Introduction to Computational Topology

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Guest Lecture

CMSC 754 – Spring 2020
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Early Topological Insights

Seven Bridges of Königsberg: find a path that crosses each bridge exactly once

The Origins of Graph Theory

- Euler observed that the subpaths within each land mass are irrelevant.
- Use an abstract model of land masses and their connectivity – a graph!
- A path enters a node through an edge, and exits through another edge.
- The solution exists if there are exactly 0 or 2 nodes of odd degree.
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More Graph Theory

Complete graph $K_5$, complete bipartite graph $K_{3,3}$, and the Petersen graph

Forbidden Graph Characterizations

- A minor $H$ of a graph $G$ is the result of a sequence of operations:
  - Contraction (merge two adjacent vertices), edge and vertex deletion.
- A graph if planar iff it does not have any $K_5$ or $K_{3,3}$ minors.
- Hadwiger conjecture: a graph is $t$-colorable iff it does not have any $K_t$ minors.

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Surfaces

Topological Invariants

Instead of edge deletion and contraction for graphs, we study surfaces under continuous deformations that do not tear or pinch the surface.

- The genus corresponds to the number of holes or handles.
- Joke: a topologist cannot distinguish his coffee mug from his doughnut!

- Topology as rubber-sheet geometry

Figures from Wikipedia [6, 7, 8, 9]
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Figures from Wikipedia [6, 7, 8, 9]
How do you compute the genus *without looking*?
Convex Polytopes

Euler’s Polyhedron Formula

- **Alternating sum** of the number of vertices (V), edges (E), and facets (F)
  \[ \chi = V - E + F \]

- As spheres can be continuously deformed into convex polytopes, they also have an Euler characteristic of 2.
- Unlike the genus, this is easily computed by simple counting or algebra.

Figures from Wikipedia [10, 11, 12, 13, 14]
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What about non-convex surfaces?
Wireframes

Rendering all triangles

Wireframe, edges only
Simplicial Complexes

A 3-simplex
Four 2-simplices
Six 1-simplices
Four 0-simplices

**Definitions**

- A **p-simplex** is the convex hull of \((p + 1)\) affinely-independent points.
  - We write this as \(\sigma = [v_0, \ldots, v_p] = \text{conv}\{v_0, \ldots, v_p\}\) and say \(\dim \sigma = p\).
- A **simplicial complex** \(K\) is a set of simplices closed under intersection, and its dimension \(\dim K\) is the maximum dimension of its simplices.
  - If \(\sigma_1, \sigma_2 \in K\), then \(\sigma_1 \cap \sigma_2 \in K\). The \((-1)\)-simplex \(\emptyset\) is always in \(K\).
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- A face $\tau$ is a $k$-simplex connecting $(k + 1)$ of the vertices of $\sigma$. We write this as $\tau \preceq \sigma$, and say that $\sigma$ is a coface of $\tau$.
- A (co)face $\tau$ of a simplex $\sigma$ is proper if $\dim \tau \neq \dim \sigma$.
- The boundary $\partial \sigma$ is the collection of proper faces of $\sigma$.
- The interior of $\sigma$ is defined as $|\sigma| = \sigma - \partial \sigma$.
- The underlying space of a complex $K$ is defined as $|K| = \bigcup_{\sigma \in K} |\sigma|$.
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How to represent a *mapping* between two surfaces?
Continuous Deformations

A continuous deformation of a cow model into a ball

Figure from Wikipedia [15]
Continuous Maps

Definition of Continuity

- Small changes in the input yield small changes in the output.
- Calculus formalizes this notion using the \((\varepsilon, \delta)\)-definition of the limit.
- For general topologies, we use neighborhoods instead of \((\varepsilon, \delta)\) intervals.

Figures from Wikipedia [16, 17]
Continuous Maps

Continuity at $x = 2$ by $(\varepsilon, \delta)$

Continuity at $x \in X$ using neighborhoods

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Definition

Two topological spaces $X$ and $Y$ are said to be homeomorphic whenever there exists a continuous map $f : X \to Y$ with a continuous inverse $f^{-1} : Y \to X$. Such a function $f$ is called a homeomorphism.

Figure from Wikipedia [15]
But, we will be using the triangulations rather than the surfaces ...
A triangulation of a topological space $X$ is a simplicial complex $\hat{X}$ such that $X$ and $|\hat{X}|$ are homeomorphic.

A topological space is triangulable if it admits a triangulation.
Triangulations

Definition

- A \textit{triangulation} of a topological space $X$ is a simplicial complex $\hat{X}$ such that $X$ and $|\hat{X}|$ are homeomorphic.
- A topological space is \textit{triangulable} if it admits a triangulation.
Continuous Maps between Simplicial Complexes

- Fix a simplicial complex $K$.
- The *star* of $\sigma$ is the collection its cofaces:
  \[ \text{St}_K(\sigma) = \{ \tau \in K \mid \sigma \leq \tau \} \]

- The *star neighborhood* of $\sigma$ is the union of the interior of its cofaces:
  \[ N_K(\sigma) = \bigcup_{\tau \in \text{St}_K(\sigma)} |\tau| \]
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Simplicial Neighborhoods

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The Star Condition

- Fix two simplicial complexes $\hat{X}$ and $\hat{Y}$ and a map $\hat{f} : |\hat{X}| \to |\hat{Y}|$.
- We say that $\hat{f}$ satisfies the star condition if for all vertices $v \in \hat{X}$
  $$\hat{f}(N_{\hat{X}}(v)) \subseteq N_{\hat{Y}}(u)$$
  for some vertex $u = \phi(v) \in \hat{Y}$.
- The map $\phi : \operatorname{Vert} \hat{X} \to \operatorname{Vert} \hat{Y}$ extends to a simplicial map that maps
every simplex $\sigma \in \hat{X}$ to some simplex $\tau \in \hat{Y}$.
- The simplicial map induces a simplicial approximation: a piecewise-linear
map $\hat{f}_\Delta : \hat{X} \to \hat{Y}$ that approximates the original function $f$. 
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What if $\hat{f} : |\hat{X}| \rightarrow |\hat{Y}|$ fails the star condition?
Simplicial Approximation Theorem

Barycentric Subdivisions

- If there exists a vertex \( v \in \hat{X} \) such that \( \hat{f}(N_{\hat{X}}(v)) \) is not contained in \( N_{\hat{Y}}(u) \) for any vertex \( u \in \hat{Y} \), then \( N_{\hat{X}}(v) \) is too large!
- Solution: refine \( \hat{X} \) without changing \( \hat{f} : \hat{X} \to \hat{Y} \).
- The barycenter of \( \sigma = [v_0, \ldots, v_p] \) is defined as \( \frac{1}{p+1} \sum_{i=0}^{p} v_i \).
- Repeated subdivisions eventually achieve the star condition.
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Simplicial Counting

- Recall the alternating sum used to compute the Euler characteristic $\chi$.
- We would like to derive a similar computation on a simplicial complex $K$.
- But, a single simplex can be shared among multiple cofaces.
- How do we keep track of the correct count?
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Recall the alternating sum used to compute the Euler characteristic $\chi$. We would like to derive a similar computation on a simplicial complex $K$. But, a single simplex can be shared among multiple cofaces. How do we keep track of the correct count? Algebra!
Chains

Counting Modulo 2

- Define a $p$-chain as a subset of the $p$-simplices in the complex $K$.
- We write a $p$-chain as a formal sum $c = \sum_i a_i \sigma_i$, where $\sigma_i$ ranges over the $p$-simplices and $a_i$ is a coefficient.
- We will work with coefficients in $\mathbb{F}_2 = \{0, 1\}$ with addition modulo 2.
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Counting Modulo 2

- Two $p$-chains can be added to obtain a new $p$-chain.
- Letting $c_1 = \sum_i a_i \sigma_i$ and $c_2 = \sum_i b_i \sigma_i$. Then, $c_1 + c_2 = \sum_i (a_i + b_i) \sigma_i$.
- As $a_i + b_i \in \mathbb{F}_2$ for all $i$, we get that $c_1 + c_2$ is a chain.
- Regarding $p$-chains as sets, we can interpret that $c_1 + c_2$ with modulo 2 coefficients is the *symmetric difference* between the two sets.
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Chain Groups

Algebra I

A group \((A, \bullet)\) is a set \(A\) together with a binary operation satisfying:

- Closure: for all \(\alpha, \beta \in A\), we have that \(\alpha \bullet \beta \in A\).
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- \(A\) has an identity element \(\omega\) such that \(\alpha + \omega = \alpha\) for all \(\alpha \in A\).

If, in addition, \(\bullet\) is commutative, we have that \(\alpha \bullet \beta = \beta \bullet \alpha\) for all \(\alpha, \beta \in A\), and we say the group \((A, \bullet)\) is abelian.

Chains as Groups

We can now recognize \(p\)-chains \((C_p, +)\) as abelian groups.

Chains as Vector Spaces

If the complex \(K\) has \(n_p\) \(p\)-simplices, then \(C_p\) is (isomorphic to) the set of binary vectors of length \(n_p\), i.e., \(\{0, 1\}^{n_p}\), with the exclusive-or operation \(\oplus\).
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Boundary of a Chain

**Linear Extensions**

- Fix a $p$-simplex $\sigma = [v_0, \ldots, v_p]$ in the complex $K$.
- Recall that the boundary of $\sigma$ is the collection of its proper faces, which we denoted by $\partial \sigma$.
- We can now express the boundary elements as a single $(p - 1)$-chain

$$\partial_p \sigma = \sum_{i=0}^{p} [v_0, \ldots, \hat{v}_i, \ldots, v_p],$$

where $\hat{v}_i$ indicates that $v_i$ is excluded in the corresponding face.
- Notice that we used the subscript to qualify the *boundary operator* as the one acting on the $p$-th chain group.
- For any $p$-chain $c = \sum_i a_i \sigma_i$, its boundary is the $(p - 1)$-chain

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The Chain Complex

Boundary Homomorphisms

- The boundary operator $\partial_p$ commutes with the group operations.

- If $c_1$ and $c_2$ are $p$-chains, then: $\partial_p(c_1 +_{(p)} c_2) = \partial_p c_1 +_{(p-1)} \partial_p c_2$, where we qualify the addition operators on each side of the equation.

- This means that $\partial_p$ induces a group homomorphism or a mapping between groups that preserves the group structures: $\partial_p : C_p \rightarrow C_{p-1}$.

- We can arrange the chain groups into a chain complex, effectively replacing the geometric complex $K$ with a series of algebraic modules.

$$\ldots \xrightarrow{\partial_{p+2}} C_{p+1} \xrightarrow{\partial_{p+1}} C_p \xrightarrow{\partial_p} C_{p-1} \xrightarrow{\partial_{p-1}} \ldots$$
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But like .. what’s the point?
Boundary Matrices

**Chains Groups as Vector Spaces**

- Let \( \{\sigma_i\}_i \) and \( \{\tau_j\}_j \) denote the \( p \)-simplices and \( (p-1) \)-simplices of \( K \).
- The boundary of a \( p \)-chain \( c = \sum_i a_i \sigma_i \) is the \( (p-1) \)-chain

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\partial_p c = \partial_p \left( \sum_i a_i \sigma_i \right) = \sum_i a_i \partial_p \sigma_i = \sum_i a_i \sum_j \partial^{j,i}_p \tau_j = \sum_j b_j \tau_j,
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where \( b_i = \sum_i (a_i \partial^{j,i}_p) \), and \( \partial^{j,i}_p \) is 1 if \( \tau_j \in \partial_p \sigma_i \) and 0 otherwise.
- With that, we can express the boundary operator \( \partial_p \) in matrix form.

\[
\partial_p c = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_{n_{p-1}} \end{bmatrix}, \quad \partial_p = \begin{bmatrix} \partial^{1,1}_p & \partial^{1,2}_p & \cdots & \partial^{1,n_p}_p \\ \partial^{2,1}_p & \partial^{2,2}_p & \cdots & \partial^{2,n_p}_p \\ \vdots & \vdots & \ddots & \vdots \\ \partial^{n_p-1,0}_p & \partial^{n_p-1,2}_p & \cdots & \partial^{n_p-1,n_p}_p \end{bmatrix}, \quad c = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_{n_p} \end{bmatrix}
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Boundaries and Cycles

Which Boundaries are Useful?

Consider the 1-chains on the torus to the right.

- We have a blue and a red loop.
- Also the boundary of the black triangle.
- Which of those help distinguish the torus from a sphere?

Chains with No Boundary

- Any such chain is called a $p$-cycle.
- A $p$-cycle that arises as the boundary of a $(p + 1)$-chain is a $p$-boundary.
- We need a way to count distinct $p$-cycles while ignoring all $p$-boundaries.
- Observe that $\partial_p \circ \partial_{p+1} = 0$.

Figure from Wikipedia [18]
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Equivalence and Quotients

Boundaries and Cycles as Subgroups

- Denote all $p$-cycles by $Z_p$ and all $p$-boundaries by $B_p$.
- As the boundary map commutes with addition, $Z_p$ is a subgroup of $C_p$.
- Likewise, $B_p$ is a subgroup of $Z_p$.
- For any $p$-cycle $\alpha \in Z_p$ and a $p$-boundary $\beta$, we get that $\alpha + \beta \in Z_p$.

Algebra II

- We define an equivalence relation that identifies a pair of elements $\alpha, \alpha' \in Z_p$ whenever $\alpha' = \alpha + \beta$ for some $\beta \in B_p$.
- The equivalence relation partitions $Z_p$ into equivalence classes or cosets; the coset $[\alpha]$ consists of all the elements identified with $\alpha$.
- Then, the collection of cosets together with the addition operator give rise to the quotient group $Z_p/B_p$ of the elements in $Z_p$ modulo the elements in $B_p$. 
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- Denote all $p$-cycles by $Z_p$ and all $p$-boundaries by $B_p$.
- As the boundary map commutes with addition, $Z_p$ is a subgroup of $C_p$.
- Likewise, $B_p$ is a subgroup of $Z_p$.
- For any $p$-cycle $\alpha \in Z_p$ and a $p$-boundary $\beta$, we get that $\alpha + \beta \in Z_p$.

Algebra II

- We define an equivalence relation that identifies a pair of elements $\alpha, \alpha' \in Z_p$ whenever $\alpha' = \alpha + \beta$ for some $\beta \in B_p$.
- The equivalence relation partitions $Z_p$ into equivalence classes or cosets; the coset $[\alpha]$ consists of all the elements identified with $\alpha$.
- Then, the collection of cosets together with the addition operator give rise to the quotient group $Z_p/B_p$ of the elements in $Z_p$ modulo the elements in $B_p$. 
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Homology

Algebra III

- Take a group \((A, \bullet)\).
  - The order of the group is the cardinality of \(A\).
  - The rank of the group is the cardinality of a minimal generator.
- For a set of binary vectors, such as \(C_p\) or \(Z_p\)
  - The order is the number of distinct binary vectors.
  - The rank is the number of basis vectors that span the entire set.

Homology Groups and Betti Numbers

- We can now define the \(p\)-th homology group as \(H_p = Z_p/B_p\).
- The rank of \(H_p\) is known as the \(p\)-th Betti number \(\beta_p\)

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Rank-Nullity

**Algebra IV**

- Let $V$ and $W$ be vector spaces and $T : V \to W$ a **linear transformation**.
- We define the *kernel* of $T$ as the subspace of $V$, denoted $\text{Ker}(T)$ of all vectors $v$ such that $T(v) = 0$.
- The remaining elements $v \in V$ for which $T(v) \neq 0$ are mapped to a subspace of $W$, i.e., the *image* of $T$.
- The *rank-nullity theorem* states that

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\dim V = \dim \text{Image}(T) + \dim \text{Ker}(T).
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**In the Context of Homology**

- $Z_p$ is the kernel of $\partial_p$, while $B_{p-1}$ is its image.
- Hence, $\text{rank } C_p = \text{rank } Z_p + \text{rank } B_{p-1}$.
- Note that $B_{-1} = \emptyset$, and for a $d$-dimensional complex, $Z_{d+1} = \emptyset$. 
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The Euler Characteristic Revisited

A Generalized Formula

Recalling the alternating sum in Euler’s polyhedron formula, we may write

\[ \chi = \sum_{p \geq 0} (-1)^p \text{rank } C_p = \sum_{p \geq 0} (-1)^p (\text{rank } Z_p + \text{rank } B_{p-1}) \]

\[ = (\text{rank } Z_0 + \text{rank } B_{-1}) - (\text{rank } Z_1 + \text{rank } B_0) + (\text{rank } Z_2 + \text{rank } B_1) - \ldots \]

\[ = (\text{rank } Z_0 - \text{rank } B_0) - (\text{rank } Z_1 - \text{rank } B_1) + (\text{rank } Z_2 - \text{rank } B_2) - \ldots \]

\[ = \sum_{p \geq 0} (-1)^p (\text{rank } Z_p - \text{rank } B_p) \]

\[ = \sum_{p \geq 0} (-1)^p \beta_p. \]

Note that the homology groups and the Betti numbers do not depend on the specific triangulation of the underlying space, i.e., they are indeed topological invariants.
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Matrix Reduction

**Rank Computations**

- To compute $\beta_p$ as the difference between $\text{rank } Z_p$ and $\text{rank } B_p$ we work with the matrix representation of the boundary map $\partial_p$.
- Using a sequence of row/column operations, the matrix is reduced without changing its rank into a simple form easily providing the ranks.
- A variant of *Gaussian elimination* is used to get the *Smith normal form*.

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What about the maps between spaces?
Induced Maps on Homology

\[ \cdots \xrightarrow{\partial_{\hat{X}}} C_{p+1}(\hat{X}) \xrightarrow{\partial_{\hat{X}}} C_p(\hat{X}) \xrightarrow{\partial_{\hat{X}}} C_{p-1}(\hat{X}) \xrightarrow{\partial_{\hat{X}}} \cdots \]

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Functoriality

- A simplicial map \( \hat{f}_\Delta : \hat{X} \to \hat{Y} \) maps simplices in \( \hat{X} \) to simplices in \( \hat{Y} \).
- A simplicial map extends to a map from the chains of \( \hat{X} \) to the chains of \( \hat{Y} \), which we denote by \( \hat{f}_\# : C_p(\hat{X}) \to C_p(\hat{Y}) \), as shown in the diagram.
- As \( \hat{f}_\# \) commutes with boundary maps, it also maps the cycles and boundaries of \( \hat{X} \) to the cycles and boundaries of \( \hat{Y} \), respectively.
- Hence, \( \hat{f}_\# \) maps the homology groups of \( \hat{X} \) to the homology groups of \( \hat{Y} \), i.e., it induces a map on homology denoted by \( H(\hat{f}) : H_p(\hat{X}) \to H_p(\hat{Y}) \).
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\[ \downarrow \hat{f}_\# \]

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... $\partial_{\hat{X}} \rightarrow C_{p+1}(\hat{X}) \rightarrow C_p(\hat{X}) \rightarrow C_{p-1}(\hat{X}) \rightarrow \cdots$

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Applications of $H(\hat{f}) : H_p(\hat{X}) \rightarrow H_p(\hat{Y})$

\[
\begin{array}{c}
\text{Y}_1 \\ \downarrow f_1 \\
\text{X} \\
\uparrow f_2 \\
\text{Y}_2
\end{array}
\]

**Indirect Inference**

If a map $f : \text{Y}_1 \rightarrow \text{Y}_2$ factors through $f_1 : \text{Y}_1 \rightarrow \text{X}$ and $f_2 : \text{X} \rightarrow \text{Y}_2$ such that $f = f_2 \circ f_1$, then we can infer the homology groups of $\text{X}$ using knowledge of the homology groups of $\text{Y}_1$ and $\text{Y}_2$. 
Brouwer’s Fixed Point Theorem

Every continuous map from the disc to itself has a fixed point

- Assume that $f : \mathbb{D} \to \mathbb{D}$ is continuous and has no fixed point.
- Define $r : \mathbb{D} \to \partial \mathbb{D}$ as the intersection of the ray from $x$ to $f(x)$ with $\partial \mathbb{D}$.
- As $f$ is continuous, so is $r$. Hence, the diagram in the middle commutes.
- Passing through homology, as shown to the right, we get that
  - $H_1(\partial \mathbb{D}) \cong \mathbb{F}_2$ while $H_1(\mathbb{D}) = 0$.
  - But then, $H(r) \circ H(\nu) \neq \text{Id}$. A contradiction!
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  - But then, \( H(r) \circ H(\nu) \neq \text{Id} \). A contradiction!
Brouwer’s Fixed Point Theorem

Every continuous map from the disc to itself has a fixed point

- Assume that \( f : \mathbb{D} \rightarrow \mathbb{D} \) is continuous and has no fixed point.
- Define \( r : \mathbb{D} \rightarrow \partial \mathbb{D} \) as the intersection of the ray from \( x \) to \( f(x) \) with \( \partial \mathbb{D} \).
- As \( f \) is continuous, so is \( r \). Hence, the diagram in the middle \textit{commutes}.
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But, how do we get triangulations in the first place?
Sampled Data and Noise

The Čech Complex

- We are given a collection of sample points from an unknown underlying manifold or surface in $\mathbb{R}^d$.
- We would like to infer some of the properties of the manifold.
- To do so, we grow a ball at each sample and take the union.
- Then, we derive an abstract simplicial complex from the union of balls.
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But, how do we choose the radii of the balls?
Scale and Persistence

Examining All Scales at Once

- As shown above, different radii may result in very different results.
- Imagine a continuous process growing the radii from $r = 0$ to $r = \infty$.
- Each topological feature will be present over an interval $[a, b]$. 
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Summary

\[ \partial_p = \begin{bmatrix} \partial_{p,1,1} & \partial_{p,1,2} & \cdots & \partial_{p,1,n_p} \\ \partial_{p,2,1} & \partial_{p,2,2} & \cdots & \partial_{p,2,n_p} \\ \vdots & \vdots & \ddots & \vdots \\ \partial_{p,n_p-1,0} & \partial_{p,n_p-1,2} & \cdots & \partial_{p,n_p-1,n_p} \end{bmatrix} \]

\[ H_p = Z_p / B_p \]

Main Concepts Introduced

- Continuous deformations
- Simplicial approximations
- Chain algebra and homology
- Functoriality

Figure from Wikipedia [15]
Summary

Key Concepts Missing

- Persistent homology
- Persistence diagrams and barcodes
- Simplicial collapses
- Sparse filtrations and interleaving