

Topological Data Analysis

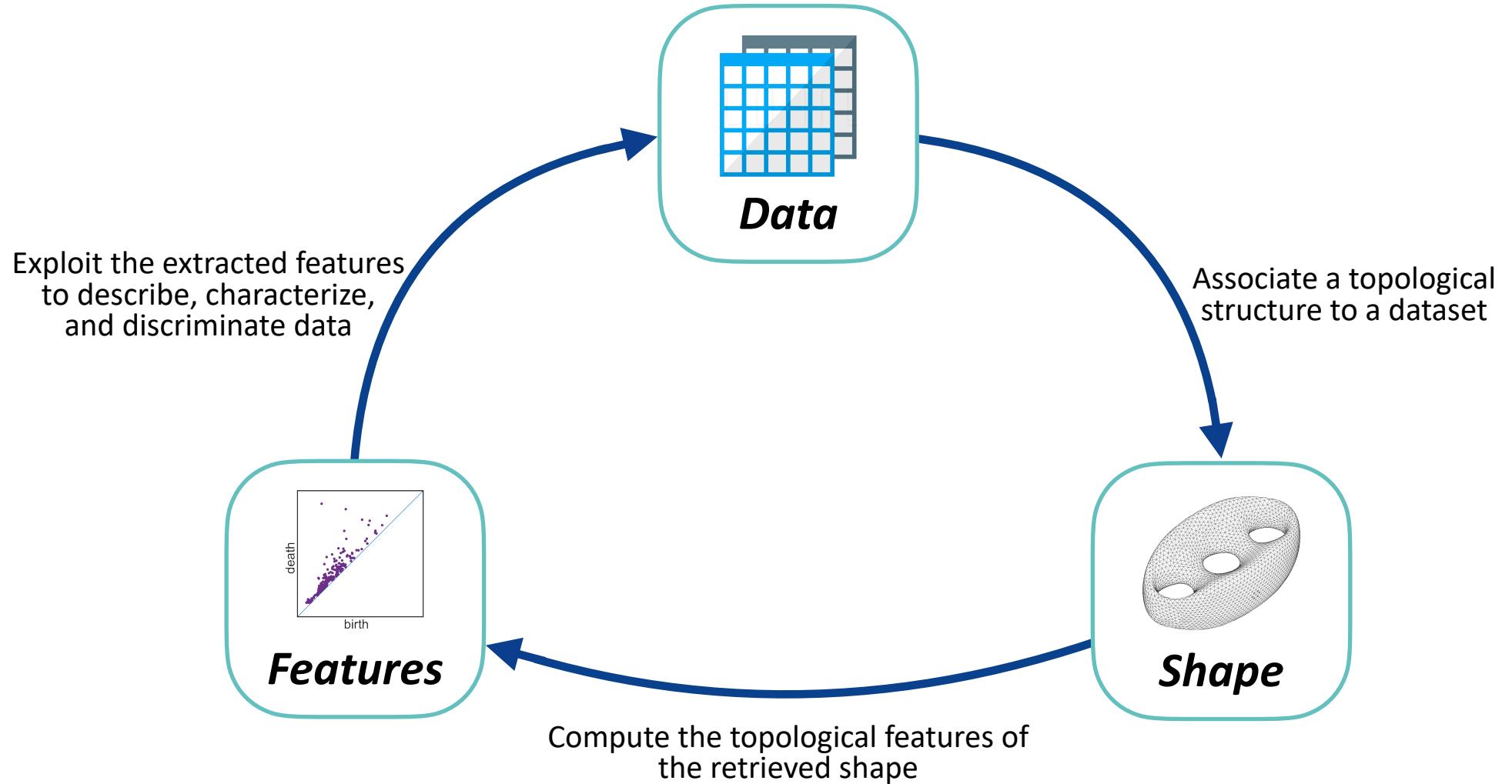
Algorithms & Structures

Ulderico Fugacci

CNR - IMATI

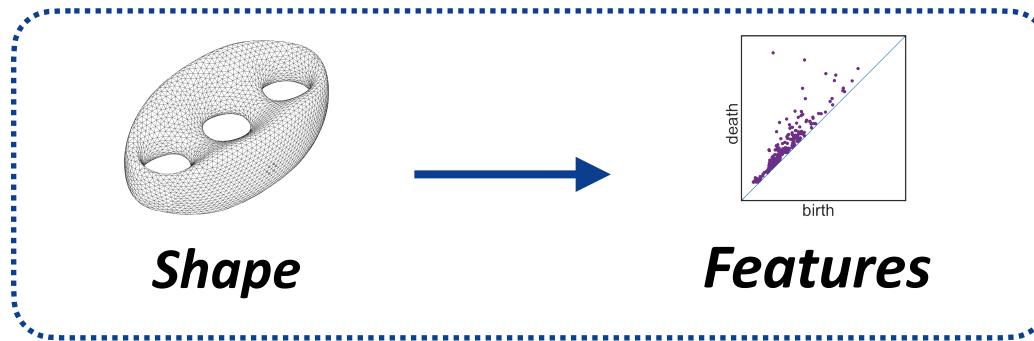
international production
computer science
excellent research
innovation engineering
mathematics
education
scientific projects
leadership participation
knowledge
productive
applied
local societal
system spreading initiatives
mission challenges
development
infrastructure
tools
high level

Topological Data Analysis



Algorithms & Structures

Topological Data Analysis allows for assigning to (almost) *any dataset* a collection of features representing a *topological summary* of the input data



Goal:

Today, we address two main questions:

- ◆ *How to efficiently compute (persistent) homology?*
- ◆ *How to compactly encode simplicial complexes of high dimension and large size?*

Algorithms & Structures

- ◆ *Computation of Persistent Homology*
- ◆ *Data Structures for Arbitrary Simplicial Complexes*

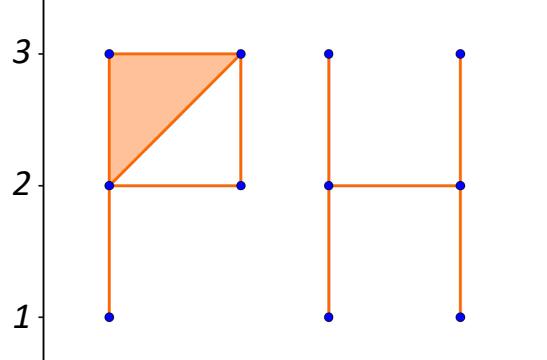
Algorithms & Structures

- ◆ *Computation of Persistent Homology*
- ◆ *Data Structures for Arbitrary Simplicial Complexes*

Persistent Homology Computation

Standard Algorithm:

From:



[Zomorodian & Carlsson 2005]

To:

[1, 2]

H₀

H_1 [3, ∞)

$[1, \infty)$

<i>i</i> \ <i>j</i>	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	
1							1																	
2								1			1													
3									1		1													
4									1		1							1	1					
5										1														
6										1											1			
7										1												1		
8																								
9																								
10																								
11																								
12																								
13																	1							
14																		1						
15																				1				
16																					1			
17																						1		
18																						1		
19																								
20																								
21																								
22																								
23																								1
<i>low</i>								4	6	7	5	3						13	14		15	16		22

Compute a *reduced boundary matrix* for K^f from which easily read the persistence pairs

Persistent Homology Computation

Given a filtered simplicial complex, let us consider its *filtering function* f :

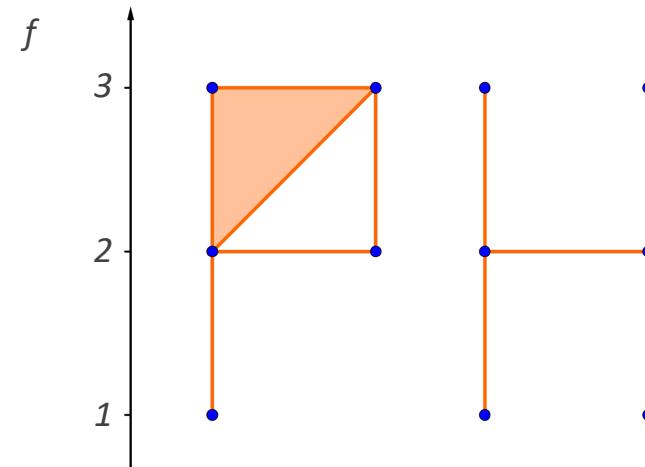
$$f(\sigma) := \min \{ p \mid \sigma \in K^p \}$$

Conversely, $K^p := \{ \sigma \in K \mid f(\sigma) \leq p \}$

Total Ordering on K^f :

A sequence $\sigma_1, \sigma_2, \dots, \sigma_n$ of the simplices of K^f such that:

- ◆ if $f(\sigma_i) < f(\sigma_j)$, then $i < j$
- ◆ if σ_i is a proper face of σ_j , then $i < j$



Persistent Homology Computation

Given a filtered simplicial complex, let us consider its *filtering function* f :

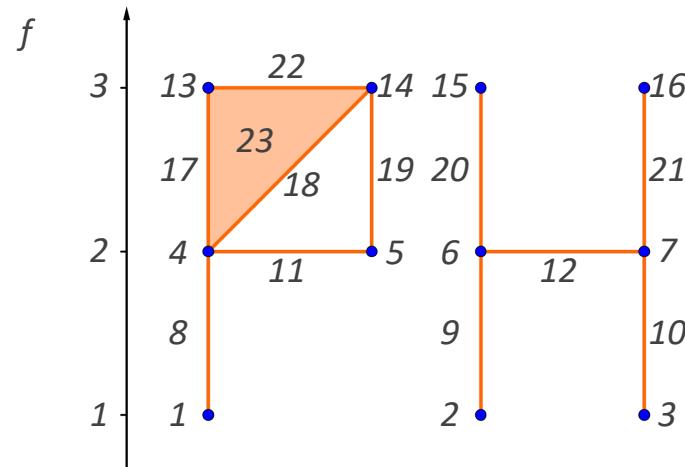
$$f(\sigma) := \min \{ p \mid \sigma \in K^p \}$$

Conversely, $K^p := \{ \sigma \in K \mid f(\sigma) \leq p \}$

A Possible Choice:

Set $\sigma < \sigma'$ if:

- ◆ $f(\sigma) < f(\sigma')$
- ◆ $f(\sigma) = f(\sigma')$ and $\dim(\sigma) < \dim(\sigma')$
- ◆ $f(\sigma) = f(\sigma')$, $\dim(\sigma) = \dim(\sigma')$, and σ precedes σ' w.r.t. the *lexicographic order* of their vertices

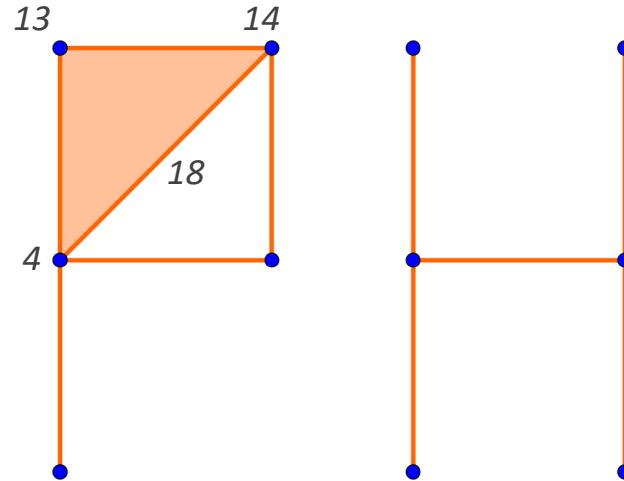


Persistent Homology Computation

Boundary Matrix:

A square matrix \mathbf{M} of size $n \times n$ defined by

$$M_{i,j} := \begin{cases} 1 & \text{if } \sigma_i \text{ is a face of } \sigma_j \text{ s.t. } \dim(\sigma_i) = \dim(\sigma_j) - 1 \\ 0 & \text{otherwise} \end{cases}$$



E.g.

- ◆ $M_{4,18} = 1$
- ◆ $M_{14,18} = 1$
- ◆ $M_{13,18} = 0$

Persistent Homology Computation

Reduced Matrix:

Given a non-null column j of a boundary matrix M ,

$$\text{low}(j) := \max \{ i \mid M_{i,j} \neq 0 \}$$

A matrix R is called **reduced** if, for each pair of non-null columns j_1, j_2 ,

$$\text{low}(j_1) \neq \text{low}(j_2)$$

Equivalently, if low function is **injective** on its domain of definition

Persistent Homology Computation

$i \setminus j$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	
1								1																
2									1															
3										1														
4										1		1						1	1					
5											1									1				
6											1		1								1			
7											1		1									1		
8																								
9																								
10																								
11																								
12																								
13																	1					1		
14																		1	1				1	
15																			1					
16																				1				
17																							1	
18																							1	
19																								
20																								
21																								
22																							1	
23																								
low								4	6	7	5	7						13	14	14	15	16	14	22

$low(10) = 7 = low(12)$



M is not reduced

Persistent Homology Computation

Reduction Algorithm:

```
Matrix  $R = M$ 
for  $j = 1, \dots, n$  do
    while  $\exists j' < j$  with  $\text{low}(j') = \text{low}(j)$  do
         $R.\text{column}(j) = R.\text{column}(j) + R.\text{column}(j')$ 
    endwhile
endfor
return  $R$ 
```

Time Complexity:

At most n^2 column additions



$O(n^3)$ in the worst case

$i \setminus j$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	
1								1																
2									1															
3										1														
4							1				1							1	1					
5											1									1				
6									1			1									1			
7										1		1										1		
8																								
9																								
10																								
11																								
12																								
13																1						1		
14																		1	1				1	
15																				1				
16																					1			
17																							1	
18																							1	
19																								
20																								
21																								
22																							1	
23																								
low								4	6	7	5	7						13	14	14	15	16	14	22

Initialize \mathbf{R} to \mathbf{M} , where

\mathbf{M} is the **boundary matrix** of K^f

expressed according with a **total ordering** of its simplices

$j < 12$

$i \setminus j$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	
1								1																
2									1															
3										1														
4								1			1							1	1					
5											1									1				
6									1			1									1			
7										1		1										1		
8																								
9																								
10																								
11																								
12																								
13																	1					1		
14																		1	1				1	
15																				1				
16																					1			
17																						1		
18																						1		
19																								
20																								
21																								
22																								1
23																								
low								4	6	7	5	7						13	14	14	15	16	14	22

For each $j < 12$,

there is no $j' < j$ such that
 $low(j') = low(j)$

So, increase j by 1

j'

j

$i \setminus j$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23		
1								1																	
2									1																
3										1															
4								1			1							1	1						
5											1									1					
6									1			1									1				
7										1			1									1			
8																									
9																									
10																									
11																									
12																									
13																	1				1				
14																		1	1			1			
15																				1					
16																					1				
17																						1			
18																						1			
19																									
20																									
21																									
22																							1		
23																									
low								4	6	7	5	7							13	14	14	15	16	14	22

For $j = 12$, $\text{low}(12) = 7$

column $j'=10$ is such that $\text{low}(j') = \text{low}(j) = 7$

So, set

column 12 := column 12 + column 10

j

$i \setminus j$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23		
1								1																	
2									1																
3										1		1													
4							1				1							1	1						
5											1									1					
6									1			1									1				
7										1												1			
8																									
9																									
10																									
11																									
12																									
13																	1				1				
14																		1	1			1			
15																				1					
16																					1				
17																						1			
18																						1			
19																									
20																									
21																									
22																							1		
23																									
low								4	6	7	5	6							13	14	14	15	16	14	22

For $j = 12$, $\text{low}(12) = 7$

column $j'=10$ is such that $\text{low}(j') = \text{low}(j) = 7$

So, set

column 12 := column 12 + column 10 $\longrightarrow \text{low}(12) = 6$

j' j

$i \setminus j$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23			
1								1																		
2									1																	
3										1		1														
4								1			1							1	1							
5											1									1						
6									1			1									1					
7										1												1				
8																										
9																										
10																										
11																										
12																										
13																	1				1					
14																		1	1			1				
15																				1						
16																					1					
17																						1				
18																						1				
19																										
20																										
21																										
22																							1			
23																										
low									4	6	7	5	6							13	14	14	15	16	14	22

For $j = 12$, $\text{low}(12) = 6$

column $j' = 9$ is such that $\text{low}(j') = \text{low}(j) = 6$

So, set

column 12 := column 12 + column 9

j

$i \setminus j$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	
1								1																
2									1			1												
3										1		1												
4								1			1							1	1					
5											1									1				
6									1												1			
7										1												1		
8																								
9																								
10																								
11																								
12																								
13																	1					1		
14																		1	1				1	
15																				1				
16																					1			
17																							1	
18																							1	
19																								
20																								
21																								
22																							1	
23																								
low								4	6	7	5	3						13	14	14	15	16	14	22

For $j = 12$, $\text{low}(12) = 6$

column $j' = 9$ is such that $\text{low}(j') = \text{low}(j) = 6$

So, set

column 12 := column 12 + column 9 $\longrightarrow \text{low}(12) = 3$

j

$i \setminus j$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	
1								1																
2									1				1											
3										1			1											
4								1			1							1	1					
5											1									1				
6									1												1			
7										1												1		
8																								
9																								
10																								
11																								
12																								
13																	1					1		
14																		1	1				1	
15																				1				
16																					1			
17																							1	
18																							1	
19																								
20																								
21																								
22																							1	
23																								
low								4	6	7	5	3						13	14	14	15	16	14	22

For each $j = 12$,

there is no $j' < j$ such that
 $low(j') = low(j) = 3$

So, increase j by 1

$$12 < j < 19$$

$i \setminus j$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23		
1									1																
2										1				1											
3											1		1												
4								1				1						1	1						
5												1								1					
6									1												1				
7										1												1			
8																									
9																									
10																									
11																									
12																									
13																	1					1			
14																		1	1				1		
15																				1					
16																					1				
17																							1		
18																							1		
19																									
20																									
21																									
22																							1		
23																									
low									4	6	7	5	3						13	14	14	15	16	14	22

For each $12 < j < 19$,

there is no $j' < j$ such that
 $low(j') = low(j)$

So, increase j by 1

j' j

$i \setminus j$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	
1								1																
2									1				1											
3										1		1												
4							1				1							1	1					
5											1									1				
6									1												1			
7										1												1		
8																								
9																								
10																								
11																								
12																								
13																	1					1		
14																		1	1				1	
15																				1				
16																					1			
17																							1	
18																							1	
19																								
20																								
21																								
22																							1	
23																								
low								4	6	7	5	3						13	14	14	15	16	14	22

For $j = 19$, $\text{low}(19) = 14$

column $j' = 18$ is such that $\text{low}(j') = \text{low}(j) = 14$

So, set

column 19 := column 19 + column 18

j

$i \setminus j$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	
1								1																
2									1				1											
3										1		1												
4								1			1							1	1	1				
5												1								1				
6									1												1			
7										1												1		
8																								
9																								
10																								
11																								
12																								
13																	1				1			
14																		1				1		
15																			1					
16																				1				
17																						1		
18																						1		
19																								
20																								
21																								
22																							1	
23																								
low								4	6	7	5	3						13	14	5	15	16	14	22

For $j = 19$, $\text{low}(19) = 14$

column $j' = 18$ is such that $\text{low}(j') = \text{low}(j) = 14$

So, set

column 19 := column 19 + column 18 $\longrightarrow \text{low}(19) = 5$

j'

j

$i \setminus j$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23		
1									1																
2									1			1													
3										1		1													
4								1			1							1	1	1					
5											1									1					
6									1												1				
7									1													1			
8																									
9																									
10																									
11																									
12																									
13																	1				1				
14																		1				1			
15																			1						
16																				1					
17																						1			
18																						1			
19																									
20																									
21																									
22																							1		
23																									
low									4	6	7	5	3						13	14	5	15	16	14	22

For $j = 19$, $\text{low}(19) = 5$

column $j' = 11$ is such that $\text{low}(j') = \text{low}(j) = 5$

So, set

column 19 := column 19 + column 11

j

$i \setminus j$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	
1								1																
2									1				1											
3										1		1												
4								1			1							1	1					
5												1												
6									1											1				
7										1											1			
8																								
9																								
10																								
11																								
12																								
13																	1				1			
14																		1				1		
15																			1					
16																				1				
17																						1		
18																						1		
19																								
20																								
21																								
22																							1	
23																								
low								4	6	7	5	3						13	14		15	16	14	22

For $j = 19$, $\text{low}(19) = 5$

column $j' = 11$ is such that $\text{low}(j') = \text{low}(j) = 5$

So, set

column 19 := column 19 + column 11 \longrightarrow low(19) undefined

j

$i \setminus j$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23		
1									1																
2										1				1											
3											1		1												
4								1			1							1	1						
5												1													
6									1											1					
7										1											1				
8																									
9																									
10																									
11																									
12																									
13																	1				1				
14																		1				1			
15																			1						
16																				1					
17																						1			
18																						1			
19																									
20																									
21																									
22																							1		
23																									
low									4	6	7	5	3						13	14		15	16	14	22

For each $j = 19$,

there is no $j' < j$ such that
 $low(j') = low(j)$

So, increase j by 1

$$19 < j < 22$$

$i \setminus j$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23		
1									1																
2										1				1											
3											1		1												
4								1			1							1	1						
5												1													
6									1											1					
7										1											1				
8																									
9																									
10																									
11																									
12																									
13																	1					1			
14																		1					1		
15																			1						
16																				1					
17																						1			
18																							1		
19																									
20																									
21																									
22																							1		
23																									
low									4	6	7	5	3						13	14		15	16	14	22

For each $19 < j < 22$,

there is no $j' < j$ such that
 $low(j') = low(j)$

So, increase j by 1

j'

j

$i \setminus j$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	
1								1																
2									1				1											
3										1		1												
4								1			1							1	1					
5												1												
6									1													1		
7										1												1		
8																								
9																								
10																								
11																								
12																								
13																1						1		
14																	1					1		
15																		1						
16																			1					
17																						1		
18																						1		
19																								
20																								
21																								
22																						1		
23																								
low								4	6	7	5	3						13	14		15	16	14	22

For $j = 22$, $\text{low}(22) = 14$

column $j' = 18$ is such that $\text{low}(j') = \text{low}(j) = 14$

So, set

column 22 := column 22 + column 18

$i \setminus j$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23		
1									1																
2										1				1											
3											1			1											
4									1				1									1			
5													1												
6										1												1			
7											1											1			
8																									
9																									
10																									
11																									
12																									
13																	1					1			
14																		1							
15																			1						
16																				1					
17																						1			
18																						1			
19																									
20																									
21																									
22																						1			
23																									
low									4	6	7	5	3						13	14		15	16	13	22

For $j = 22$, $\text{low}(22) = 14$

column $j' = 18$ is such that $\text{low}(j') = \text{low}(j) = 14$

So, set

column 22 := column 22 + column 18 $\longrightarrow \text{low}(22) = 13$

j'

j

$i \setminus j$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	
1								1																
2									1			1												
3										1		1												
4								1			1						1	1				1		
5											1													
6									1											1				
7										1											1			
8																								
9																								
10																								
11																								
12																								
13																1						1		
14																	1							
15																		1						
16																			1					
17																						1		
18																						1		
19																								
20																								
21																								
22																						1		
23																								
low								4	6	7	5	3					13	14			15	16	13	22

For $j = 22$, $\text{low}(22) = 13$

column $j' = 17$ is such that $\text{low}(j') = \text{low}(j) = 13$

So, set

column 22 := column 22 + column 17

$i \setminus j$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23
1								1															
2									1				1										
3										1			1										
4								1				1						1	1				
5													1										
6									1													1	
7										1												1	
8																							
9																							
10																							
11																							
12																							
13																	1						
14																		1					
15																			1				
16																				1			
17																						1	
18																						1	
19																							
20																							
21																							
22																						1	
23																							
low								4	6	7	5	3						13	14		15	16	22

For $j = 22$, $\text{low}(22) = 13$

column $j' = 17$ is such that $\text{low}(j') = \text{low}(j) = 13$

So, set

column 22 := column 22 + column 17 \longrightarrow low(22) undefined

$i \setminus j$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	
1									1															
2										1				1										
3											1			1										
4								1				1									1			
5													1											
6										1												1		
7											1												1	
8																								
9																								
10																								
11																								
12																								
13																	1							
14																		1						
15																			1					
16																				1				
17																						1		
18																							1	
19																								
20																								
21																								
22																							1	
23																								
low									4	6	7	5	3						13	14		15	16	22

For each $j = 22$,

there is no $j' < j$ such that
 $low(j') = low(j)$

So, increase j by 1

$i \setminus j$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	
1									1															
2										1				1										
3											1			1										
4									1				1											
5													1											
6										1													1	
7											1												1	
8																								
9																								
10																								
11																								
12																								
13																	1							
14																		1						
15																			1					
16																				1				
17																							1	
18																							1	
19																								
20																								
21																								
22																							1	
23																								
low									4	6	7	5	3						13	14		15	16	22

For each $j = 23$,

there is no $j' < j$ such that
 $low(j') = low(j) = 22$

So, matrix R is reduced

$i \setminus j$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23
1									1														
2										1				1									
3											1		1										
4								1			1							1	1				
5												1											
6									1												1		
7										1												1	
8																							
9																							
10																							
11																							
12																		1					
13																							
14																		1					
15																			1				
16																				1			
17																					1		
18																						1	
19																							
20																							
21																							
22																							1
23																							
low									4	6	7	5	3					13	14		15	16	22

The algorithm returns the above **reduced matrix R**

Persistent Homology Computation

Retrieving Persistence Pairs:

- ◆ For each $i = 1, \dots, n$,
if there exists j such that $\text{low}(j) = i$  $[i, j]$ is a pair for R
- ◆ Once every i has been parsed,
if i is an **unpaired** value  $[i, \infty)$ is a pair for R

From pairs of R to the “**actual**” persistence pairs of K^f :

$[i, j]$ corresponds to $[f(\sigma_i), f(\sigma_j)]$

(homological degree = $\dim(\sigma_i)$)

$[i, \infty)$ corresponds to $[f(\sigma_i), \infty)$

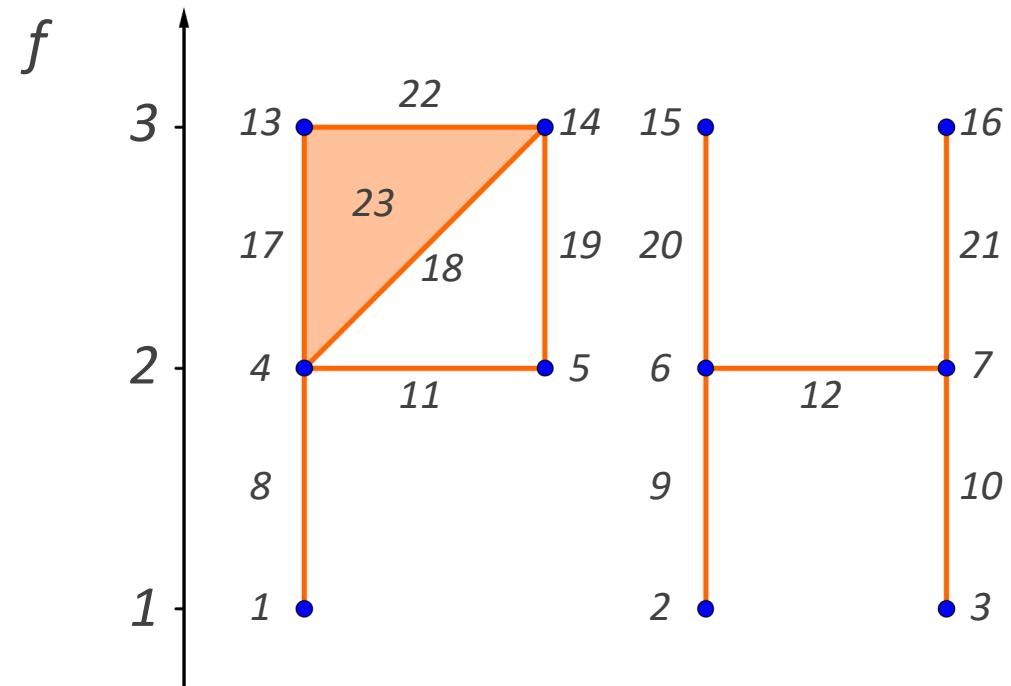
Persistent Homology Computation

 H_0 $[1, \infty)$ $[2, \infty)$ $[3, 12]$ $[4, 8]$ $[5, 11]$ $[6, 9]$ $[7, 10]$ $[13, 17]$ $[14, 18]$ $[15, 20]$ $[16, 21]$ H_1 $[19, \infty)$ $[22, 23]$

$i \setminus j$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23
1								1															
2									1					1									
3										1				1									
4										1				1						1	1		
5											1												
6											1											1	
7											1												1
8																							
9																							
10																							
11																				1			
12																							
13																			1				
14																				1			
15																					1		
16																						1	
17																							1
18																							1
19																							
20																							
21																							
22																							1
23																							
low								4	6	7	5	3						13	14		15	16	22

Persistent Homology Computation

	H_0
$[1, \infty)$	$[1, \infty)$
$[2, \infty)$	$[1, \infty)$
$[3, 12]$	$[1, 2]$
$[4, 8]$	$[2, 2]$
$[5, 11]$	$[2, 2]$
$[6, 9]$	$[2, 2]$
$[7, 10]$	$[2, 2]$
$[13, 17]$	$[3, 3]$
$[14, 18]$	$[3, 3]$
$[15, 20]$	$[3, 3]$
$[16, 21]$	$[3, 3]$



H_1 $[19, \infty)$ $[3, \infty)$
 $[22, 23]$ \rightarrow $[3, 3]$

Persistent Homology Computation

Standard algorithm to compute (persistent) homology [Zomorodian & Carlsson 2005]:

- ◆ Based on a **matrix reduction**
- ◆ **Linear complexity** in practical cases
- ◆ **Cubic complexity** in the worst case

Several different strategies:

Direct approaches:

- ◆ **Zigzag persistent homology** [Milosavljević et al. '05]
- ◆ **Computation with a twist** [Chen, Kerber '11]
- ◆ **Dual algorithm** [De Silvia et al. '11]
- ◆ **Output-sensitive algorithm** [Chen, Kerber '13]
- ◆ **Multi-field algorithm** [Boissonnat, Maria '14]
- ◆ **Annotation-based methods** [Boissonnat et al. '13; Dey et al. '14]

Distributed approaches:

- ◆ **Spectral sequences** [Edelsbrunner, Harer '08; Lipsky et al. '11]
- ◆ **Constructive Mayer-Vietoris** [Boltcheva et al. '11]
- ◆ **Multicore coreductions** [Murty et al. '13]
- ◆ **Multicore homology** [Lewis, Zomorodian '14]
- ◆ **Persistent homology in chunks** [Bauer et al. '14a]
- ◆ **Distributed persistent computation** [Bauer et al. '14b]

Coarsening approaches:

- ◆ **Topological operators and simplifications** [Mrozek, Wanner '10; Dłotko, Wagner '14]
- ◆ **Morse-based approaches** [Robins et al. '11; Harker et al. '14; Fugacci et al. '14]

Persistent Homology Computation

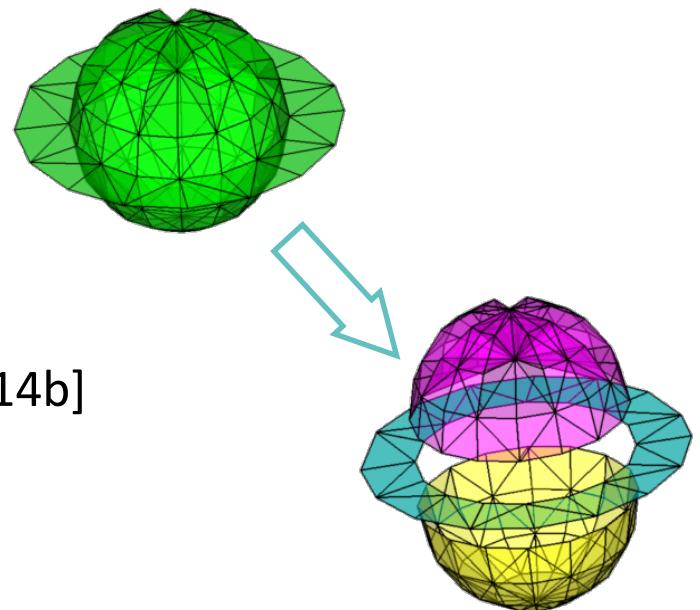
Direct Approaches:

- ◆ **Zigzag persistent homology** [Milosavljević et al. '05]
- ◆ **Computation with a twist** [Chen, Kerber '11]
- ◆ **Dual algorithm** [De Silvia et al. '11]
- ◆ **Output-sensitive algorithm** [Chen, Kerber '13]
- ◆ **Multi-field algorithm** [Boissonnat, Maria '14]
- ◆ **Annotation-based methods** [Boissonnat et al. '13; Dey et al. '14]

Persistent Homology Computation

Distributed Approaches:

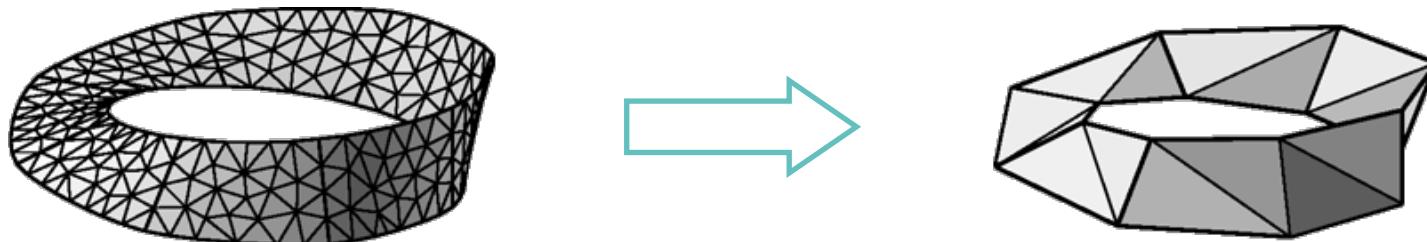
- ◆ **Spectral sequences** [Edelsbrunner, Harer '08; Lipsky et al. '11]
- ◆ **Constructive Mayer-Vietoris** [Boltcheva et al. '11]
- ◆ **Multicore coreductions** [Murty et al. '13]
- ◆ **Multicore homology** [Lewis, Zomorodian '14]
- ◆ **Persistent homology in chunks** [Bauer et al. '14a]
- ◆ **Distributed persistent computation** [Bauer et al. '14b]



Persistent Homology Computation

Coarsening Approaches:

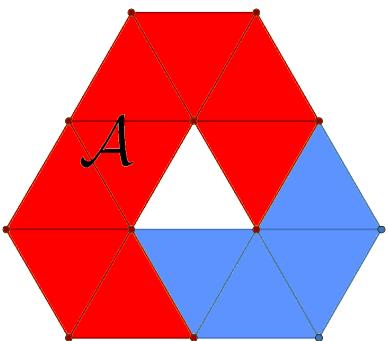
- ◆ ***Topological operators and simplifications*** [Dłotko, Wagner '14]
 - ❖ Acyclic subcomplexes [Mrozek et al. '08]
 - ❖ Reductions and coreductions [Mrozek et al. '10]
 - ❖ Edge contractions [Attali et al. '11]
- ◆ ***Morse-based approaches*** [Robins et al. '11; Harker et al. '14; Fugacci et al. '14]



Persistent Homology Computation

Coarsening Approaches:

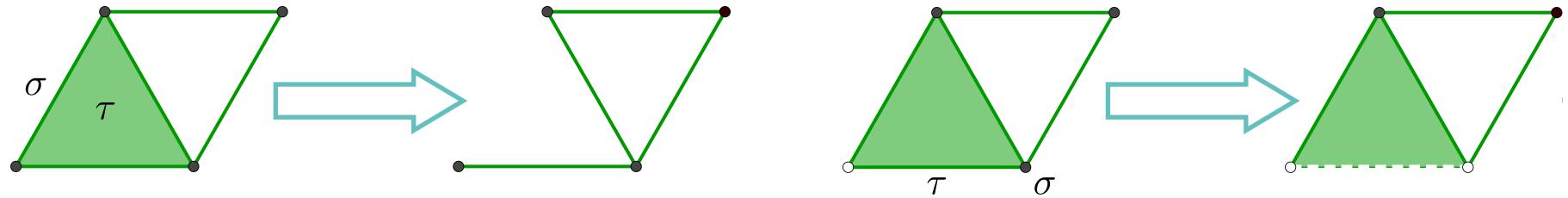
- ◆ ***Topological operators and simplifications*** [Dłotko, Wagner '14]
 - ❖ ***Acyclic subcomplexes*** [Mrozek et al. '08]
 - ❖ Reductions and coreductions [Mrozek et al. '10]
 - ❖ Edge contractions [Attali et al. '11]
- ◆ ***Morse-based approaches*** [Robins et al. '11; Harker et al. '14; Fugacci et al. '14]



Persistent Homology Computation

Coarsening Approaches:

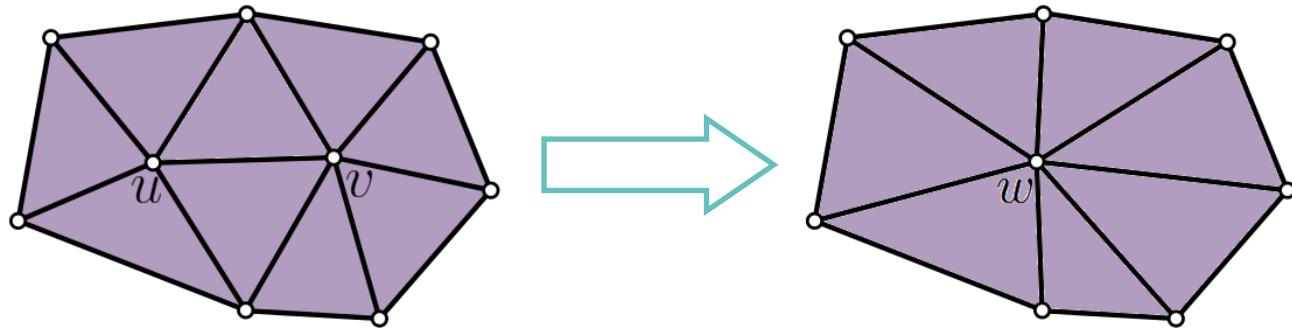
- ◆ **Topological operators and simplifications** [Dłotko, Wagner '14]
 - ❖ Acyclic subcomplexes [Mrozek et al. '08]
 - ❖ **Reductions and coreductions** [Mrozek et al. '10]
 - ❖ Edge contractions [Attali et al. '11]
- ◆ **Morse-based approaches** [Robins et al. '11; Harker et al. '14; Fugacci et al. '14]



Persistent Homology Computation

Coarsening Approaches:

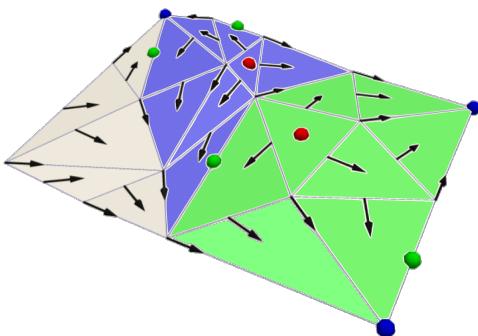
- ◆ **Topological operators and simplifications** [Dłotko, Wagner '14]
 - ❖ Acyclic subcomplexes [Mrozek et al. '08]
 - ❖ Reductions and coreductions [Mrozek et al. '10]
 - ❖ *Edge contractions* [Attali et al. '11]
- ◆ **Morse-based approaches** [Robins et al. '11; Harker et al. '14; Fugacci et al. '14]



Persistent Homology Computation

Coarsening Approaches:

- ◆ ***Topological operators and simplifications*** [Dłotko, Wagner '14]
 - ❖ Acyclic subcomplexes [Mrozek et al. '08]
 - ❖ Reductions and coreductions [Mrozek et al. '10]
 - ❖ Edge contractions [Attali et al. '11]
- ◆ ***Morse-based approaches*** [Robins et al. '11; Harker et al. '14; Fugacci et al. '14]



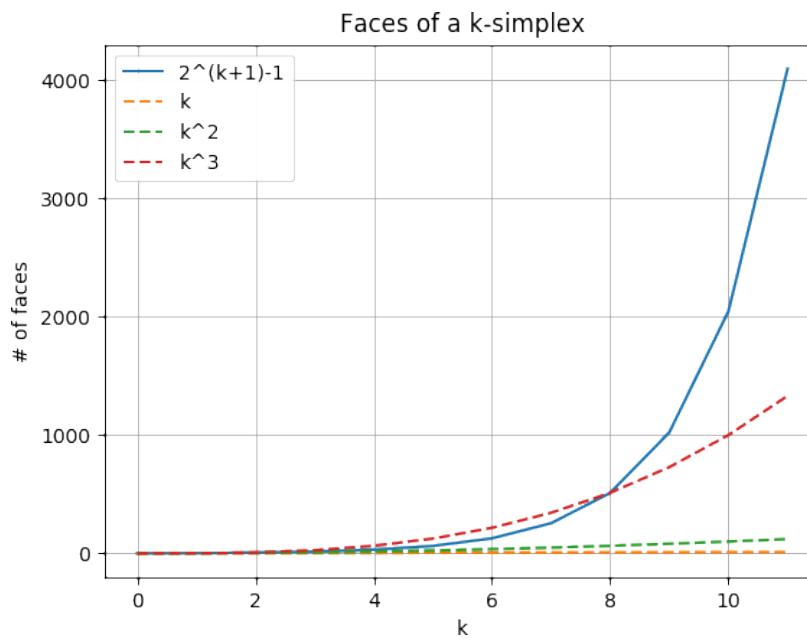
Algorithms & Structures

- ◆ *Computation of Persistent Homology*
- ◆ ***Data Structures for Arbitrary Simplicial Complexes***

Encoding Simplicial Complexes

Issue:

*It is enough to have a point cloud consisting of at least **30 points** for having to deal with an associated filtered simplicial complex of more than a **billion** of simplices*



Solution:

*Development of **compact** and **efficient data structures** for encoding arbitrary simplicial complexes*

Encoding Simplicial Complexes

Outline:

- ◆ **Which info to be stored?**
- ◆ **Data Structures**
 - ❖ *Simplex-based* representations
 - ❖ *Top-based* representations
 - ❖ *Operator-driven* representations
- ◆ **Comparisons**
- ◆ **Issues and solutions in adopting top-based representations**

Out Of Scope:

- ◆ **Data structures for specific classes of complexes**
 - ❖ E.g. *manifold* or complexes of *low dimension*

Encoding Simplicial Complexes

Data Structure:

The *entities* which a simplicial complex consists of are:

- its *simplices*

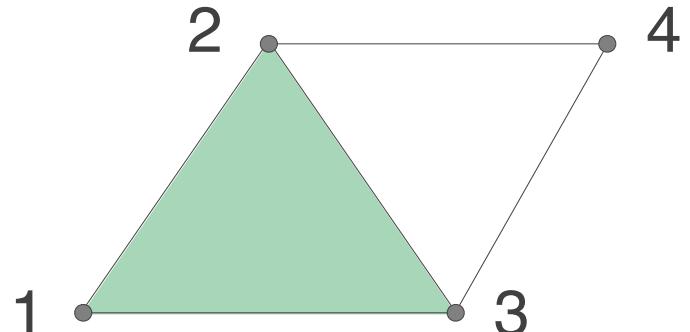
$$K = K_0 \cup K_1 \cup \dots \cup K_d$$

where K_i is the collection of the i -simplices of K

- the *topological relations*

$$R_{i,j} \subseteq K_i \times K_j$$

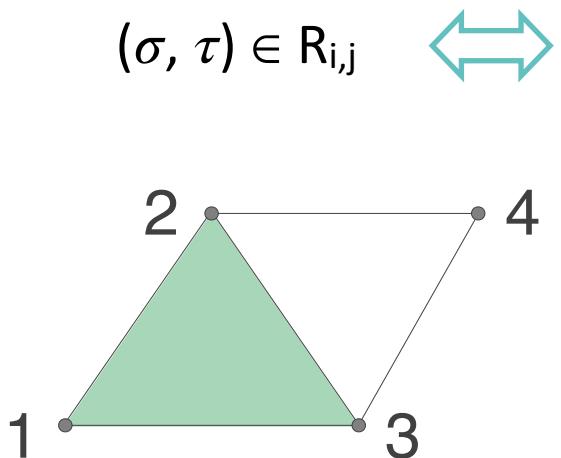
between the simplices of K encoding the (co-)boundary of each simplex



A *data structure* for K has to explicitly *store* a portion of the above information and to (efficiently) *retrieve* the remaining part

Encoding Simplicial Complexes

Topological Relations:



Given an i -simplex σ and a j -simplex τ of K ,

$$\left\{ \begin{array}{ll} \sigma \subseteq \tau & \text{for } i < j \\ |\sigma \cap \tau| = i \text{ (equivalently, } \sigma \cap \tau \in K_{i-1}) & \text{for } i = j \\ \tau \subseteq \sigma & \text{for } i > j \end{array} \right.$$

$(12, 123) \in R_{1,2}$

$(12, 24) \in R_{1,1}$

$(12, 1) \in R_{1,0}$

An i -simplex σ is called a **top simplex** of K if there is no simplex τ of K such that $(\sigma, \tau) \in R_{i,i+1}$

Encoding Simplicial Complexes

Store all the entities



- **Simplex-based** representations
- **Top-based** representations
- **Operator-driven** representations

Encoding Simplicial Complexes

Store all the entities

Incidence Graph

Efficiency

Compactness

- **Simplex-based** representations
- **Top-based** representations
- **Operator-driven** representations

Store only the top-simplices

Encoding Simplicial Complexes

Store all the entities

Incidence Graph

Simplex Tree

Efficiency

Compactness

- **Simplex-based** representations
- **Top-based** representations
- **Operator-driven** representations

Store only the top-simplices

Encoding Simplicial Complexes

Store all the entities

Incidence Graph

Simplex Tree

Efficiency

IA* Data Structure

Compactness

- **Simplex-based** representations
- **Top-based** representations
- **Operator-driven** representations

Store only the top-simplices

Encoding Simplicial Complexes

Store all the entities

Incidence Graph

Simplex Tree

Efficiency

IA* Data Structure

Stellar Tree

Compactness

- **Simplex-based** representations
- **Top-based** representations
- **Operator-driven** representations

Store only the top-simplices

Encoding Simplicial Complexes

Store all the entities

Incidence Graph

Simplex Tree

Efficiency

IA* Data Structure

Stellar Tree

Compactness

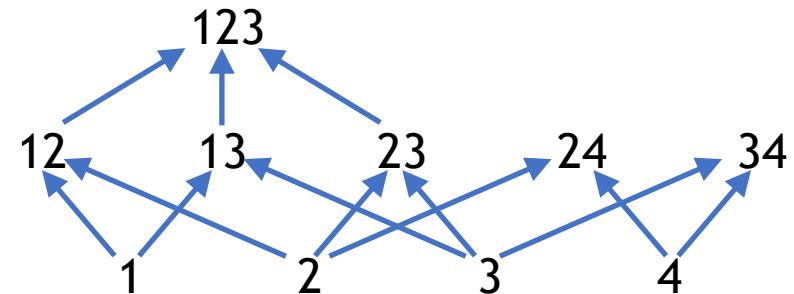
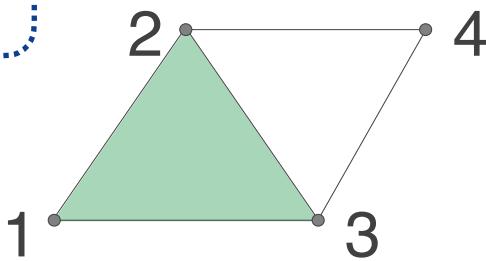
Skeleton Blocker

Store only the top-simplices

- **Simplex-based** representations
- **Top-based** representations
- **Operator-driven** representations

Simplex-based Representations

Incidence Graph:



The simplicial complex K is encoded via a *directed graph* $G = (N, A)$:

$$N \longleftrightarrow K$$

$$(\sigma, \tau) \in A \longleftrightarrow (\sigma, \tau) \in R_{i,i+1}$$



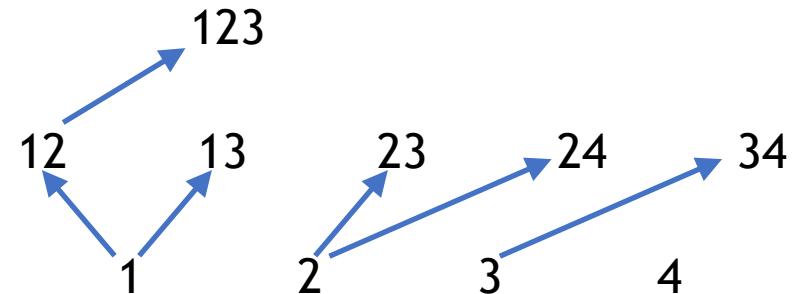
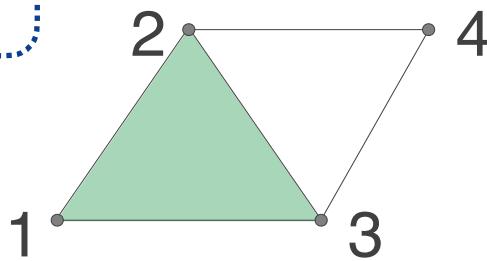
All the relations between simplices can be immediately retrieved



The representation *size exponentially increases* with the complex dimension

Simplex-based Representations

Simplex Tree:



The simplicial complex K is encoded via a *directed graph* $G = (N, A)$:

$$N \leftrightarrow K$$

$$(\sigma, \tau) \in A \leftrightarrow (\sigma, \tau) \in R_{i,i+1} \text{ and } I(\sigma) < I(\tau)$$

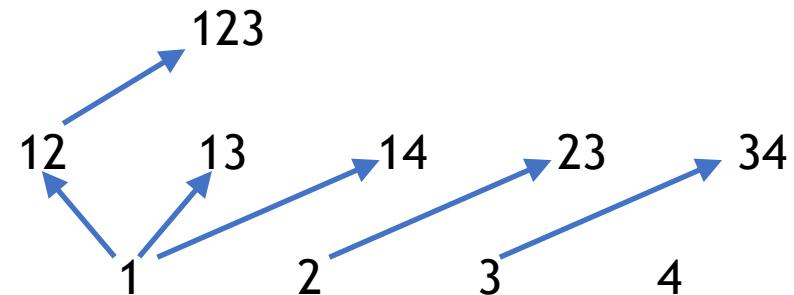
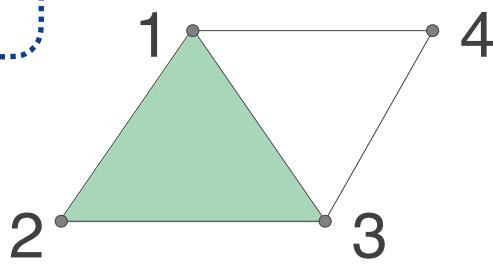
where $I(\sigma)$ denotes the *maximum value* taken by the vertices of σ w.r.t. a *total order* on K_0



Graph is *not uniquely determined* but it depends on the chosen vertex order

Simplex-based Representations

Simplex Tree:



The simplicial complex K is encoded via a *directed graph* $G = (N, A)$:

$$N \leftrightarrow K$$

$$(\sigma, \tau) \in A \leftrightarrow (\sigma, \tau) \in R_{i,i+1} \text{ and } I(\sigma) < I(\tau)$$

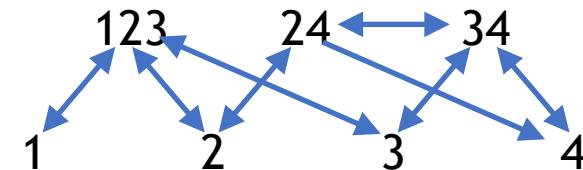
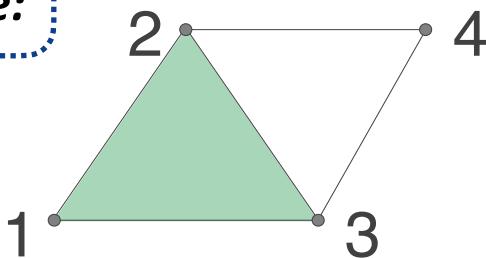
where $I(\sigma)$ denotes the *maximum value* taken by the vertices of σ w.r.t. a *total order* on K_0



Graph is *not uniquely determined* but it depends on the chosen vertex order

Top-based Representations

IA* Data Structure:



The simplicial complex K is encoded via a *directed graph* $G = (N, A)$:

$$N \longleftrightarrow K_0 \cup K_{top}$$

$$(\sigma, \tau) \in A \iff \begin{cases} \sigma \in K_{top} \text{ and } (\sigma, \tau) \in R_{i,0} \\ \sigma, \tau \in K_{top} \text{ and } (\sigma, \tau) \in R_{i,i} \\ \tau \in K_{top} \text{ and } (\sigma, \tau) \in (R_{0,i})^* \end{cases}$$



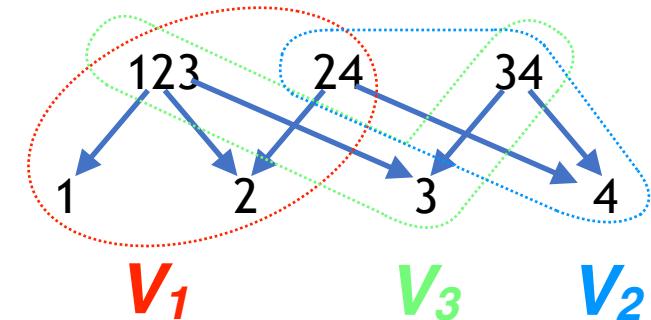
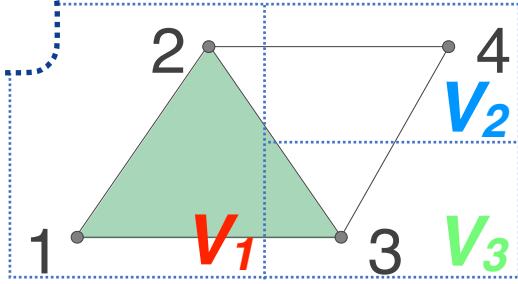
Compact: it explicitly stores just a fraction of the entities of a simplicial complex



Not all the relations between simplices are *immediately available*

Top-based Representations

Stellar Tree:



Given a decomposition of K_0 , the simplicial complex K is encoded via a *directed graph* $G = (N, A)$:

$$N \longleftrightarrow K_0 = V_1 \cup V_2 \cup \dots \cup V_n$$

$$(\sigma, \tau) \in A \longleftrightarrow \sigma \in K_{top} \text{ and } (\sigma, \tau) \in R_{i,0}$$

plus a *map* returning, for each j , the vertices of K in V_j and the top simplices with at least one vertex in V_j



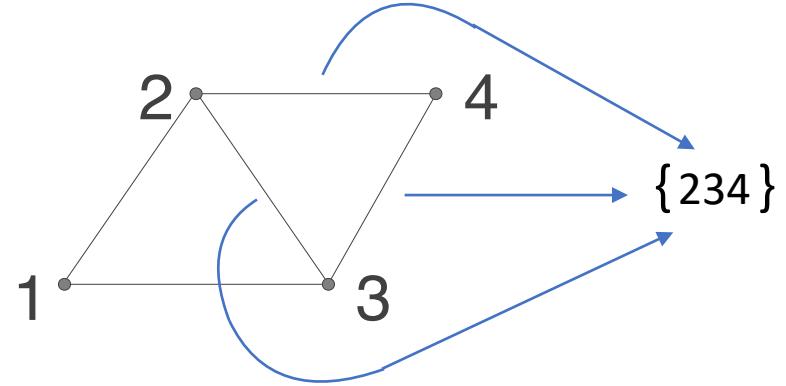
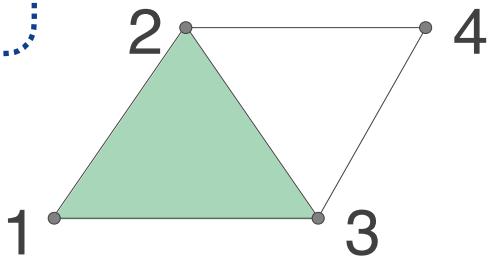
Compact and highly adjustable (e.g. choice of the decomposition, of the maximum number of vertices in each region)



Not all the relations between simplices are immediately available

Operator-driven Representations

Skeleton Blocker:



The simplicial complex K is encoded by storing its **1-skeleton** (i.e. the graph consisting of the 0- and the 1-simplices) and a **map** returning, for each 1-simplex σ , the blockers of K containing σ , where:

*A simplex τ is a **blocker** if τ does not belong to K but all its faces do*



Designed for flag complexes (e.g. **VR complexes**) and edge contraction



Too specific: **inefficient in any other task**

Encoding Simplicial Complexes

Top-based vs Simplex-based:

Dataset	d	$ \Sigma_0 $	$ \Sigma_{top} $	$ \Sigma $	Storage Cost		
					IA^*	IG	ST
DTI-SCAN	3	0.9M	5.5M	24M	0.97	11.9	2.4
VISMALE	3	4.6M	26M	118M	4.7	-	9.7
ACKLEY4	4	1.5M	32M	204M	6.8	-	12.8
AMAZON01	6	0.2M	0.4M	2.2M	0.12	1.6	0.3
AMAZON02	7	0.4M	1.0M	18.4M	0.28	9.8	1.5
ROADNET	3	1.9M	2.5M	4.8M	0.8	3.3	1.0
SPHERE-1.0	16	100	224	0.6M	0.003	0.9	0.04
SPHERE-1.2	21	100	285	26M	0.0032	-	1.5
SPHERE-1.3	23	100	382	197M	0.0034	-	11.01

Encoding Simplicial Complexes

Top-based vs Simplex-based:

PROB.5D
(607 MB)

PROB.7D
(7.9 GB)

PROB.40D
(2.6 GB)

VISMALE7D
(134 MB)

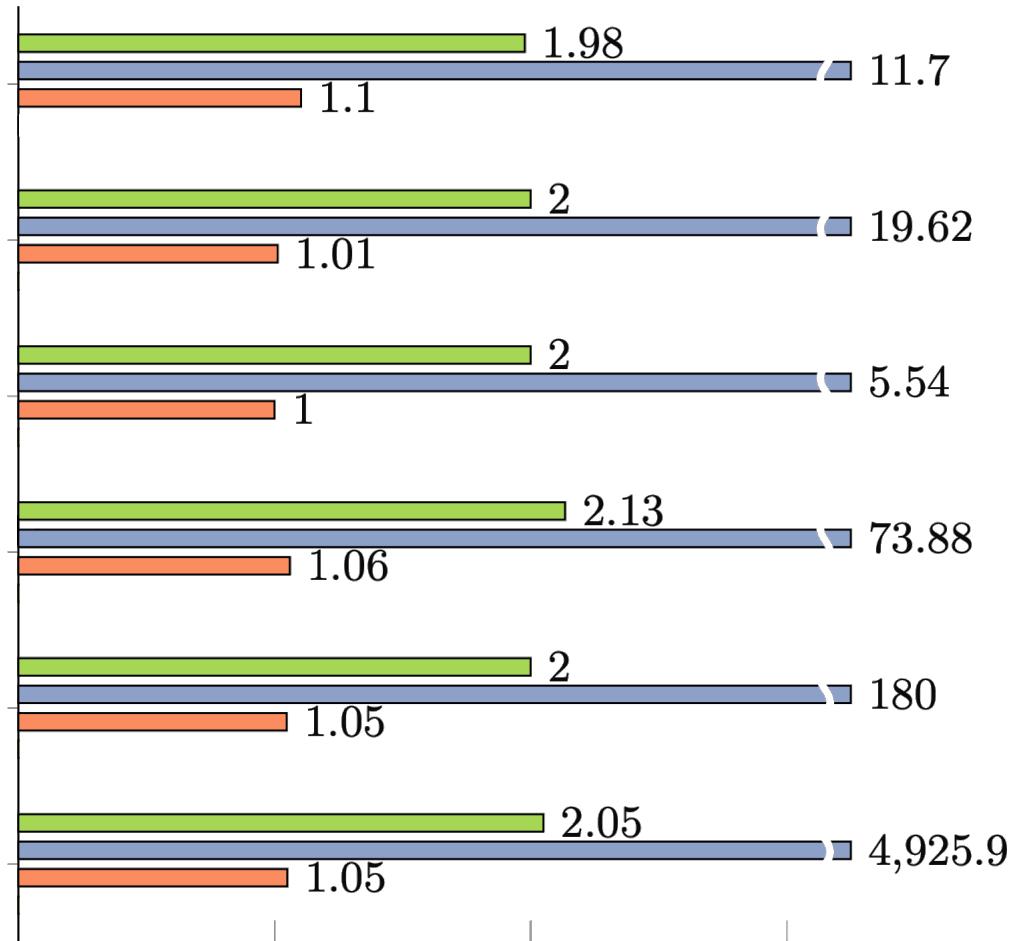
FOOT10D
(2.1 GB)

LUCY34D
(2.0 GB)

IA*

Simplex tree

Stellar tree



Encoding Simplicial Complexes

Top-based vs Operator-driven:

data	ω	contr. edges	timings			memory peak	
			check	contr.	tot	gen.	simpl.
CHICAGO	28	weak	9.15h	2.27m	9.19h	5.6	57.2K
		top	0.01s	0.02s	0.09s	7.6	—
		Skel.	0.00s	0.15s	0.15s	7.8	7.8
	56	weak	out-of-memory			6.2	—
		top	7.99K	0.04s	0.06s	0.23s	10.8
		Skel.	0.00s	0.71s	0.71s	14.1	14.1
ATHENS	63	weak	out-of-memory			11.6	—
		top	27.9K	0.08s	0.11s	0.38s	14.9
		Skel.	0.00s	0.74s	0.75s	26.4	26.8
	126	weak	out-of-memory			10.0	—
		top	31.2K	0.40s	0.49s	1.36s	25.9
		Skel.	0.01s	7.73s	7.74s	66.1	66.7
VISMAL	3.5	weak	34.3m	1.28m	40.4m	1.0K	2.0K
		top	4.23M	4.34m	0.89m	7.20m	2.0K
		Skel.	0.76m	3.34h	3.35h	8.0K	8.0K
	4.5	weak	killed after 25 hours			7.5K	—
		top	4.69M	2.89h	26.0m	3.32h	10.7K
		Skel.	killed after 25 hours			19.4K	—
LUCY	1.5	weak	killed after 25 hours			7.5K	—
		top	14.0M	11.9m	14.8m	32.0m	15.4K
		Skel.	23.19s	14.6h	14.6h	50.9K	52.1K

Encoding Simplicial Complexes

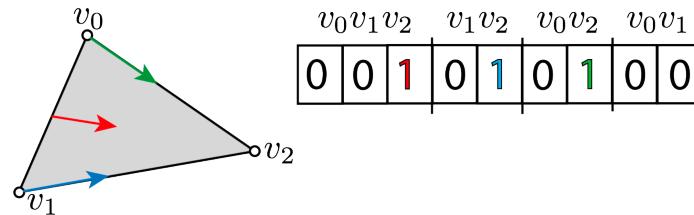
Possible Issues in Top-based Representations:

Top-based representations are promising data structures for encoding a simplicial complex K

but, how to ...

- ◆ *Store information associated to each simplex of K (e.g. labels, gradient, ...)?*

Attach information to the
top simplices only



- ◆ *Efficiently perform operators having explicitly stored a fraction of the entities of K?*

Re-define the algorithms performing the operators trying to extract
the lowest possible amount of non-explicitly stored entities

Bibliography

General References:

- ♦ **Books on TDA:**
 - ❖ A. J. Zomorodian. *Topology for computing*. Cambridge University Press, 2005.
 - ❖ H. Edelsbrunner, J. Harer. *Computational topology: an introduction*. American Mathematical Society, 2010.
 - ❖ R. W. Ghrist. *Elementary applied topology*. Seattle: Createspace, 2014.
- ♦ **Papers on TDA:**
 - ❖ G. Carlsson. *Topology and data*. Bulletin of the American Mathematical Society 46.2, pages 255-308, 2009.

Today's References:

- ♦ **Persistent Homology Computation:**
 - ❖ A. Zomorodian, G. Carlsson. *Computing persistent homology*. Discrete & Computational Geometry, 33.2, pages 249-274, 2005.
 - ❖ N. Otter, M.A. Porter, U. Tillmann, P. Grindrod, H.A. Harrington. *A roadmap for the computation of persistent homology*. EPJ Data Science, 6.1, 2017.

Bibliography

Today's References:

- ◆ **Data Structures for Arbitrary Simplicial Complexes:**
 - ❖ D. Canino, L. De Floriani, K. Weiss. **IA*: an adjacency-based representation for non-manifold simplicial shapes in arbitrary dimensions.** Computers & Graphics, 35.3, pages 747-753, 2011.
 - ❖ D. Attali, A. Lieutier, D. Salinas. **Efficient data structure for representing and simplifying simplicial complexes in high dimensions.** International Journal of Computational Geometry & Applications, 22.4, pages 279-303, 2012.
 - ❖ J.D. Boissonnat, C. Maria. **The simplex tree: An efficient data structure for general simplicial complexes.** Algorithmica, 70.3, pages 406-427, 2014.
 - ❖ R. Fellegara, K. Weiss, L. De Floriani. **The Stellar tree: a compact representation for simplicial complexes and beyond.** arXiv preprint:1707.02211, 2017.
 - ❖ U. Fugacci, F. Iuricich, L. De Floriani. **Computing discrete Morse complexes from simplicial complexes.** Graphical models, 103, 101023, 2019.
 - ❖ R. Fellegara, F. Iuricich, L. De Floriani, U. Fugacci. **Efficient Homology-Preserving Simplification of High-Dimensional Simplicial Shapes.** Computer Graphics Forum, 39.1, pages 244-259, 2020.