The Gudhi Library: Simplicial Complexes and Persistent Homology

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Introduction
Simplicial Complex

Given a set $V = \{1 \cdots n\}$ of vertices, an abstract simplicial complex $\mathcal{K}$ on $V$ is a family of subsets of vertices s.t.:

$$\forall \sigma \in \mathcal{K} : \tau \subseteq \sigma \Rightarrow \tau \in \mathcal{K}$$

Such $\sigma$ is called a simplex

Boundary of a simplex $\sigma$: $\partial \sigma = \{\tau \subset \sigma | \dim(\sigma) = \dim(\tau) + 1\}$
Introduction to Homology

$K^p$: set of $p$-simplices of $K$

$C_p$: Abelian group of formal sums of $p$-simplices with $\mathbb{Z}$-coefficients

$\{e_1, e_2, e_3, e_4, e_5, e_6, \ldots\}$

$\partial^2 = - + [a, b, c]$
Introduction to Homology

\[ e_1 + e_2 + e_3 + e_4 + e_5 + e_6 \]

\[ \{e_1, e_2, e_3, e_4, e_5, e_6, \cdots \} \]

\( K^p \): set of \( p \)-simplices of \( K \)

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\( C_1 = (\{\sum_i k_i e_i\}, +) \)
Introduction to Homology

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\[ C_1 = (\{ \sum_i k_i e_i \}, +) \]

\[ \partial_p : C_p \to C_{p-1} \): Boundary operator

\[ \partial_2 [a, b, c] = [ab] - [bc] + [ca] \]
Introduction to Homology

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Field \( \mathbb{Z}_p \) or \( \mathbb{Q} \)

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Introduction to Homology

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Introduction to Homology

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\[ \partial_2 [a, b, c] = [ab] - [bc] + [ca] \]

\[ Z_p = \ker \partial_p : \text{the } p\text{-cycles} \]

\[ \partial_1 = \begin{array}{c}
\times 2 \\
\times 2 \\
\times 2 \\
\times 2 \\
\times 2
\end{array} = 0 \]
\( \partial_p : C_p \rightarrow C_{p-1} : \) Boundary operator

\[
\partial_2 [a, b, c] = [ab] - [bc] + [ca]
\]

\( Z_p = \ker \partial_p : \) the \( p \)-cycles

\( B_p = \text{im} \partial_{p+1} : \) the \( p \)-boundaries

\[
\partial_1 = \begin{array}{c}
\times 2 \\
\times 2 \\
\times 2 \\
\times 2 \\
\times 2 \\
\end{array}
\]

\[
= 0
\]

\[
\partial_2 = \begin{array}{c}
\times 2 \\
\times 2 \\
\times 2 \\
\times 2 \\
\times 2 \\
\end{array}
\]

Fundamental property:

\( \partial_p \circ \partial_{p+1} = 0 \)

\( H_p = Z_p / B_p : \) \( p \)-th homology group
Introduction to Homology

\[ \partial_p : C_p \to C_{p-1} : \text{Boundary operator} \]
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Fundamental property: \[ \partial_p \circ \partial_{p+1} = 0 \]
**Introduction to Homology**

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Fundamental property: \( \partial_p \circ \partial_{p+1} = 0 \)

\[ H_p = Z_p / B_p : p^{\text{th}} \text{ homology group} \]
Persistent Homology

Indexing

Complex

Homology

Persistence diagram

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Persistent Homology in Practice

$\mathbb{H}_1$ 

$\varepsilon_1 \quad \varepsilon_2 \quad \varepsilon_3 \quad \varepsilon_4 \quad \varepsilon_5 \quad \varepsilon_6 \quad \varepsilon_7$
Persistent Homology: Standard Algorithm

- Store the matrix of the boundary operator of the final complex
- Reduce it from left-to-right with column operations
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Challenge
Practical Performance

[Boissonnat, Dey, M. '13]

On a machine with 3.00 GHz processor and 32 GB RAM, on a variety of datasets, with different coefficients for cohomology:

Maximal complex size \(^1\): \(\approx 500 \cdot 10^6\) simplices
Timings \(^2\): \(2.7 \cdot 10^{-7} \leq \cdot \leq 9.1 \cdot 10^{-7}\) s. per simplex
Size cohomology groups: negligible compared to complex

Running time: less than 5 minutes

\(^1\) with a Simplex Tree
\(^2\) with a Compressed Annotation Matrix for persistent cohomology
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(Recent) Solutions

Standard Persistence: Simplicial Complexes connected by Inclusions
(Recent) Solutions

Standard Persistence: Simplicial Complexes connected by Inclusions

General Cell Complexes \[ \Rightarrow \] \[\text{[Mischaikow, Nanda '13]}\]
(Recent) Solutions

Standard Persistence: Simplicial Complexes connected by Inclusions

General Cell Complexes \( \cong \) General Simplicial Maps

\[\text{[Mischaikow, Nanda '13]}\]
(Recent) Solutions

Standard Persistence: Simplicial Complexes connected by Inclusions

General Cell Complexes

General Simplicial Maps

[Carlsson, de Silva '10]

Standard Persistence...

[Dey, Fan, Wang '13]

[Mischaikow, Nanda '13]

[Schehy '13]

[Dey, Fan, Wang '13]
(Recent) Solutions

Standard Persistence: Simplicial Complexes connected by Inclusions

General Cell Complexes

General Simplicial Maps

[Carlsson, de Silva '10]

[Dey, Fan, Wang '13]

[Mischaikow, Nanda ’13]

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[Sheehy ’13]

[Dey, Fan, Wang ’13]
(Recent) Solutions

Standard Persistence: Simplicial Complexes connected by Inclusions

\[
\bullet \rightarrow \bullet \rightarrow \bullet \rightarrow \bullet \rightarrow \bullet \rightarrow \bullet \rightarrow \bullet \rightarrow \bullet \rightarrow \bullet \rightarrow \bullet
\]

General Cell Complexes

\[
\bullet \rightarrow \bullet \rightarrow \bullet \rightarrow \bullet \rightarrow \bullet \rightarrow \bullet \rightarrow \bullet \rightarrow \bullet \rightarrow \bullet \rightarrow \bullet
\]

\[\Rightarrow\]

\[\circ\]

[Mischaikow, Nanda ’13]

[Sheehy ’13]

[Dey, Fan, Wang ’13]

General Simplicial Maps

\[
\bullet \rightarrow \bullet \rightarrow \bullet \rightarrow \bullet \rightarrow \bullet \rightarrow \bullet \rightarrow \bullet \rightarrow \bullet \rightarrow \bullet \rightarrow \bullet
\]

[Zigzag Persistence

\[
\bullet \rightarrow \bullet \rightarrow \bullet \rightarrow \bullet \rightarrow \bullet \rightarrow \bullet \rightarrow \bullet \rightarrow \bullet \rightarrow \bullet \rightarrow \bullet
\]

[Carlsson, de Silva, Morozov ’09]

[M, Oudot ’15]
(Recent) Solutions

Standard Persistence: Simplicial Complexes connected by Inclusions

General Cell Complexes

General Simplicial Maps

Zigzag Persistence

[Oudot, Sheehy ’13]

[Mischaikow, Nanda ’13]

[Sheehy ’13]

[Dey, Fan, Wang ’13]

[Carlsson, de Silva, Morozov ’09]

[M, Oudot ’15]
(Recent) Solutions

Standard Persistence: Simplicial Complexes connected by Inclusions

General Cell Complexes

General Simplicial Maps

Zigzag Persistence

\[ \sigma_1 \rightarrow \cdots \rightarrow \sigma_n \]

\[ \partial \]

\[ \sigma_1 \cdots \sigma_n \]

\[ \partial^* \]

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Software Design
Distinguish Indexing - Complex - Homology
Distinguish Indexing - Complex - Homology

Indexing 0 ↔ 1 ↔ 2 ↔ 3 ↔ 4 ↔ 5 ↔ 6 ↔ 7

Complex

Homology 0 → 0 → 0 → ⟨[c]⟩ → ⟨[c]⟩ → ⟨[c], [c']⟩ → ⟨[c]⟩ → 0
Distinguish Indexing - Complex - Homology

Creation of a concept *IndexingTag*

- linear-indexing-tag for standard persistence
- zigzag-indexing-tag for zigzag persistence

Complex

Homology

0 → 0 → 0 → \langle [c] \rangle → \langle [c] \rangle → \langle [c], [c'] \rangle → \langle [c] \rangle → 0
Distinguish Indexing - Complex - Homology

Creation of a concept **IndexingTag**
- linear-indexing-tag for standard persistence
- zigzag-indexing-tag for zigzag persistence

Creation of a concept **FilteredComplex**
- type Simplex-handle
- function `int dimension(Simplex-handle)`
- function `Boundary-simplex-range boundary-simplex-range(Simplex-handle)`

Homology

$$\langle [c] \rangle \rightarrow \langle [c] \rangle \rightarrow \langle [c], [c'] \rangle \rightarrow \langle [c] \rangle \rightarrow 0$$
Distinguish Indexing - Complex - Homology

Indexing

Creation of a concept *IndexingTag*

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Complex

Creation of a concept *FilteredComplex*

- type Simplex-handle
- function int dimension(Simplex-handle)
- function Boundary-simplex-range boundary-simplex-range(Simplex-handle)

Homology

Creation of a concept *PersistentHomology*

- type Coefficient-field

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Concepts and Relations

FilteredComplex
typedef ...
... Filtered complex
Coefficient field
Indexing tag
PersistentHomology
CoefficientField
IndexingTag
Concept Model
FilteredComplex
typedef ... Indexing_tag
PersistentHomology
typedef ... Coefficient_field
typedef ... Filtered_complex
Live in the Present
Live in the Present

Persistence diagram

Indexing

Complex

Homology

Persistence
Live in the Present

Persistence diagram

Indexing 0 \rightarrow 1 \rightarrow 2 \rightarrow 3 \rightarrow 4 \rightarrow 5 \rightarrow 6 \rightarrow 7

Complex 0 \rightarrow 0 \rightarrow \langle [c] \rangle \rightarrow \langle [c] \rangle \rightarrow \langle [c], [c'] \rangle \rightarrow \langle [c] \rangle \rightarrow 0

Homology 0 \rightarrow \langle [c] \rangle \rightarrow \langle [c] \rangle \rightarrow \langle [c], [c'] \rangle \rightarrow \langle [c] \rangle \rightarrow 0

Persistence diagram
Live in the Present

![Diagram of indexing, complex, homology, and persistence diagram]

Indexing 0 → 1 → 2 → 3 → 4 → 5 → 6 → 7
Complex
Homology 0 → 0 → 0 → \langle [c] \rangle → \langle [c] \rangle → \langle [c], [c'] \rangle → \langle [c] \rangle → 0

Persistence diagram
Live in the Present

Indexing
Complex
Homology

Persistence diagram
Live in the Present
Live in the Present

Indexing
Complex
Homology

Persistence diagram
4 Implementation
Model of *FilteredComplex*: **Simplex_tree**

*Simplex Tree* for Simplicial Complexes:  
[Boissonnat, M. ’12]

- $O(1)$ memory word per simplex (optimal)
- fast boundary computation
- fast construction of geometric complexes (Rips complex, etc)
- very dynamic: addition/removal simplices, edge contraction ...
Model of *PersistentHomology*: Persistent_cohomology

*Compressed Annotation Matrix*: [Boissonnat, Dey, M. ’13]

- begin with an empty structure (represent the cohomology groups)
- remain very small all along the computation
- very dynamic: fast update under simplex addition, edge contraction
Model of *CoefficientField*: Field\_Zp and Multi\_field

Multi-Field Persistent Homology:

[Boissonnat, M. '14]

<table>
<thead>
<tr>
<th>Field:</th>
<th>(\mathbb{Z})</th>
<th>(\mathbb{Z}_2)</th>
<th>(\mathbb{Z}_p \geq 3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(H_0(\mathbb{Z}))</td>
<td>(\mathbb{Z})</td>
<td>(\mathbb{Z}_2)</td>
<td>(\mathbb{Z}_p)</td>
</tr>
<tr>
<td>(H_1(\mathbb{Z}))</td>
<td>(\mathbb{Z} \oplus \mathbb{Z}_2)</td>
<td>(\mathbb{Z}_2 \oplus \mathbb{Z}_2)</td>
<td>(\mathbb{Z}_p)</td>
</tr>
<tr>
<td>(H_2(\mathbb{Z}))</td>
<td>0</td>
<td>(\mathbb{Z}_2)</td>
<td>0</td>
</tr>
</tbody>
</table>

- \(\mathbb{Z} \oplus \mathbb{Z}_2^{*}\)
- \(\mathbb{Z}^3 \oplus \mathbb{Z}_2^{*}\)
- \(\mathbb{Z}_2\) only in \(\mathbb{Z}_2\)
- \(\mathbb{Z}_3\) only in \(\mathbb{Z}_3\)
- \(\mathbb{Z}_2\) and \(\mathbb{Z}_3\)
### Some Experiments

| Data | $|P|$ | $D$ | $d$ | $r$  | $|K|$   | $T_{st}$ | $T_{\mathbb{Z}_2}^{ph}$ | $T_{\mathbb{Z}_{1223}}^{ph}$ | $T_{\mathbb{Z}_2}^{ph}$ |
|------|------|-----|-----|------|--------|---------|-----------------|-----------------|-----------------|
| **Bud** | 49,990 | 3   | 2   | 0.09 | $127 \cdot 10^6$ | 5.7 | 161 | 161 | 252 |
| **Bro**  | 15,000 | 25  | ?   | 0.04 | $142 \cdot 10^6$ | 5.8 | 252 | 252 | 380 |
| **Cy8**  | 6,040  | 24  | 2   | 0.8  | $193 \cdot 10^6$ | 8.4 | 249 | 249 | 325 |
| **KL**   | 90,000 | 5   | 2   | 0.25 | $114 \cdot 10^6$ | 8.3 | 228 | 227 | 401 |
| **S3**   | 50,000 | 4   | 3   | 0.65 | $134 \cdot 10^6$ | 7.2 | 176 | 176 | 310 |

**Figure**: Timings in seconds for the various algorithms.
Future Directions

- Prototype for zigzag persistence [M., Oudot ’15]
- more complexes: witness complex, alpha complex, … + general cell complexes
- edge contractions and persistence for simplicial maps
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general cell complexes
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Thank you! Any question?