.
We call $C_i(K)$ the i-dimensional chain group of K



Let K be an abstract simplicial complex.

Recall for each $i = 0, 1, 2, \ldots$,
We define $C_i(K)$ to be the binary vector space with basis the i-simplies in K

"the ith chain group of K"



$\partial_2(\Delta) = A+B+E$ → interestingly enough, $\partial_1(\partial_2(\Delta)) = 0$ Which generalizes

$$\ldots C_3(K) \xrightarrow{\partial_3} C_2(K) \xrightarrow{\partial_2} C_1(K) \xrightarrow{\partial_1} C_0(K) \longrightarrow 0$$

Define $Z_i(K) := \ker \partial_i$, the group of i-cycles of K.

Boundary maps

"Boundary 1"

Define $\partial_1 : C_1(K) \to C_0(K)$. Suppose α is an edge with vertices x and y.
Then define $\partial_1(\alpha) := x+y$.
Now, extend by linearity. e.x. $\partial_1(A+B) = \partial_1(A) + \partial_1(B)$
$= (a+b) + (b+d)$
$= a+d$

What does the kernel of ∂_1 look like?

$$\partial_1(A+B+E) = \partial_1(A) + \partial_1(B) + \partial_1(E)$$
$$= (a+b)+(b+d)+(d+a)$$
$$= 0$$

$Z_1(K)$:
0
$\alpha = A+B+E$
$\gamma = D+E+C$
$\delta = A+B+C+D = \alpha+\gamma$

had even though we have 4 loops, we only have 2 holes...

So far, we've gotten: $C_2(k) \xrightarrow{\partial_2} C_1(k)$. Let's look at $\partial_2 : C_2(k) \to C_1(k)$.

Given a triangle Δ with edges E_1, E_2, E_3
Define $\partial_2(\Delta) = E_1 + E_2 + E_3$.
Extend by linearity.

Def For each i, the image of $\partial_{i+1} : C_{i+1} \to C_i$ is denoted $B_i(k)$ and is the group of i-boundaries in k

In the above case, $B_1(k) = \{0, \alpha = A+B+E\} \subset Z_1(k)$

Now we can do fun quotient stuff with our lil subspace $B_1(k)$

Claim [HW]: $\forall i,\ \partial_i \circ \partial_{i+1} = 0$.

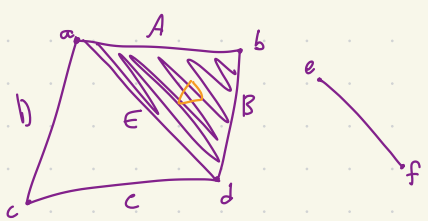
$$\cdots \to C_{i+1} \xrightarrow{\partial_{i+1}} C_i \xrightarrow{\partial_i} C_{i-1} \to \cdots$$

going down twice gives 0 every time.

As a consequence, $\forall i$ B_i is a subspace of Z_i.
(B_i: image of ∂_{i+1}; Z_i: kernel of ∂_i)

Def (the big one)
The i-th homology group of k is $H_i(k) := Z_i(k)/B_i(k) = \ker \partial_i / \operatorname{Im} \partial_{i+1}$
it's dimension is $\beta_i(k)$, the ith Betti number of k.

Recall: K



$\dim H_1 = 1$
basis: $\{[\gamma]\}$
$\beta_1(k) = 1$

In H_1, consider $[\alpha] = [0]$ (though in Z_1, $\alpha \neq 0$)
we also have $[\gamma] = [\delta]$ because $\gamma + \delta = \alpha \in B_1$
($[\gamma]$: homology class of γ)

note $\partial_0 : C_0 \to 0$ is the zero transformation

$C_1 \xrightarrow{\partial_1} C_0 \xrightarrow{\partial_0} 0$

By definition $Z_0 = C_0$ and $B_0 = \operatorname{Im} \partial_1$.

Then $H_0 = Z_0 / B_0$.

Elements of C_0 are just combinations of vertices.

$a+b = \partial_1(A)$ so $a+b \in B_0$

hence $[a] = [b] \in H_0$

$b+c = \partial_1(B+C)$ so $[a] = [b] = [c] \in H_0$

note $a+e \notin B_0$ so $[a] \neq [e] \notin H_0$

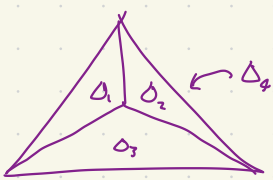
Note $\beta_0(K) = \dim H_0(K) = 2$ with one possible choice of basis being $\{[a], [e]\}$

Return to shapes!

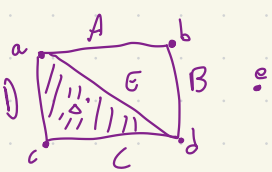


$[\alpha] = [\beta]$ but $[\delta] \neq [\alpha]$

$C_3 \xrightarrow{\partial_3} C_2 \xrightarrow{\partial_2} C_1$



$\partial_2(\Delta_1 + \Delta_2 + \Delta_3 + \Delta_4) = 0$



$H_1(K) = \ker \partial_1 / \operatorname{Im} \partial_2$

Kernel of ∂_1: $\alpha = A+B+G$

$\gamma = C+D+E$

$\delta = A+B+C+D$

0

$Z_1(K)$ has dimension 2

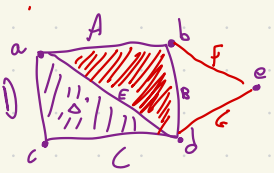
$H_1(K) = Z_1(K) / B_1(K)$

$B_1(K) = \{\partial_2(\Delta)\}$

$= \{C+D+E = \gamma\}$

Since $\alpha + \delta = \gamma \in B_1(K)$,

$[\alpha] = [\delta]$



Consider $\cdots \to C_3(K) \xrightarrow{\partial_3} C_2(K) \xrightarrow{\partial_2} C_1(K) \xrightarrow{\partial_1} C_0(K) \xrightarrow{\partial_0} 0$

In general, define $\partial_i : C_i(K) \to C_{i-1}(K)$. Let

$\sigma = \langle v_0 v_1 \dots v_i \rangle$ be a typical i-simplex in K.

We define $\partial_i(\sigma) := \sum_{j=0}^{i} (-1)^j \langle v_0 \cdots \hat{v_j} \cdots v_i \rangle$ (remove this v_j)

If $i=2$, $\partial(\langle v_0 v_1 v_2 \rangle) = \langle \hat{v_0} v_1 v_2 \rangle + \langle v_0 \hat{v_1} v_2 \rangle + \langle v_0 v_1 \hat{v_2} \rangle$ (edge b/w v_1 & v_2)

Claim: [HW] $\forall i$, $\partial_i \circ \partial_{i+1} = 0$.

That is, for any $(i+1)$-simplex τ,

$\partial_i(\partial_{i+1}(\tau)) = 0$.

$C_{i+1}(K) \xrightarrow{\partial_{i+1}} C_i(K) \xrightarrow{\partial_i} C_{i-1}(K)$

Corollary $\forall i$, $B_i(K) \subseteq Z_i(K)$

Simplicial maps:

Suppose K and L are 2 simplicial complexes.

Suppose $f : \text{Vert}(K) \to \text{Vert}(L)$ is a set map.

We say that f is a simplicial map if whenever

$\{v_0, v_1, \dots, v_i\}$ form a simplex in K,

$\{f(v_0), f(v_1), \dots, f(v_i)\}$ form a simplex in L.





$\{a,b,c,d\} \to \{x,y,z\}$

$f(a) = y$ $f(c) = x$ $f(d) = z$

$f(b) = y$

Induced Maps:

Suppose $f : K \to L$ is a simplicial map.

For each i, f induces a linear transformation via if σ is an i-simplex in K,

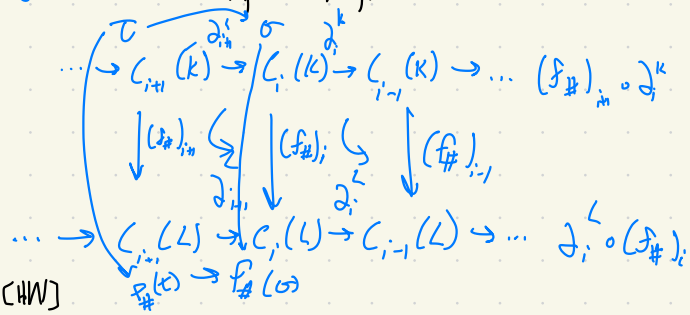
$(f_\#)_i : C_i(K) \to C_i(L)$

$$f_\#(\sigma) = \begin{cases} f(\sigma) & \text{if } \dim(f(\sigma)) = \dim(\sigma) \\ 0 & \text{if } \dim(f(\sigma)) < \dim(\sigma) \end{cases}$$

Ex from above $f_\#(\langle a b \rangle) = \langle xy \rangle$

$f(\langle abb \rangle) = \langle yyz \rangle$

Suppose $f: K \to L$ is a simplicial map.



[HW]

Lemma

$\forall i$, diagram commutes

Corollary: $f_\#(Z_i(K)) \subseteq Z_i(L)$

Corollary: $f_\#(B_i(K)) \subseteq B_i(L)$

As a consequence, a simplicial map $f: K \to L$ induces linear transformations on homology groups

$(f_*)_i : H_i(K) \to H_i(L)$ $\forall i$

$\| \qquad\qquad \|$

$Z_i(K)/B_i(K) \qquad Z_i(L)/B_i(L)$

defined by

$$f_*([\alpha]) = [f_\#(\alpha)]$$

Linear Algebra

Suppose V and V' are vector spaces and $T: V \to V'$ is a linear transformation

Suppose W is a subspace of V and W' is a subspace of V'

And suppose $T(W) \subseteq W'$

Then T induces a well-defined linear transformation $T_*: V/W \to V'/W'$ defined by $T_*([v]_W) = [T(v)]_{W'}$

Persistent Homology

How can we do topology on this point cloud?

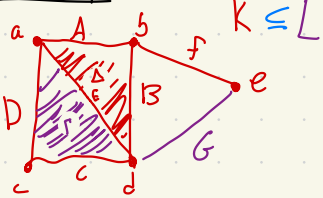


To fix this, let each point be a disk of radius ε; increase ε and watch the data disks overlap.

Literally, $\beta_0 = 69, \beta_1 = 0$

but visually, $\beta_0 = 2, \beta_1 = 2$

Warm up:



$K \subseteq L$

Consider the inclusion $i: K \to L$ of K into L $\quad \{a\} \to \{a\}$

Consider $i_*: H_0(K) \to H_0(L)$

$i_*: H_1(K) \to H_1(L)$

$[A+B+C+D] \to [A+F+G+C+D]$

$\hookrightarrow 0$

$[A+B+C+D] \neq [0] \in H_1(K)$

but

$i_*([A+B+C+D]) = [0] \in H_1(L)$

Simplest case of Persistent Homology:

Def A simplex stream is a sequence of simplicies

$$\sigma_1, \sigma_2, \sigma_3, \cdots, \sigma_N$$

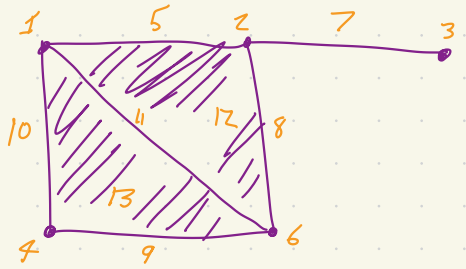
Satisfying if σ_i is a face of σ_j then $i \leq j$.

Def for each i, define $K^i = \{\sigma_1, \cdots, \sigma_i\}$

Note $\forall i$, K^i is a simplicial complex.

Also note if $i < j$, then K^i includes into K^j

Example:



Consider the sequence of inclusions:

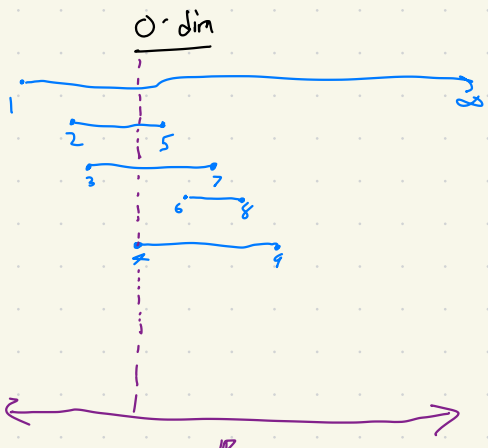
$$\phi = K^0 \subseteq K^1 \subseteq K^2 \subseteq \dots \subseteq K^{N-1} \subseteq K^N$$

This induces a sequence of linear transformations:

fix p.

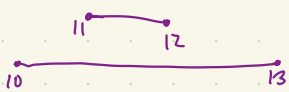
$$0 \to H_p(K^1) \to H_p(K^2) \to \dots \to H_p(K^{N-1}) \to H_p(K^N)$$

Barcode:



$\beta_0 = 4$ @ $t = 4$

1-dim



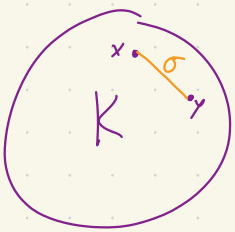
Let's look at how to compute persistent homology: The Persistence Algorithm

Suppose I have a simplicial complex K and I add to it a single simplex σ of dimension p. Call the new simplex p.

Then either β_{p-1} goes down by 1 XOR β_p goes up by 1

"σ is a negative p-simplex"

"σ is a positive p-simplex"



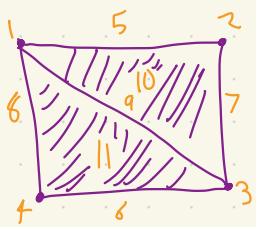
Now for the algorithm: (Edelsbrunner, Letscher, Zomorodian 1999
Zomorodian + Carlsson 2002)

Suppose K has N simplices which stream in as $\sigma_1, \sigma_2, \dots, \sigma_N$
We create an $N \times N$ binary matrix D where $D_{ij} = 1$ only if σ_i is a boundary face of σ_j

low(5) = 2, low(8) = 4, low(11) = 8

	5	6	7	8	9	10	11
1	1			1	1		
2	1		1				
3		1	1		1		
4				1	1		
5						1	
6							1
7						1	
8							1
9						1	1

not reduced



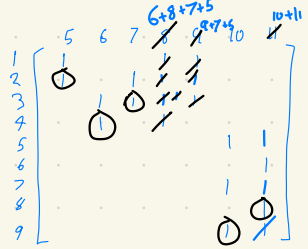
Leave off vertex columns and triangle rows.

Def Let M be any $N \times N$ binary matrix.
Define $low_M : \{1, 2, \dots, N\} \to \{0, 1, 2, \dots, N\}$ by

$$low_M(j) = \begin{cases} 0 & \text{if column } j \text{ of } M \text{ empty} \\ i & \text{if lowest (bottommost) } 1 \text{ in column } j \text{ of } M \text{ lies in row } i \end{cases}$$

Def M is reduced if the lowest 1 in each column is in a unique row. That is, if $low_M(j) = low_M(j') \neq 0$ then $j = j'$.

Algorithm: Loosely, we reduce D via left-to-right column additions



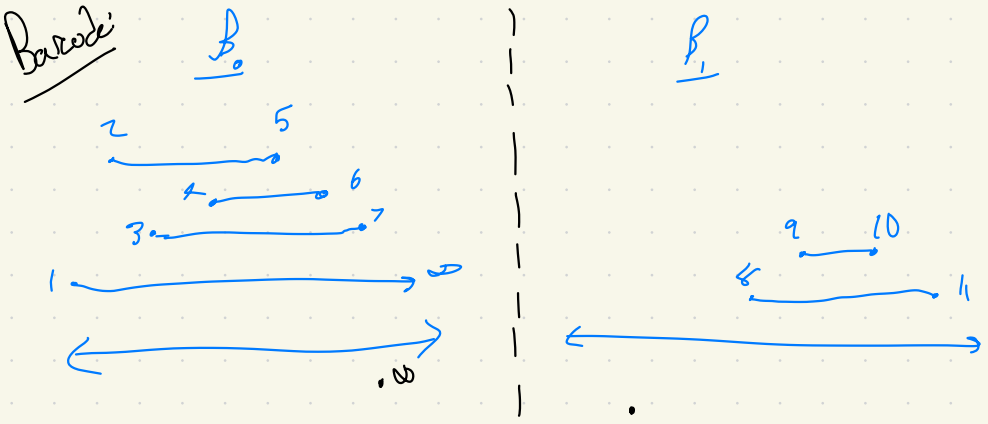
β_0: $(2, 5)$, $(4, 6)$, $(3, 7)$, $(1, \infty)$

β_1: $(9, 10)$, $(10, 11)$

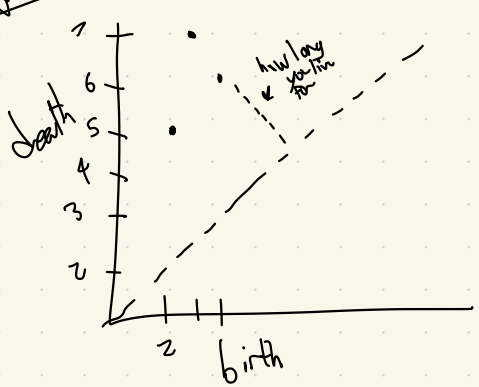
Note: this algorithm has worst case complexity $O(N^3)$

Visual representation of algorithm output

Barcode



Persistence diagram



Suppose K is a simplicial complex and suppose $f: K \to \mathbb{R}$ is a function



Def. f is a filter function if whenever σ is a face of τ, we have

$$f(\sigma) \leq f(\tau).$$

Def Let $r \in \mathbb{R}$. Define → sublevel set / threshold set

$$K_r = \{\sigma \in K \mid f(\sigma) \leq r\}$$

Claim $\forall r$ K_r is a subcomplex of K

Note: $\forall r \leq s$, $K_r \subseteq K_s$

Now suppose K has N simplicies and suppose the distinct values taken by f are $r_1 \leq r_2 \leq \cdots \leq r_m$. (note $m \leq N$)

$\forall i$, define $K_i := K_{r_i}$

Consider the complex K_i:

$$\emptyset \subseteq K_1 \subseteq K_2 \subseteq \cdots \subseteq K_m = K$$

for any p, we get:

$$0 \to H_p(K_1) \to H_p(K) \to \cdots \to H_p(K_m) = H_p(K)$$

For any $i<j$, let $f_p^{i,j}: H_p(K_i) \to H_p(K_j)$ be the map induced by including K_i into K_j

Def suppose $[\alpha] \in H_p(K_i)$. $[\alpha]$ is born at r_i if

$$[\alpha] \notin \operatorname{Im} f_p^{i-1,i}$$

Def suppose $[\alpha] \in H_p(K_i)$ is born at r_i.
we say $[\alpha]$ lies at r_j if

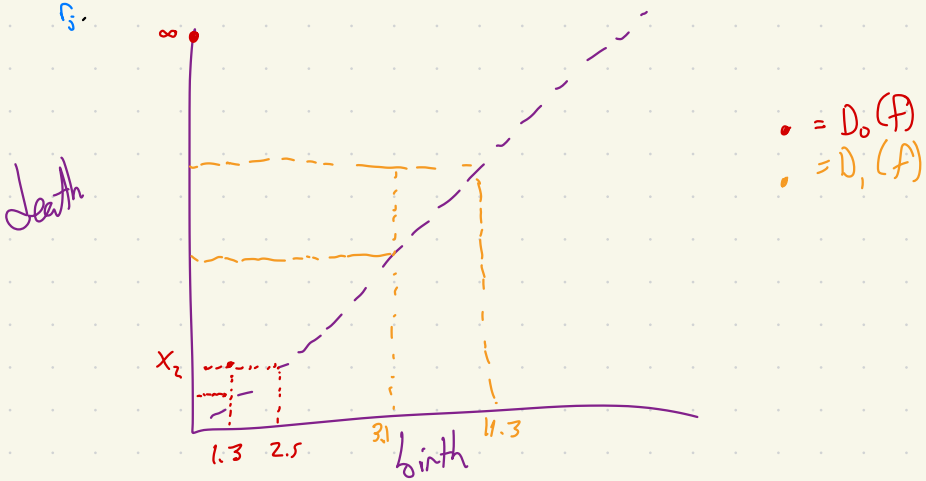
- $f_p^{i,j}[\alpha] \in \operatorname{Im} f_p^{i-1,j}$
- $f_p^{i,j-1}[\alpha] \notin \operatorname{Im} f_p^{i-1,j-1}$

(if $i=j-1$ this is vacuously true.)

$$H_p(K_{i-1}) \to H_p(K_i) \to \cdots \to H_p(K_{j-1}) \to H_p(K_j)$$

$$[\alpha_i] \longmapsto f_p^{i,j}([\alpha_i])$$

Def: The p-dimensional persistence diagram of f, $\operatorname{Dgm}_p(f)$ $[D_p(f)]$ contains a dot (r_i, r_j) for each p-dimensional homology class born at r_i and dead at r_j.



Def Let A be any set. A metric/distance ρ on A is a function $\rho: A \times A \to \mathbb{R}$ satisfying:

- $\forall a, b \in A,\ \rho(a,b) \geq 0$ (non-negativity)
- $\forall a, b \in A,\ \rho(a,b) = 0 \Leftrightarrow a = b$ (discernability)
- $\forall a, b \in A\ \ \rho(a,b) = \rho(b,a)$ (symmetry)
- $\forall a, b, c \in A,\ \rho(a,c) \leq \rho(a,b) + \rho(b,c)$ (triangle inequality)

(A, ρ) is a metric space

Examples: consider $A = \mathbb{R}^n$

1) $\rho(\vec{x}, \vec{y}) = \left[\sum_{i=1}^{n} (x_i - y_i)^2\right]^{1/2}$ (l_2, Euclidean)

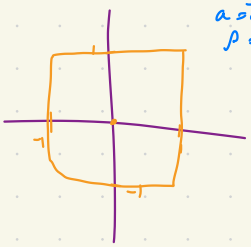
2) $\rho(\vec{x},\vec{y}) = \sum_{i=1}^{n} |x_i - y_i|$ (ℓ_1, "taxicab metric")

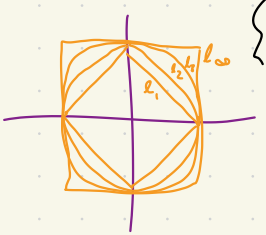
3) $\rho(\vec{x},\vec{y}) = \left[\sum_{i=1}^{n} |x_i - y_i|^p\right]^{1/p}$ for any $p > 0$ (ℓ_p)

4) $\rho(\vec{x},\vec{y}) = \max_i |x_i - y_i|$ (ℓ_∞)

5) $\rho(\vec{x},\vec{y}) = \#i$ s.t. $x_i \neq y_i$ (ℓ_0)

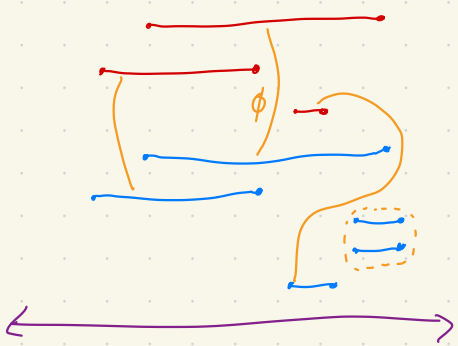
Def Let (A,ρ) be a metric space. Fix $a \in A$ and a radius $R > 0$.
The closed ball of radius R centered at a is
$$B_\rho(a,R) := \{x \in A \mid \rho(a,x) \leq R\}$$

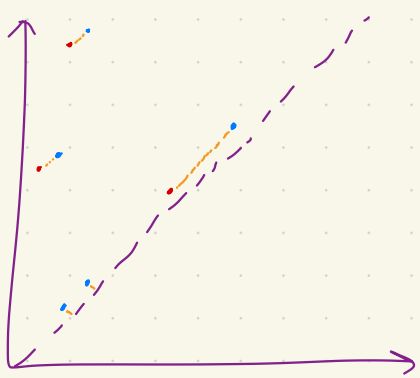




{Curse / blessing} of dimensionality
↳ point distribution of ℓ_p in $\mathbb{R}^n$

Let's look at metrics applied to position diagrams!





Suppose $\mathcal{D}$ and $\mathcal{D}'$ are two different diagrams. How far apart are they?

Let D, D' be two barcodes. A matching between D and D' is a bijection ϕ between a subset E of D and $\phi(E)$

Given ϕ, fixing $p > 0$, the cost of ϕ is $[C_p(\phi)]^p = \sum_{\text{bars not in } E} [\text{length(bars)}]^p + \sum_{\text{bars not in } \phi(E)} [\text{length(bars)}]^p + \sum_{(a,b)\in\phi} |a-\phi(a)|^p + |b-\phi(b)|^p$

Finally, the pth Wasserstein distance between D and D' is

$$W_p(D,D') := \inf_{\substack{\text{matchings} \\ \phi: D \to D'}} C_p(\phi)$$

How do we choose p? Well... basically it's arbitrary and up to us.

Claim [HW]: for any $p > 0$, W_p is a metric on the space of persistence diagrams

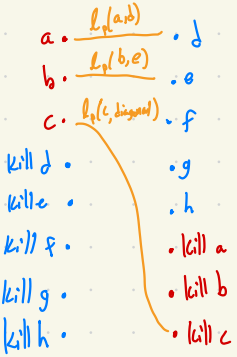
Hint: composing bijections gives you a bijection... but it may not be the best one.

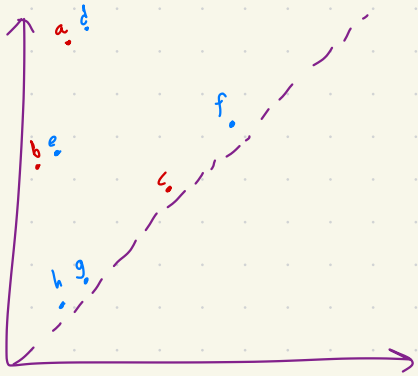
$$W_p(D,D') = \inf_{\phi: D \to D'} C_p(\phi)$$

Turns out, this is reasonably efficiently computable

Create bipartite graph with edge weights the cost of moving a point to where we matched it

$\exists$ some algorithm to find best bijection in $O(n^3)$





Digression: doing statistics in a metric space.

Suppose (A, ρ) is a metric space.
Suppose we have a finite set $X = \{x_1, \ldots, x_n\} \subseteq A$.
What's the mean of X?

Let's define $\widetilde{F}_X : A \to \mathbb{R}$ via $\widetilde{F}_X(a) = \sum_{i=1}^{n} [\rho(x_i, a)]^2$

↳ The fréchet function of X.

Def: The fréchet mean of X is

$$\mu_X := \operatorname{argmin}_{a \in A} \widetilde{F}_X(a).$$

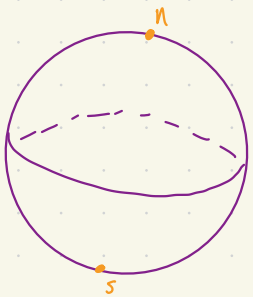
↳ argument which achieves minimum

$\min_{x \in [0, 2\pi]} (\sin(x)) = -1$

$\operatorname{argmin}_{x \in [0, 2\pi]} (\sin(x)) = 3\pi/2$

$\sin(3\pi/2) = -1$

Claim: Consider the metric space $(\mathbb{R}, d_2)$. The fréchet mean of a finite set is the mean you know (and love).

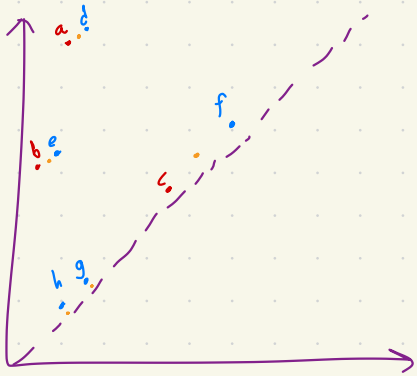


$X = \{n, s\}$

$\mu_X = \{\text{equator?}$ yikes...

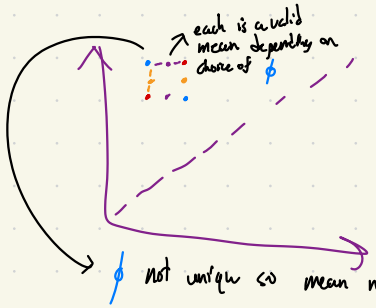
$\mathbb{R}^2 - \{0\}$, $X = \{-5, 5\}$

μ_X DNE



μ_X is a diagram!

- is that μ_X, as it turns out



$\Rightarrow$ Space of persistence diagrams basically has infinite curvature :)

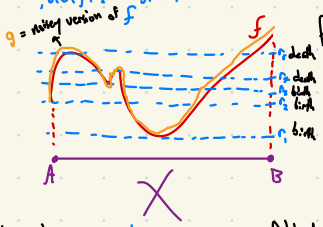
Stability of persistent homology

Prototypical example: changing a set of numbers a little bit changes the mean only a little bit

$(4, 4.5, 5.5, 6) \mapsto 5$

$(4.01, 4.501, 5.501, 6.01) \mapsto \sim 5.01$

Suppose X some topological space.
Suppose $f: X \to \mathbb{R}$ a function.

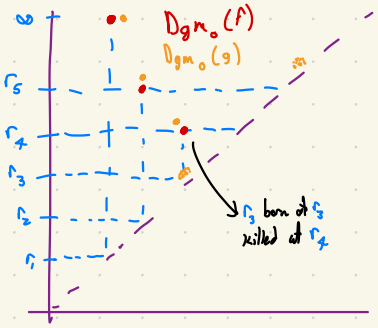


For each threshold value $r \in \mathbb{R}$, consider $X_r := f^{-1}((-\infty, r]) = \{x \in X \mid f(x) \le r\}$

note if $r \le s$, then $X_r \subseteq X_s$.

$H_p(X_r) \to H_p(X_s)$.

Let's look at the 0-dimensional homology of X under the filtration induced by X_r.

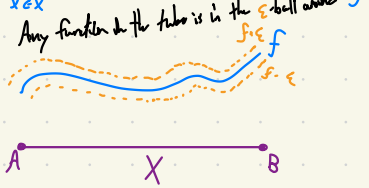


Suppose f and g are two real-valued function on X.

The ℓ_∞-distance between f and g is

$\ell_\infty(f,g) := \sup_{x \in X} |f(x) - g(x)|$

$\|f - g\|_\infty$



Theorem (Stability theorem): [Chazal, Edelsbrunner, Cohen-Steiner 2007]

If f and g are [reasonable] real-valued functions on X

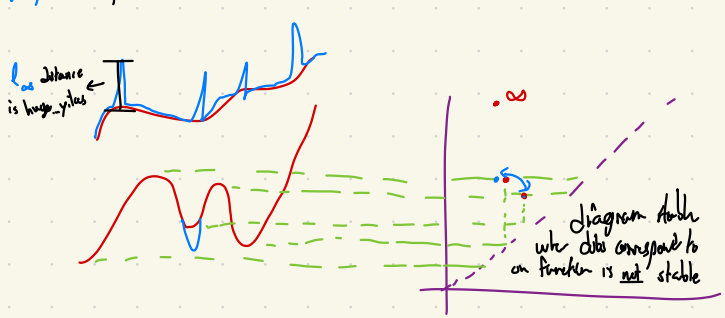
Then $\forall p$, $W_\infty(Dgm_p(f), Dgm_p(g)) \le \ell_\infty(f,g)$.

(W_∞: bottleneck distance; $\inf(\sup(\text{whatever}))$: "min-max")

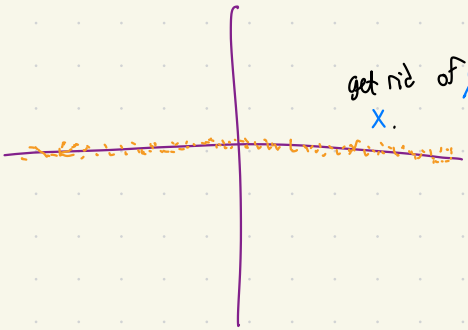
Nice thing: small change in R$\to$R^k leads to small change in R$\to$R^k

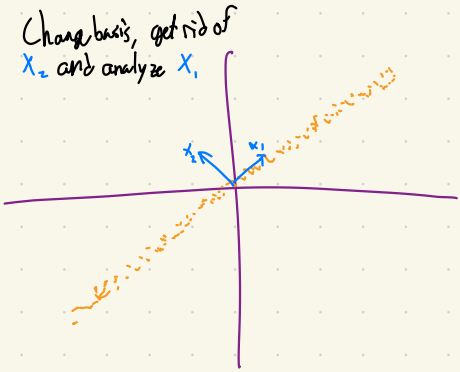
$f \mapsto Dgm_p(f)$ respects the metric structure

Not so nice things: outliers

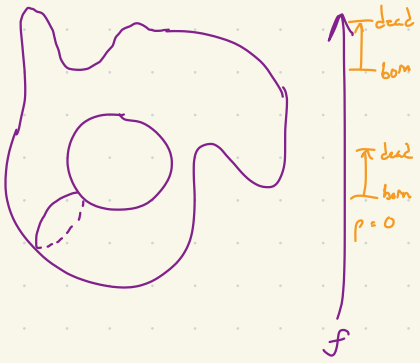


Principle Components Analysis (PCA)





Recall if X is a topological space and $f: X \to \mathbb{R}$ is a function. We have $\mathrm{Dgm}_p(f)$ for each homological dimension p.



Question: how do we compute this?

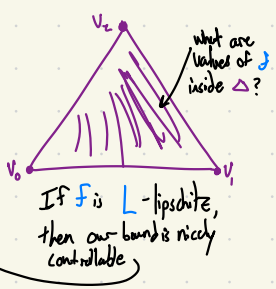
Procedure [cone-star filtration]:

- Triangulate X with a simplicial complex K.
- To each vertex of K, just associate it's f-value. $\hat{f}(v) = f(v)$.
- To each higher order simplex σ in K, set $\hat{f}(\sigma) = \max_{v \in \sigma} f(v)$.
- Now consider the filtration of K via subsets of $\hat{f}$.
- Compute, for each p, $\mathrm{Dgm}_p(\hat{f})$.

[UW]
Claim: $\hat{f}$ is a filter function on K.

Questions:

1) What is relation between $\mathrm{Dgm}_p(\hat{f})$ and $\mathrm{Dgm}_p(f)$?
2) How efficient is this algorithm?



We know (from stability theorem) that $W_\infty(\mathrm{Dgm}_p(f), \mathrm{Dgm}_p(\hat{f})) \leq \|f - \hat{f}\|_\infty$

To bound RHS, assume f is L-Lipschitz, assume you have many many simplices in K and that they are super small.

"many many cubed is very many many"

Point Cloud Triangulations:



Let $X = \{x_1, x_2, \dots, x_N\} \subseteq \mathbb{R}^D$ (or really any metric space).
be a "point cloud."

Define $d_X : \mathbb{R}^D \to \mathbb{R}$ via $d_X(y) := \min_{x \in X} \|y - x\|$.

Abuse (of notation): for any ε, let $X_\varepsilon := \{y \in \mathbb{R}^D \mid d_X(y) \leq \varepsilon\}$.
Note for any ε, $X_\varepsilon = \bigcup_{x \in X} B_\varepsilon(x)$ (closed ε-balls).
And for $\varepsilon < \varepsilon'$, $X_\varepsilon \subseteq X_{\varepsilon'}$.
for every p, we get $Dgm_p(X) := Dgm_p(d_X)$

Question: how do we compute this?

Čech Complex: how can we feed the persistence monster

for any $\varepsilon > 0$, define $\check{C}_\varepsilon(X)$ to be a simplicial complex with X as its vertices and where $\sigma \in \check{C}_\varepsilon(X)$ if

$$\bigcap_{x \in \sigma} B_\varepsilon(x) \neq \emptyset$$



Note:

- for any ε, $\check{C}_\varepsilon(X)$ is indeed a simplicial complex because if τ is a face of σ, then

$$\bigcap_{x \in \tau} B_\varepsilon(x) \supseteq \bigcap_{x \in \sigma} B_\varepsilon(x).$$

- for any $\varepsilon < \varepsilon'$, $\check{C}_\varepsilon(X)$ is a subcomplex of $\check{C}_{\varepsilon'}(X)$

Thus we can compute persistent diagrams $Dgm_p(\check{C}(X))$ associated with this filtration.

Nice fact: $Dgm_p(\check{C}(X)) = Dgm_p(X)$ $\forall p$. Magic ingredient: Nerve Lemma.

Not fun facts:

- $\check{C}(X)$ has a lot of simplices!
  In fact, it has 2^N simplices.

  But if we want $Dgm_p(X)$, or we can just bound ϵ.
  we only need consider $(p+1)$-skeleton
  of $\check{C}(X)$. this is size $\binom{N}{p+1} = O(N^{p+1})$

- figuring out when a simplex appears in $\check{C}(X)$... is not that fun. $O(N^{\lfloor D/2 \rfloor})$ ← complexity depends on ambient space is bad.

Housekeeping: no class thursday!

Recall: Suppose $X = \{X_1, \dots, X_N\} \subseteq \mathbb{R}^D$ is a point cloud
We are interested in $Dgm_p(X)$ associated to the filtration
of $\mathbb{R}^D$ given by the growing balls around points in X.

Last time, we defined the Čech complex $\check{C}(X)$.
Where for any $\alpha \in \mathbb{R}$, $\sigma \in \check{C}_\alpha(X)$ if

$$\bigcap_{x \in \sigma} B_\alpha(x) \neq \emptyset.$$

Vietoris-Rips Complex: again given $X = \{X_1, \dots, X_N\} \subseteq \mathbb{R}^D$ (or any metric space)
for any $\alpha \in \mathbb{R}$, define $R_\alpha(X)$ to be the simplicial complex with vertex X
and $\sigma \in R_\alpha(X)$ iff $\forall x_i, x_j \in \sigma$, $B_\alpha(x_i) \cap B_\alpha(x_j) \neq \emptyset$.

Problem: $R_\alpha(X)$ doesn't give same Betti #'s as X_α

However: $\forall \alpha$, $\check{C}_\alpha(X) \subseteq R_\alpha(X) \subseteq \check{C}_{2\alpha}(X)$ [HW]
Because $\forall i,j$ $\bigcap_{x \in \sigma} B_\alpha(x) \subseteq B_\alpha(x_i) \cap B_\alpha(x_j)$

In fact in $\mathbb{R}$, $R_\alpha(X) \subseteq C_{\alpha\sqrt{\frac{2D}{D+1}}}(X)$ [Ghrist, deSilva, Zeb]

Rips alternate definition: $R_\alpha(X)$ is the maximal simplicial complex which shares the same 1-skeleton of $\check{C}_\alpha(X)$.

2 negatives, 2 positives:
- Rips theoretically wrong
- Rips has a ton of simplices

But
- Easier to check stuff (can just check edges)

interleaving → gives nice stuff about birth and death

We care about the homology of top row

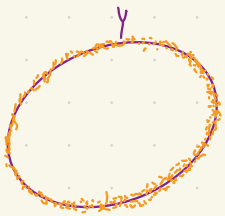
but we can much more easily compute bottom row

$$\check{C}_\alpha(X) \subseteq R_\alpha(X) \subseteq \check{C}_{2\alpha}(X) \subseteq R_{2\alpha}(X) \subseteq \check{C}_{4\alpha}(X) \subseteq \cdots$$

$$R_{\alpha/2}(X)$$

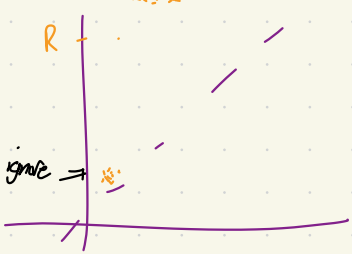
Homology inference:

Suppose Y is a topological space embedded in $\mathbb{R}^D$.
Suppose $X = \{X_1, \ldots, X_N\}$ is a point sampled from/near Y.



Problem: can we use X to infer homological things about Y?

Def: Suppose Y is a topological space embedded in $\mathbb{R}^D$. Consider $d_Y : \mathbb{R}^D \to \mathbb{R}$ defined by $d_Y(z) := \inf_{y \in Y} \|z - y\|$.
For any $\alpha \in \mathbb{R}$, define $Y_\alpha := \{z \in \mathbb{R}^D \mid d_Y(z) \leq \alpha\}$



Def: If X and Y are 2 topological spaces embedded in $\mathbb{R}^D$.
The Hausdorff distance between X and Y is

$$d_H(Y, X) := \inf\{\varepsilon \mid Y \subseteq X_\varepsilon \text{ and } X \subseteq Y_\varepsilon\}$$

"is X a good point sample of Y?" — controls density & bounds outliers



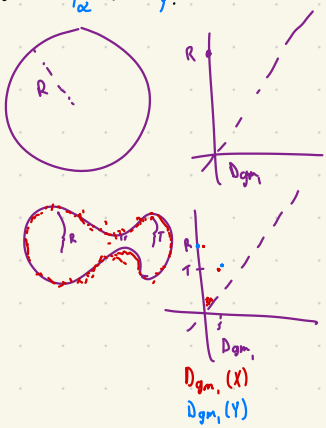
$Y \subseteq X_\varepsilon$
$X \not\subseteq Y_\varepsilon$

Problem:



If Y is a space and X is a point-cloud, and $d_H(X, Y) \leq \varepsilon$
Then we say "X is an ε-sample of Y"

Note for any space Y embedded in $\mathbb{R}^D$ we can filter $\mathbb{R}^D$ via sublevel sets Y_α of d_Y.
So for any p, we get persistence diagram $Dgm_p(Y) := Dgm_p(d_Y)$.



Q: How do I read $\beta_p(Y)$ from $Dgm_p(Y)$?
A: # of dots on y-axis.

Claim: [HW] If Y and X are shapes embedded in $\mathbb{R}^D$, then
$$d_H(Y,X) = \|d_Y - d_X\| = \sup_{x \in \mathbb{R}^D} |d_Y(x) - d_X(x)|$$
Therefore for all p, $W_\infty(Dgm_p(Y), Dgm_p(X)) \leq d_H(Y,X)$ (by stability theorem).

(recall)
Problem: Given a topological space Y and a point cloud X sampled from/near Y, can we infer homology of Y from X

Two major players: first, "how good is the sample?"

Recall: If X and Y are 2 topological spaces embedded in $\mathbb{R}^D$.
The Hausdorff distance between X and Y is
$$d_H(Y,X) := \inf\{\varepsilon \mid Y \subseteq X_\varepsilon \text{ and } X \subseteq Y_\varepsilon\}$$
"is X a good point sample of Y?" — controls density & bounds outliers

HW: $d_H(X,Y) = \|d_X - d_Y\|_\infty$

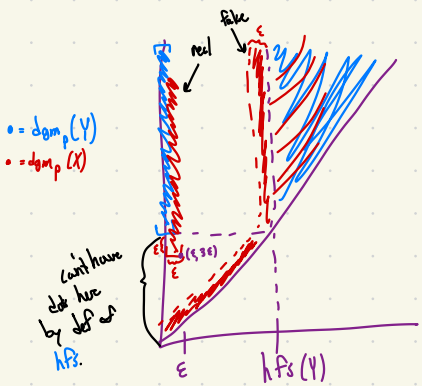
Now by stability $W_\infty(Dgm_p(Y), Dgm_p(X)) \leq d_H(Y,X)$

Second major player: resolution
Let's define the homological feature size of Y, denoted $hfs(Y)$ to be the first nonzero birth and/or death value in the filtration defined by d_Y.

Theorem: (Homology inference theorem) [Cohen-Steiner, Edelsbrunner, Harer, 2007]

Suppose X is a point sample from near Y with $d_H(X,Y) = \varepsilon < \frac{hfs(Y)}{4}$. Then for all p, $\beta_p(Y)$ is equal to the # of dots born before ε and dead after 3ε.

Proof: HW



Today (10/26): Project

Dates:

Project Choice – Due via email in 2 weeks (11/9)
↳ email in advance to discuss before finalizing
↳ no annotated bibliography

Presentation → final exam block: 20min
Paper → due by final exam block

Paper itself: 2 options

① research
- doesn't have to be publishable
- graded on effort and creativity

② expository lecture
- don't expect this to be easy!
- held to high-ish standards :)

Details on option 1
- find a dataset → make sure you're allowed to use this data!
- do some tda
- find some patterns

Page limit: 6 pages (using template)

Not graded on correct hypothesis!

Option 2
- Choose something we've said Paul didn't cover
- Teach a good class in 20 minutes.

Python package: giotto-tda (calls ripser)

Relative Homology (on the simplicial homology)

Suppose K is a simplicial complex and L is a subcomplex



for each $p \in \{0,1,\dots\}$ define the pth relative chain group to be $C_p(K,L) := C_p(K)/C_p(L)$

Observe that if γ is a p-chain in $C_p(L)$, then $\partial_p(\gamma)$ is a $(p-1)$-chain in $C_{p-1}(L)$.

$$\cdots \to C_{p+1}(K) \xrightarrow{\partial_{p+1}} C_p(K) \xrightarrow{\partial_p} C_{p-1}(K) \to \cdots$$
$$\cup \qquad\qquad \cup \qquad\qquad \cup$$
$$C_{p+1}(L) \quad C_p(L) \to C_{p-1}(L)$$



Consider $\gamma = A+B$
Then $\gamma = \Delta \in C_2(K,L)$

Thus we can define a map on quotient spaces $\partial_p : C_p(K,L) \to C_{p-1}(K,L)$
The group of relative p-cycles is $Z_p(K,L)$ is the kernel of this map
The group of relative p-boundaries is $B_p(K,L)$ is the image of $\partial_{p+1} : C_{p+1}(K,L) \to C_p(K,L)$.
Finally, $H_p(K,L) := Z_p(K,L)/B_p(K,L)$ is the relative pth homology group of K mod L.

$\beta_1(K,L) = 1$
$\beta_0(K,L) = 0$ $\quad C_1(K,L) \xrightarrow{\partial_1} C_0(K,L) \xrightarrow{\partial_0} 0$

# of connected components in K not "hit" by L



K/L = pinched torus

$\beta_0(K) = 1$ — $\beta_0(K,L) = 0$
$\beta_1(K) = 1$ — $\beta_1(K,L) = 1$
$\beta_2(K) = 0$ — $\beta_2(K,L) = 1$

result of manifold mashed out by boundary



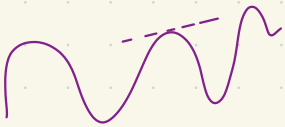
$\beta_0(K,L) = 0$
$\beta_1(K,L) = 0$
$\beta_2(K,L) = 1$

Local Homology



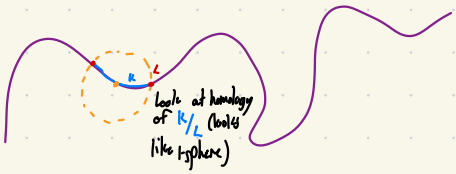


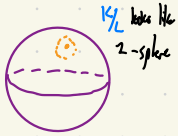
Technically dimension 3 but locally dimension 2.



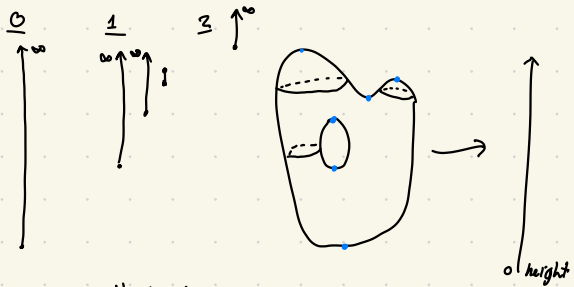
technically dim 2, locally dim 1

local dimension = # of parameters needed (ish)



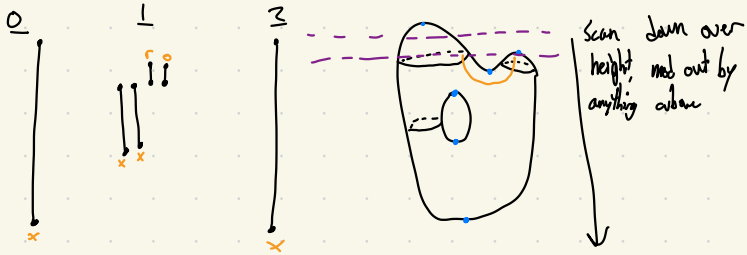


Extended Persistence



Ascend via sublevel sets

Descend via modding out by superlevel sets



Poincaré Duality

Manifold of dim d: $\beta_i = \beta_{d-i}$

Elevation function

Suppose X is a smooth, compact, orientable, d-dimensional manifold embedded in $\mathbb{R}^{d+1}$

Given a unit vector $u \in S^d$ (unit sphere in $d+1$ dimensions), consider the filtration function f_u which measures height in direction u. Formally, $f_u : X \to \mathbb{R}$ via $f_u(x) = x \cdot u$.

Note that every point $x \in X$ is a critical point for precisely 2 functions f_u, where u is either the inward or outward pointing normal vector to X at x.

Fact: X is paired with the same point $p(x)$ for both these directions!

We can define a function on X, called elevation $E : X \to \mathbb{R}$, where

$$E(x) = \left| f_u(x) - f_u(p(x)) \right|$$

where u is either the inward or outward facing normal vector to X at x.

Persistent Homology Transform (PHT; Turner, Mukherjee, Boyer)

If X is d-dimensional manifold inside $\mathbb{R}^{d+1}$

Consider $PHT_X : S^d \to \{\text{all persistence diagrams}\}$

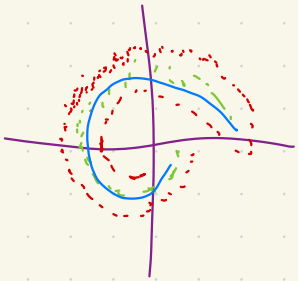
$u \mapsto$ Extended PD of u

Theorem: if $PHT_X = PHT_Y$, then $X = Y$. ...but this is still uncountable...

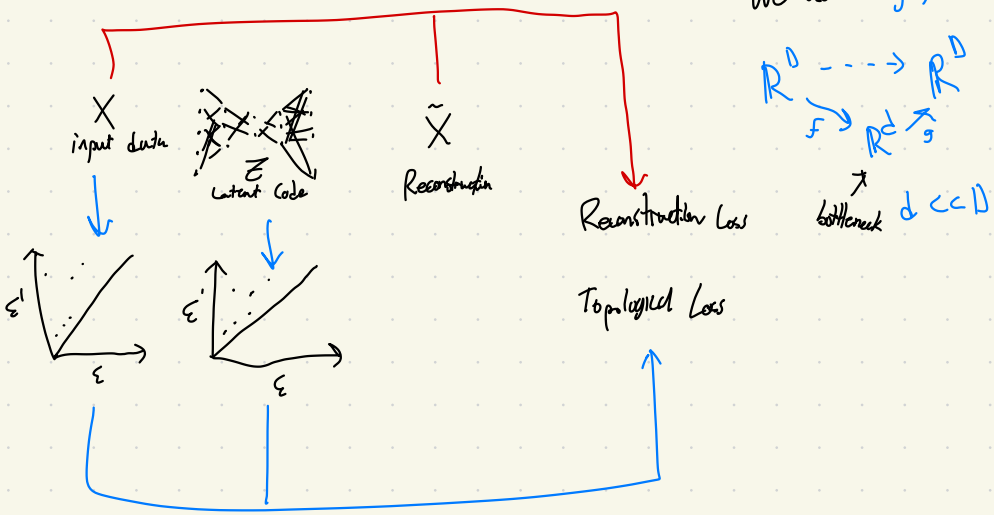
"How many directions determine a shape?" (Turner, Mukherjee, Curry)

IDA for deep learning

Motivation: Draw me a line that separates these two point sets.



Make topological loss function – restrict connected components instead of smoothness



we want $g \circ f \approx id$

$\mathbb{R}^D \dashrightarrow \mathbb{R}^D$, $f: \mathbb{R}^D \to \mathbb{R}^d$, $g: \mathbb{R}^d \to \mathbb{R}^D$

Turns out we can compute gradients for topological functions based on persistence homology