Fantastic barcode algorithms and where to find them

Barbara Giunti

Topology of Data in Rome, 15-16 September 2022

TU Graz

SCIENCE
PASSION
TECHNOLOGY

Matrices and interval spheres

$$\begin{bmatrix} 1 & & 1 & 1 \\ & 1 & 1 & \\ 1 & & 1 & \\ & 1 & & 1 \\ 1 & & & \\ & & 1 & 1 \end{bmatrix}$$

Motivation

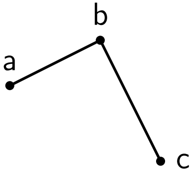
Motivation

http://www.zotero.org/groups/TDA-Applications

Boundary matrices

n-**simplex:** collection of $n + 1$ points

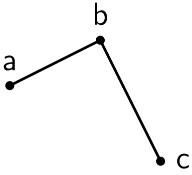
Boundary matrices



***n*-simplex:** collection of $n + 1$ points

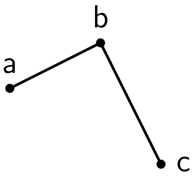
Simplicial complex: collection of simplices

Boundary matrices



n-simplex: collection of $n+1$ points
Simplicial complex: collection of simplices
Boundary of a n-simplex: all $(n-1)$-simplices without one of its points

Boundary matrices



	ab	bc
a	1	
b	1	1
c		1

***n*-simplex:** collection of $n + 1$ points
Simplicial complex: collection of simplices
Boundary of a *n*-simplex: all $(n - 1)$-simplices without one of its points
(n)-boundary matrix: boundary of all the (n)-simplices

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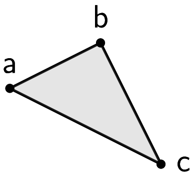

$$\begin{array}{c} \\ a \\ b \\ c \end{array} \begin{array}{c} \begin{array}{cc} ab & bc \end{array} \\ \begin{bmatrix} 1 & \\ 1 & 1 \\ & 1 \end{bmatrix} \end{array} \qquad \begin{array}{c} \\ ab \\ ac \\ bc \end{array} \begin{array}{c} abc \\ \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \end{array}$$

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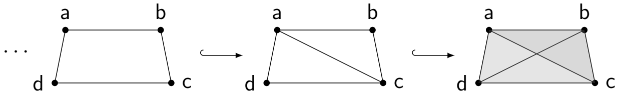
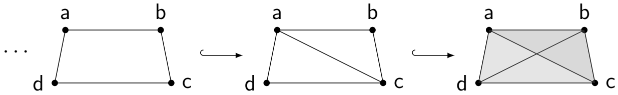
Filtrations



Filtration: nested sequence of simplicial complexes

Filtrations



	abc	acd	abd	bcd
bc	1			1
ad		1	1	
ab	1		1	
cd		1		1
ac	1	1		
bd			1	1

Filtration: nested sequence of simplicial complexes

(Total) boundary matrix: boundary matrix of the final complex

Chain complexes and homology

Chain complex: sequence of (boundary) maps of vector spaces such that the composition of two consecutive maps is 0

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degree n k

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degree $n+1$ k

$$\downarrow$$

degree n k   k

Chain complexes and homology

Chain complex: sequence of (boundary) maps of vector spaces such that the composition of two consecutive maps is 0

$$\begin{array}{lcc} \text{degree } n+1 & & \mathsf{k} \\ & & \downarrow \\ \text{degree } n & \mathsf{k} & \mathsf{k} \end{array}$$

Homology: the quotient of the kernel of a map by the image of the previous one

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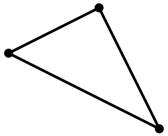

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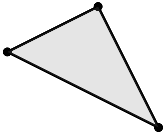

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Decomposition into interval spheres

Theorem (Chachólski, G., Landi, HHA 2020)

Every filtration decomposes uniquely into direct sum of interval spheres.

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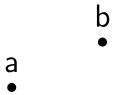

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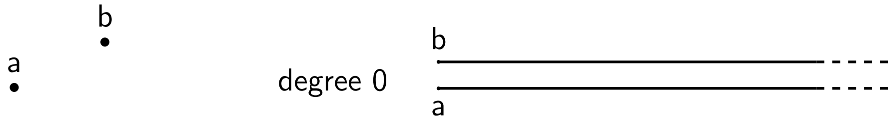

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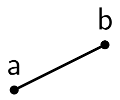

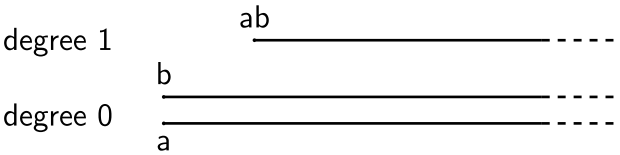

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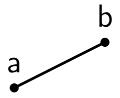

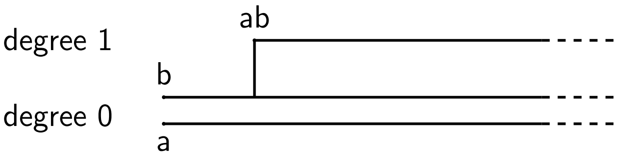

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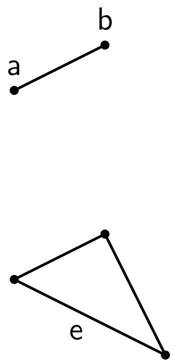

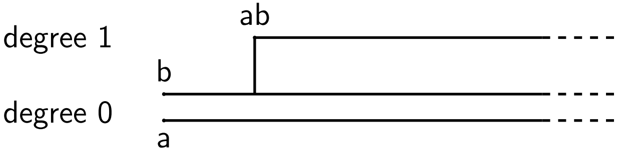

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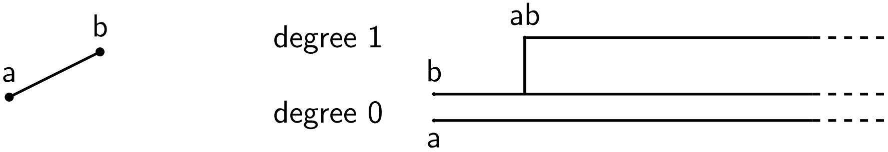

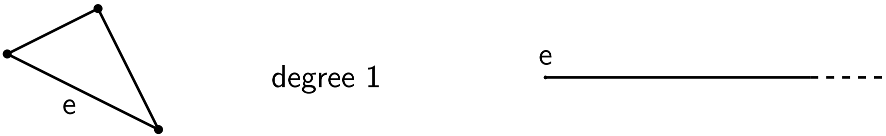

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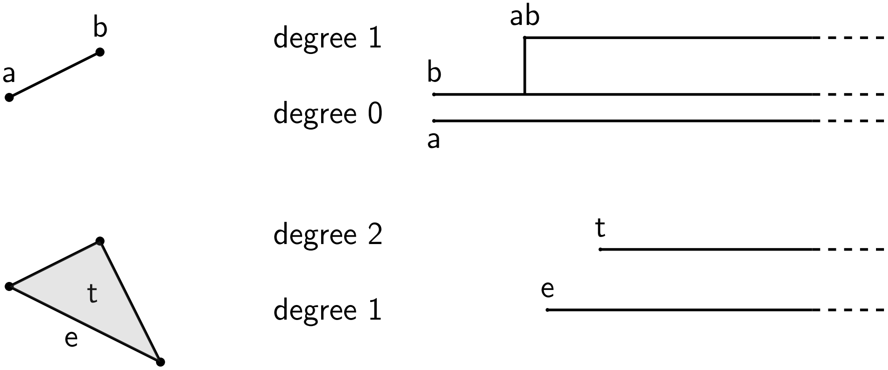

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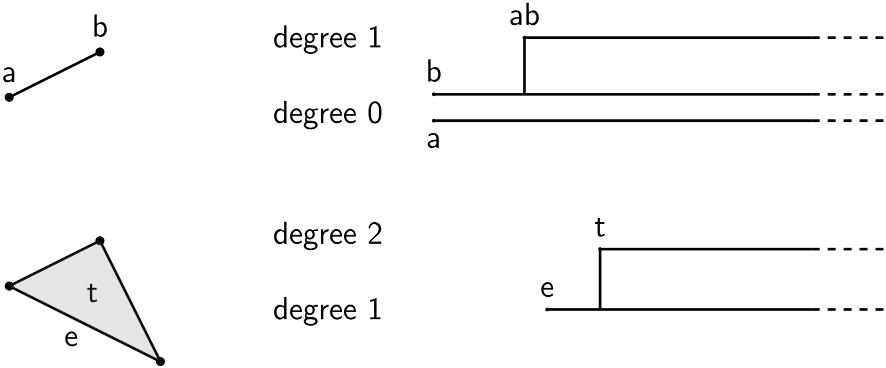

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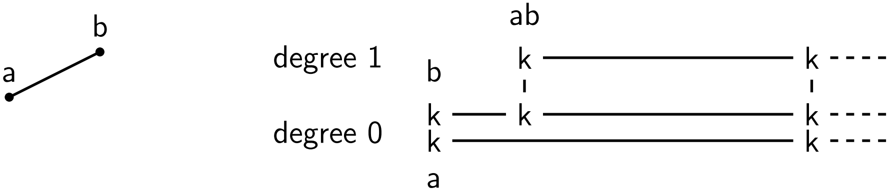

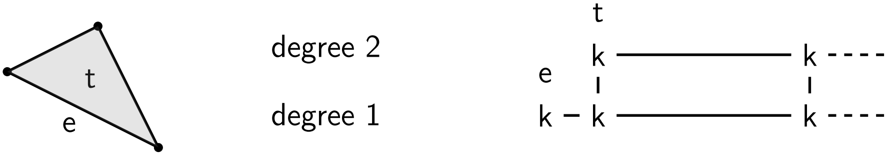

Pairing

	abc	**acd**	abd	bcd
bc				
ad				
ab				
cd				
ac				
bd				

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Two elements are paired if and only if the sum of the differences of the ranks is 1

Topological persistence and simplification, Edelsbrunner, Letscher, Zomorodian, *FOCS*, 2000

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Two elements are paired if and only if the sum of the differences of the ranks is 1

$\Longrightarrow$ Any reduction that preserves these ranks is legit

Topological persistence and simplification, Edelsbrunner, Letscher, Zomorodian, *FOCS*, 2000

Standard barcode algorithm

Pivot $low(j)$: index of lowest nonzero element of column j

Input: Boundary matrix D
Output: Reduced matrix R

$R = D$
for $j = 1, \ldots, \#$ *of simplices* **do**
  while $low(j) = low(i) \neq 0$ *for* $i < j$ **do**
    add column i to column j

Topological persistence and simplification, Edelsbrunner, Letscher, Zomorodian, *FOCS*, 2000

Example

$$
\left[\begin{array}{cccc|c|cccc}
* & * & * & * & * & * & * & * & * \\
\hline
 & & & 1 & & & & & \\
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\end{array}\right]
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Example

$$
\begin{bmatrix}
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$$

Standard barcode algorithm with clear

Input: Boundary matrix D
Output: Reduced matrix R

```
R = D
for j = 1, ..., # of simplices do
    while low(j) = low(i) ≠ 0 for i < j do
        add column i to column j
    if the column j is nonzero then
        Set column i to 0 for i = low(j)
```

Each interval sphere has two generators:

- If we find the “upper”, we can remove the “lower”
- If we find the “lower”, we can remove the “upper”

Persistent homology computation with a twist, Chen, Kerber, *EuroCG*, 2011

Standard barcode algorithm with clear

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$R = D$

for $j = 1, \dots, \#$ *of simplices* **do**

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Each interval sphere has two generators:

- If we find the "upper", we can remove the "lower" CLEAR
- If we find the "lower", we can remove the "upper" COMPRESS

Persistent homology computation with a twist, Chen, Kerber, *EuroCG*, 2011

Cohomology

The coboundary of a $(n-1)$-simplex s is the collection of all n-simplices that have s in their boundary.

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The anti-transpose of a boundary matrix is (almost) the coboundary matrix of the filtration and its pairing is in bijection with the pairing of the boundary matrix[1].

[1] Dualities in persistent (co)homology, de Silva, Morozov, Vejdemo-Johansson, *Inverse Problems*, 2011

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On some inputs, the standard barcode algorithm with clear is much more efficient on the coboundary than on the boundary matrix.

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On some inputs, the standard barcode algorithm with clear is much more efficient on the coboundary than on the boundary matrix. Nothing comparable happens for the compress optimisation.

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Row barcode algorithm

Pivot *left* (i): index of leftmost nonzero element of row i

```
Input: Boundary matrix D
Output: Reduced matrix R
R = D
for i = # of simplices, ..., 1 do
    while left(i) = left(j) ≠ 0 for j > i do
        add row j to row i
```

Tripartitions and bases of an ordered complex, Edelsbrunner, Ölsböck, *Discrete & Computational Geometry*, 2020

Row barcode algorithm with compress

Pivot $\mathit{left}(i)$: index of leftmost nonzero element of row i

Input: Boundary matrix D
Output: Reduced matrix R

$R = D$
for $i = \#$ *of simplices*$, \ldots, 1$ **do**
  while $\mathit{left}(i) = \mathit{left}(j) \neq 0$ *for* $j > i$ **do**
    add row j to row i
  if *the row* i *is nonzero* **then**
    Set row j to 0 for $j = \mathit{left}(i)$

Tripartitions and bases of an ordered complex, Edelsbrunner, Ölsböck, *Discrete & Computational Geometry*, 2020 / Notes on pivot pairings, G., *EuroCG*, 2021

Row barcode algorithm with compress

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If the filtration is full, then # of column operations with clear on the coboundary matrix is equal to # of row operations with the compress on the boundary matrix.

Implementations

- JavaPlex
- Dionysus
- Gudhi
- Phat
- Ripser
- Giotto-PH

A roadmap for the computation of persistent homology, Otter, Porter, Tillmann, Grindrod, Harrington, *EPJ Data Science*, 2017

Memory and data type

The choice of how to store the boundary matrix has big impact on the performances, as boundary matrices are initially sparse[1].

[1] PHAT-persistent homology algorithms toolbox, Bauer, Kerber, Reininghaus, Wagner, *Journal of symbolic computation*, 2017

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$\Longrightarrow$ use data types whose size is proportional to the number of nonzero entries in a column

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$\Longrightarrow$ use data types whose size is proportional to the number of nonzero entries in a column

- The cost of adding column i to column j is $\#i$;
- The **cost of a matrix reduction** is the added cost of all column additions;
- The **fill-up** of is the number of entries in the reduced matrix.

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\hline
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\end{array}\right]
$$

What if we try to keep the matrix sparse during the reduction?

Swap barcode algorithm

Input: Boundary matrix D

Output: Reduced matrix R

$R = D$

for $j = 1, \ldots, \#$ *of simplices* **do**

  while $low(j) = low(i) \neq 0$ *for* $i < j$ **do**

    if $\#j < \#i$ **then**

      swap j and i

    add column i to j

  if *column* j *is nonzero* **then**

    Set i to 0 for $i = low(j)$

Keeping it sparse: Computing Persistent Homology revised, Bauer, Bin Masood, G., Houry, Kerber, Rathod, *to appear*

Example

$$
\left[\begin{array}{cccc|c|cccc}
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Example

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Example

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\end{array}\right]
$$

Retrospective barcode algorithm

Input: Boundary matrix D
Output: Reduced boundary matrix R

$R = D$
for $j = 1, \ldots, \#$ *of simplices* **do**
    Remove the negative entries from j
    while *column* j *is nonzero and* $R_j^{low(i)} \neq 0$ *for* $i < j$ **do**
        add column i to column j
    for *every column* $i < j$ *with* $R_i^{low(j)} \neq 0$ **do**
        add column j to column i

Keeping it sparse: Computing Persistent Homology revised, Bauer, Bin Masood, G., Houry, Kerber, Rathod, *to appear*

Example

$$
\left[\begin{array}{cccc|c|cccc}
* & * & * & * & * & * & * & * & * \\
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Example

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\left[\begin{array}{cccc|c|cccc}
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Example

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Example

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\end{array}\right]
$$

Experiments

	Alpha shape			Lower star			Vietoris–Rips		
Algorithm	Fill-up	Col.ops	Bitflips	Fill-up	Col.ops	Bitflips	Fill-up	Col.ops	Bitflips
clear	6.35M	2.17M	62.30M	34.70M	4.90M	29.43M	14,975	5.35M	19.02M
clear*	6.90M	1.41M	84.09M	33.18M	4.91M	30.06M	0.51M	222	38,342
swap	1.56M	1.10M	7.37M	33.61M	4.83M	26.79M	14,887	5.19M	17.29M
swap*	2.04M	1.54M	20.72M	31.59M	4.86M	27.15M	0.51M	224	33,830
retro	1.14M	2.34M	19.93M	8.13M	21.51M	34.70M	5,049	0.48M	0.49M
retro*	7.94M	3.51M	40.87M	7.35M	21.94M	31.73M	6.41M	9,944	14.32M
mix	1.04M	15.04M	140.34M	10.85M	120.02M	239.17M	5,172	0.52M	0.57M
mix*	1.41M	14.03M	71.37M	10.79M	76.24M	150.20M	0.49M	0.22M	21.84M

Table: "M" stands for millions. The $*$ means via row barcode algorithm.

Experiments

	Alpha shape			Lower star			Vietoris–Rips			Shuffled		
Algorithm	40K	80K	160K	Tooth	Lobster	Skull	104	297	445	50	75	100
clear	*6.5	*18.6	*49.8	2.0	25.8	23.9	*0.0	*0.1	*0.1	*0.1	*1.3	*11.2
swap	*9.8	*28.2	*74.2	2.4	38.6	25.4	*0.0	*0.1	*0.2	0.1	0.6	2.9
retro	4.3	11.8	30.9	*4.9	*29.0	*61.6	0.1	1.4	7.2	0.0	0.1	0.3

Table: Best running times (in seconds) on various data sets. The $*$ means via row barcode algorithm.

Experiments

	List	Vector	Set	Heap	P-Heap	P-Set	P-Full	P-Bit-Tree
clear	58.3	1.9	7.9	7.1	6.5	7.5	2.2	**0.9**
clear*	144.6	2.8	11.9	9.5	8.9	9.8	3.2	0.9
swap	45.9	1.2	1.1	68.8	63.7	1.1	**0.5**	27.7
swap*	+5m	3.0	4.0	275.6	213.6	4.1	1.6	122.8
retro	2.8	**0.6**	2.9	6.5	6.3	9.4	4.6	3.3
retro*	72.7	2.6	20.3	128.0	167.5	182.3	103.8	54.6
mix	40.1	**4.0**	17.7	44.5	38.0	14.5	6.5	22.1
mix*	+5m	14.0	15.5	+5m	+5m	12.5	6.5	268.2

Table: Alpha filtration on 10000 points on a torus. All timings are in seconds but for the timeout (minutes). The $*$ means via row barcode algorithm.

Step columns and critical pivots

A **clique filtration** is a filtration where the n-simplices are added as soon as their boundary $(n-1)$-simplices are added.

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A **step column** is a column that is not modified during the reduction.

	abc	acd	abd	bcd
bc	1			1
ad		1	1	
ab	1		1	
cd		1		1
ac	1	1		
bd			1	1

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	abc	acd	abd	bcd
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ad		1	1	
ab	1		1	
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bd			1	1

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ab	1	1	1	
cd		1		
ac	1			
bd			1	

Lemma (G., Houry, Kerber, *ISSAC*, 2022)

In a clique filtration, there is an critical pivot if and only if at the corresponding simplex is a "lower" generator of a new interval sphere.

Average complexity

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The cost of a matrix reduction is bounded by $\#$ of columns $\times$ the fill-up of the reduced matrix.

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For every random clique filtration model for which we can bound the probability of obtaining a new interval sphere, we have a bound on the average complexity of the barcode algorithm.

Average complexity

Theorem (G., Houry, Kerber, *ISSAC*, 2022)

Let R be the reduced 1-boundary matrix of a Vietoris–Rips filtration. Then $\mathbb{E}[\textit{fill-up of } R] = O(n^2 \log^2 n)$ and $\mathbb{E}[\textit{cost of matrix reduction}] = O(n^5 \log^2 n)$.

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Let R be the reduced 1-boundary matrix of an Erdős–Rényi filtration. Then $\mathbb{E}[\text{fill-up of } R] = O(n^3 \log n)$ and $\mathbb{E}[\text{cost of matrix reduction}] = O(n^6 \log n)$.

Average complexity

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Let R be the reduced 1-boundary matrix of a Vietoris–Rips filtration. Then $\mathbb{E}[\text{fill-up of } R] = O(n^2 \log^2 n)$ and $\mathbb{E}[\text{cost of matrix reduction}] = O(n^5 \log^2 n)$. Let R be the reduced 1-boundary matrix of an Erdős–Rényi filtration. Then $\mathbb{E}[\text{fill-up of } R] = O(n^3 \log n)$ and $\mathbb{E}[\text{cost of matrix reduction}] = O(n^6 \log n)$.

The worst-case complexities are, respectively, $O(n^4)$ and $O(n^7)$, and they are realized for the Erdős–Rényi filtration.

Take home

- The pairs links the matrices (combinatorial) to the barcode (homological/geometrical)
- Any reduction that maintains the pairs is valid
- Things can go (sort of) bad but they usually don't

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Thank you for your attention!