A Space and Time Efficient Implementation for Computing Persistent Homology

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1 Introduction

Background

Abstract Simplicial Complex.

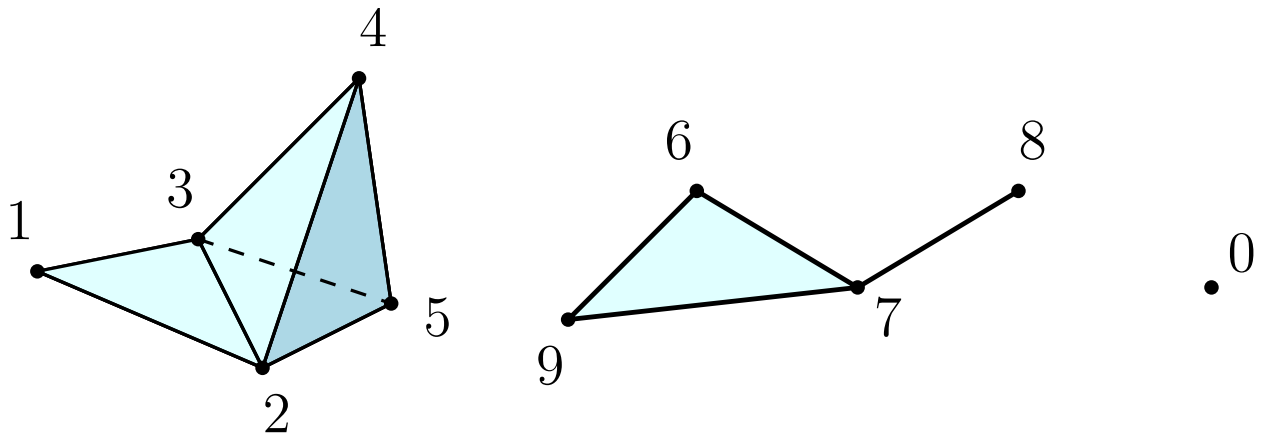
Given a set $V = \{1 \cdots n\}$ of vertices, an **abstract simplicial complex** $\mathcal{K}$ on V is a family of subsets of vertices s.t.:

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

Such σ is called a simplex

Dimension of a simplex σ: $\dim(\sigma) = |\sigma| - 1$

Dimension of the simplicial complex $\mathcal{K}$: $\dim(\mathcal{K}) = \max_{\sigma \in \mathcal{K}} \dim(\sigma)$.



Really Short Introduction to Persistent Homology with $\mathbb{Z}_2$ Coefficients

Given a simplicial complex $\mathcal{K}$, $\mathcal{K}^p$ the p-dimensional simplices:

$C_p = 2^{\mathcal{K}^p}$

$$\begin{array}{lccl} \partial_p : & C_p & \rightarrow & C_{p-1} \\ & \sigma = \{v_0, \cdots, v_p\} & \rightarrow & \partial\sigma = \sum_{i=0\cdots p} \{v_0, \cdots, \widehat{v_i}, \cdots, v_p\} \\ & \partial_p \partial_{p+1} = 0 & & \end{array}$$

$$\left\{ \begin{array}{rcl} Ker(\partial_p) & = & Z_p \\ Im(\partial_{p+1}) & = & B_p \end{array} \right. \qquad \begin{array}{l} \partial_p \partial_{p+1} = 0 \Rightarrow B_p \subseteq Z_p \\ H_p = Z_p / B_p \end{array}$$

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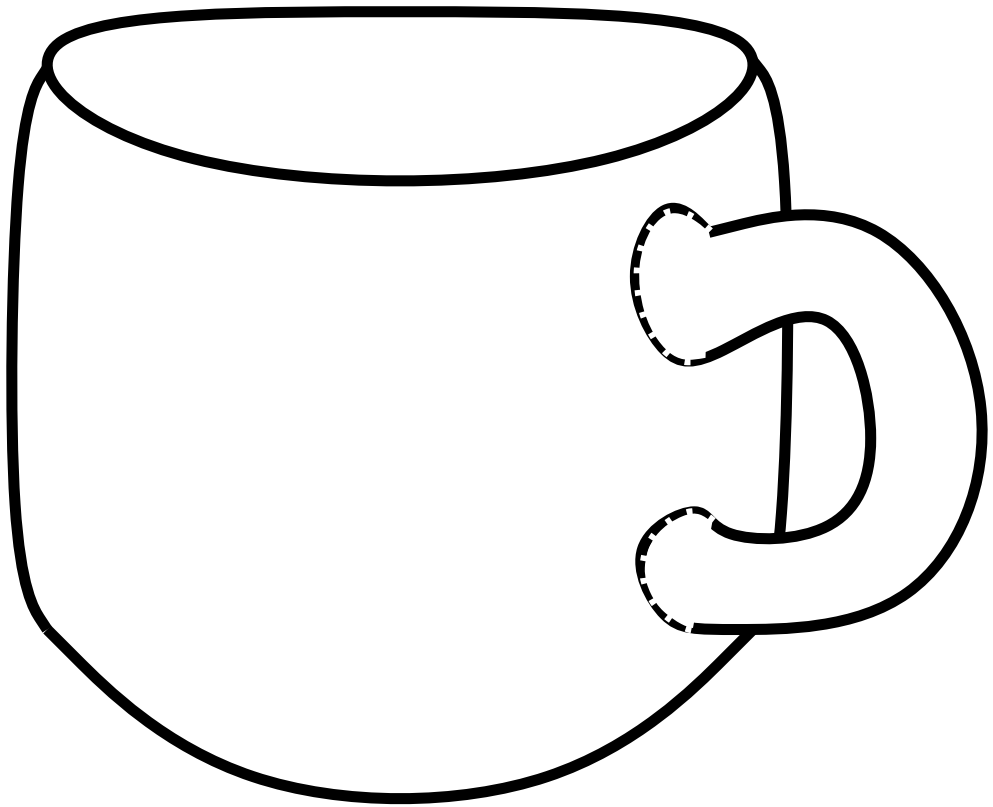

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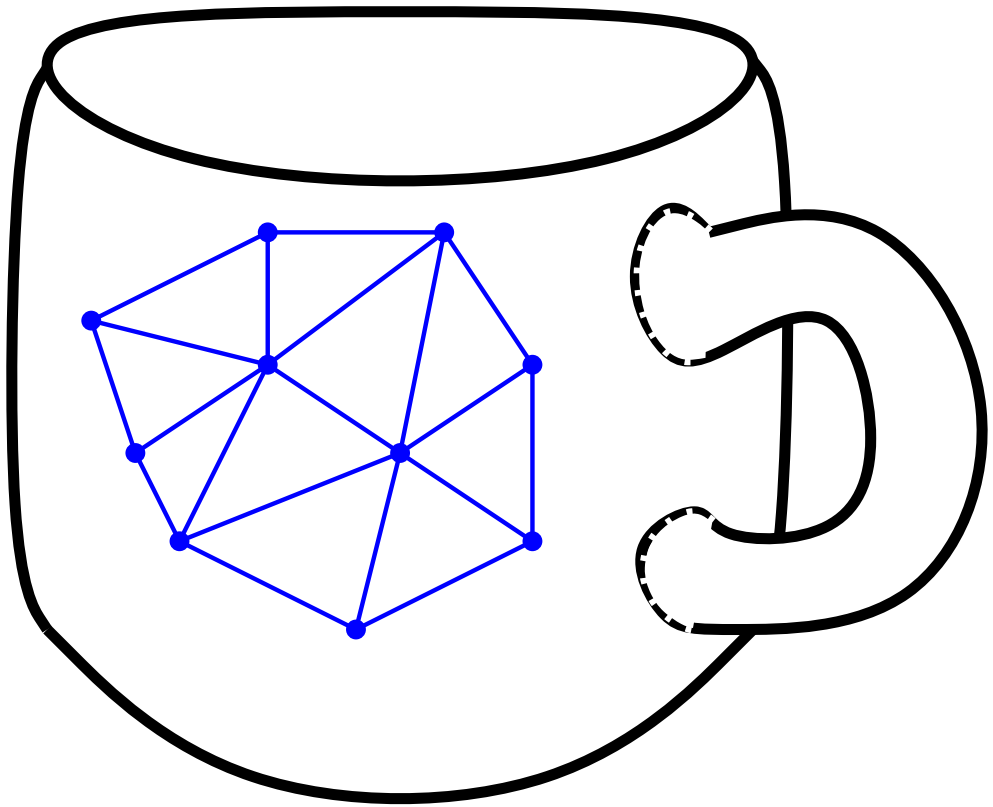

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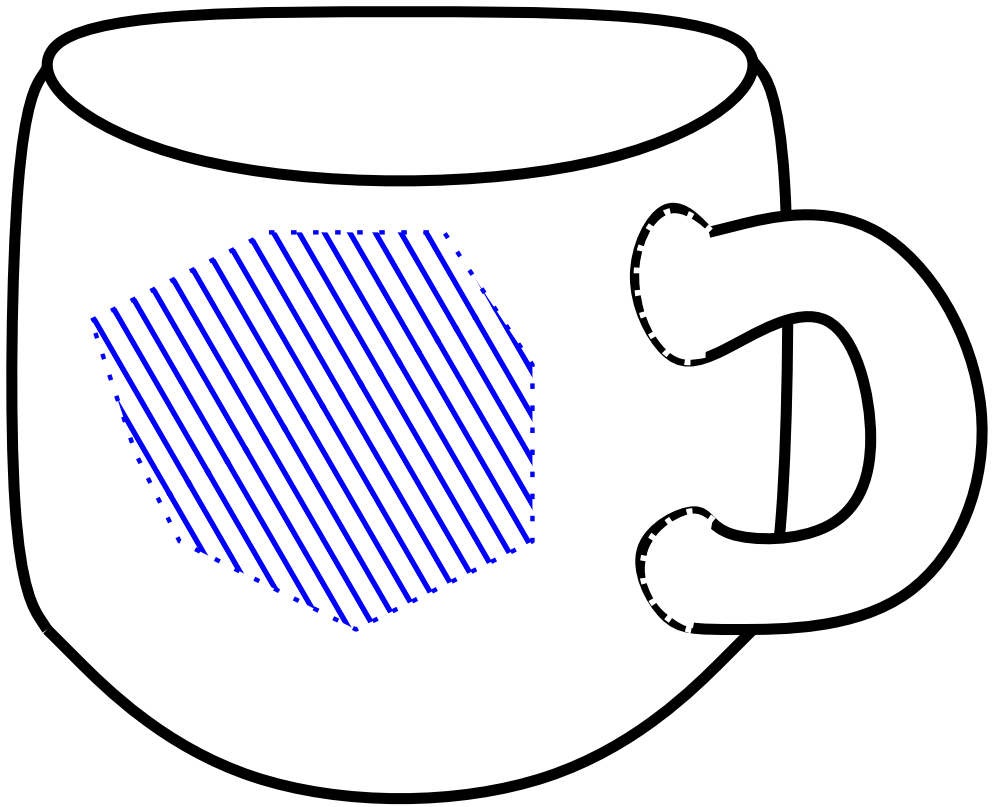

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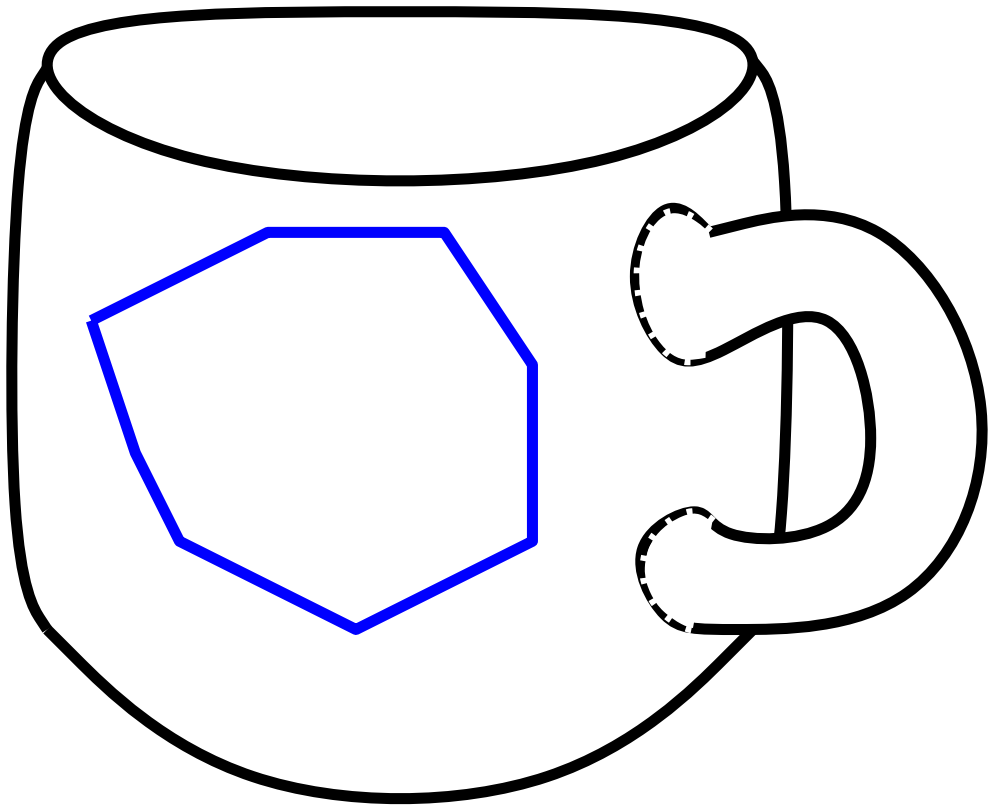

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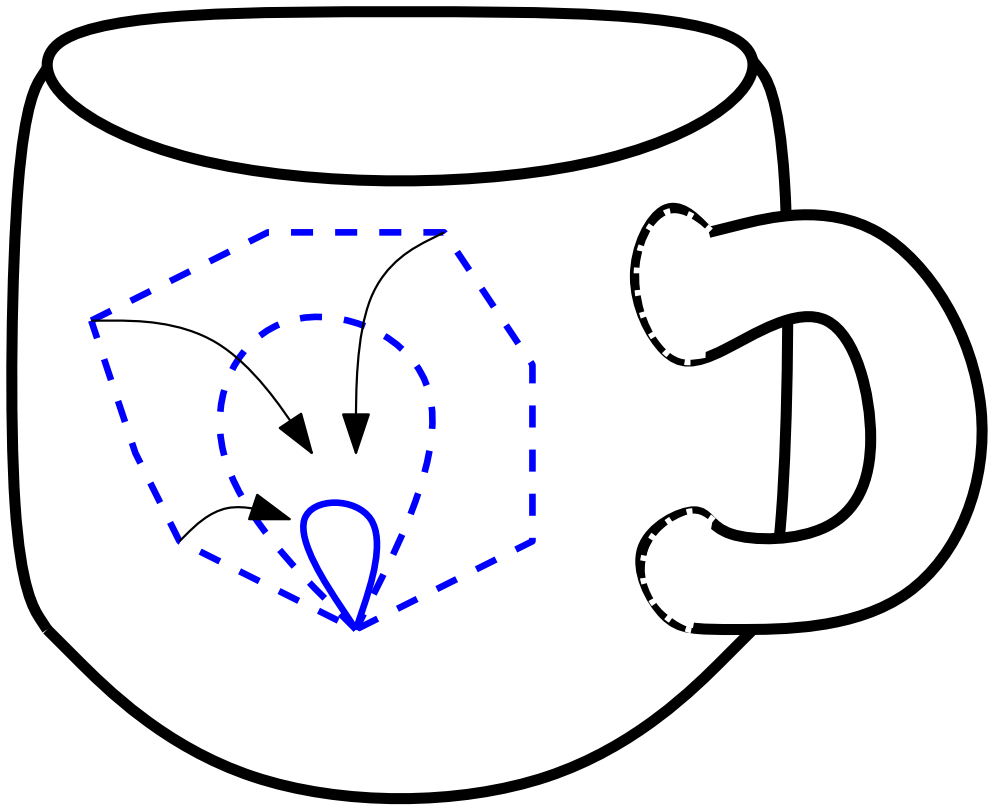

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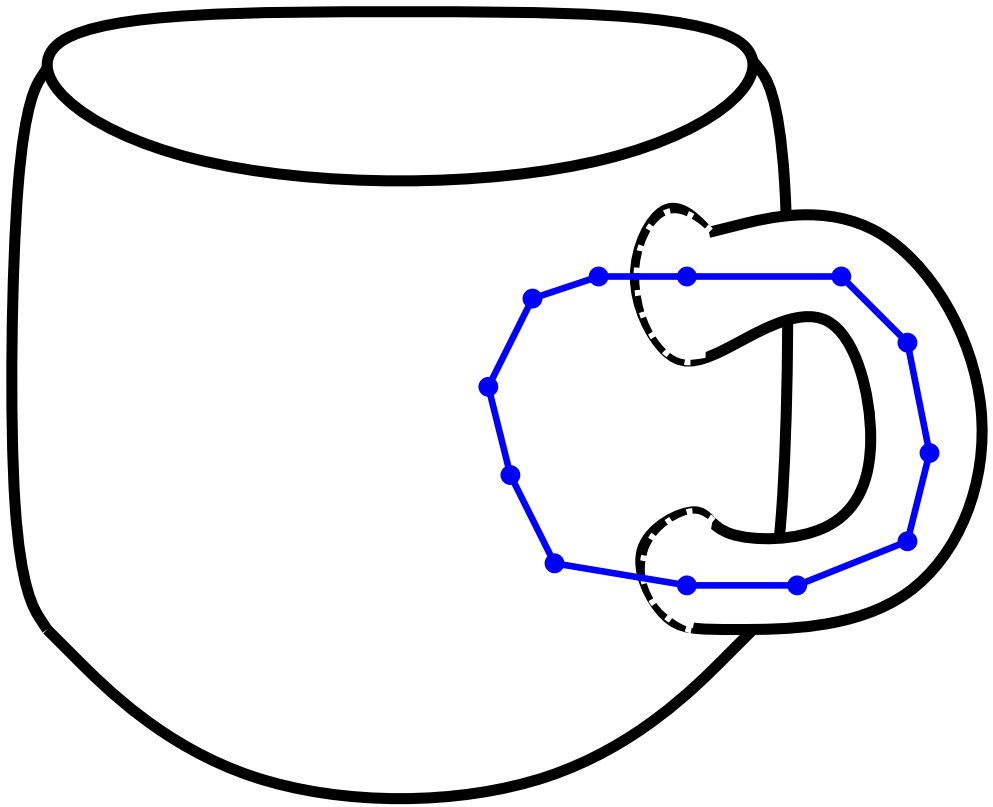
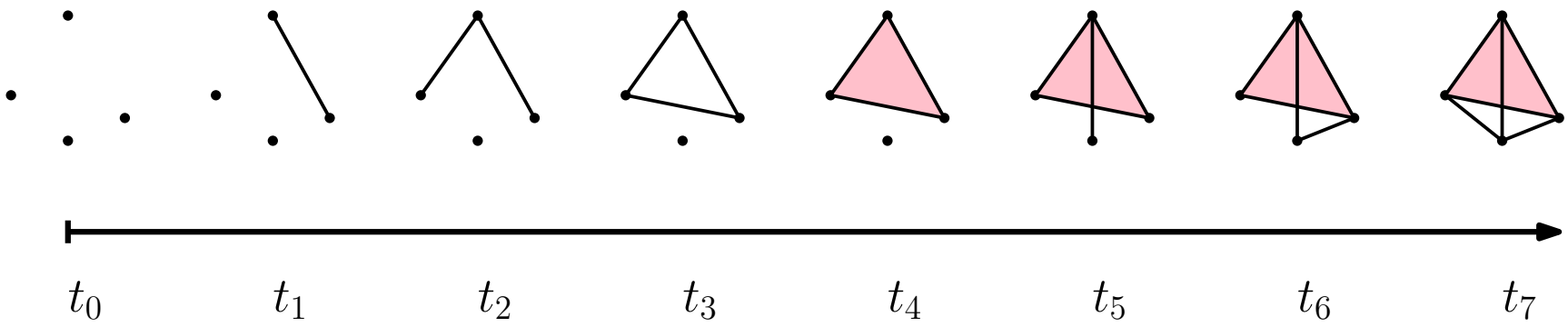


Filtration of a Simplicial Complex

A *filtration* of a simplicial complex $\mathcal{K}$ is defined by an indexed family of simplicial complexes $(\mathcal{K}_{t_i})_{i=0\cdots n}$ such that:

$$\emptyset = \mathcal{K}_{t_0} \subset \mathcal{K}_{t_1} \subset \cdots \subset \mathcal{K}_{t_{n-1}} \subset \mathcal{K}_{t_n} = \mathcal{K}$$

We can attach to each face of $\mathcal{K}$ a *time of appearance* t_i.



Incremental Algorithm: $\sigma = \mathcal{K}_i \setminus \mathcal{K}_{i-1}, \dim(\sigma) = p$
If σ belongs to a p-cycle **then** $\beta_p + +$
else $\beta_{p-1} - -$

Persistence Diagram

Incremental Algorithm: $\sigma = \mathcal{K}_i \setminus \mathcal{K}_{i-1}, \dim(\sigma) = p$
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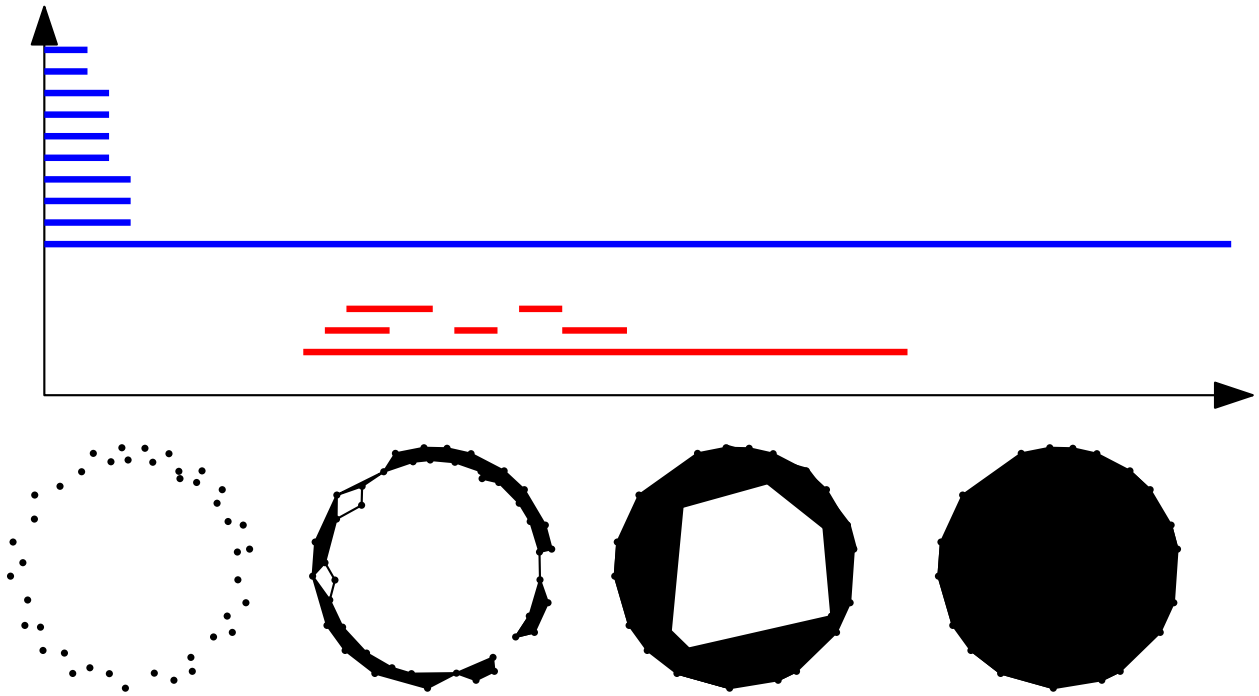


Implementation for Computing Persistent Homology

Focus on simplices:

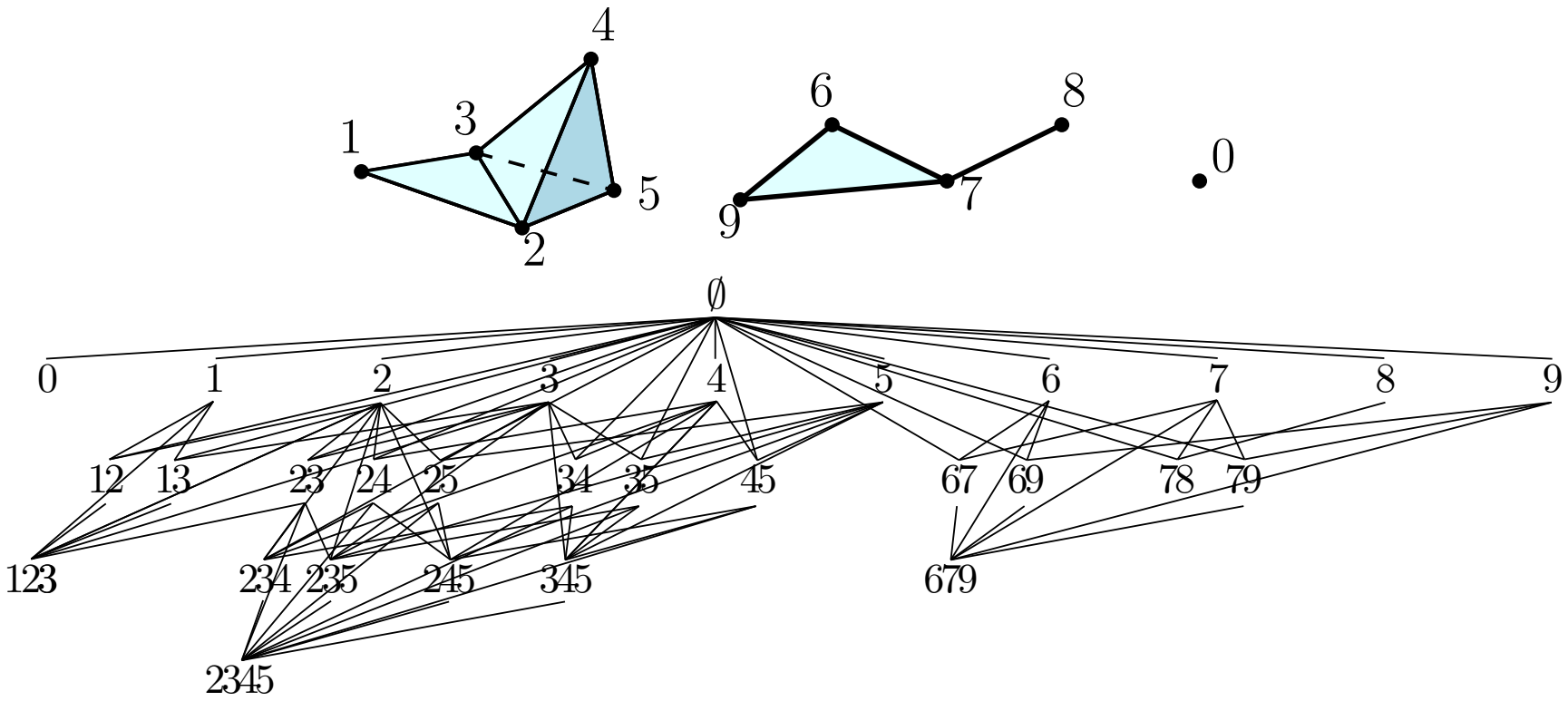
1. Represent the filtered simplicial complex:
   - Represent the simplices and their time of appearance
   - Retrieve incidence relation (compute $\partial\sigma$)
2. Attach topological information to simplices
   - Check if a new simplex is in a cycle or not
   - Update the topological information under insertion of a simplex
3. Interface the two structures

2
The Simplex Tree
[Boissonnat, M. '12]

an Efficient Data Structure for General Simplicial Complexes

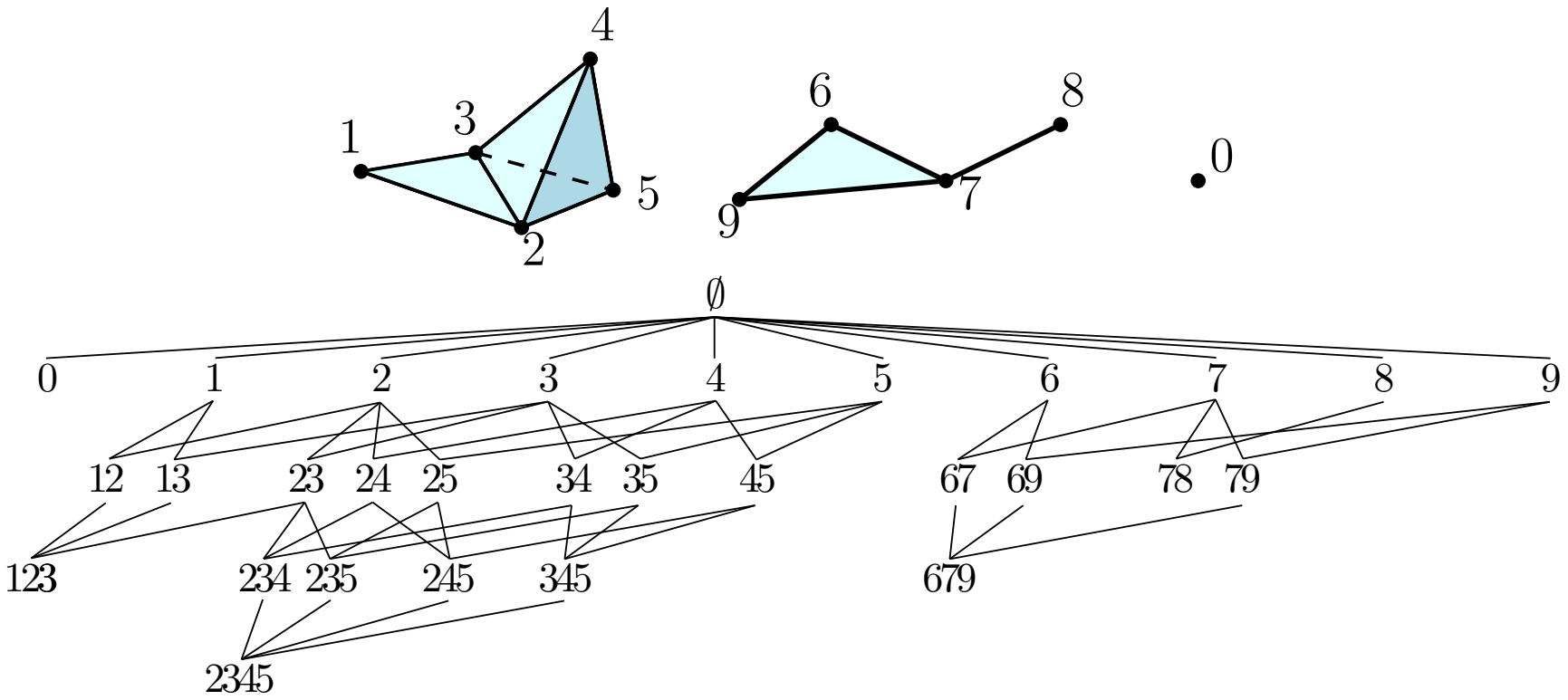
The Simplex Tree

A simplicial complex is a partially ordered set with regard to inclusion. All the incidences are represented in the following:



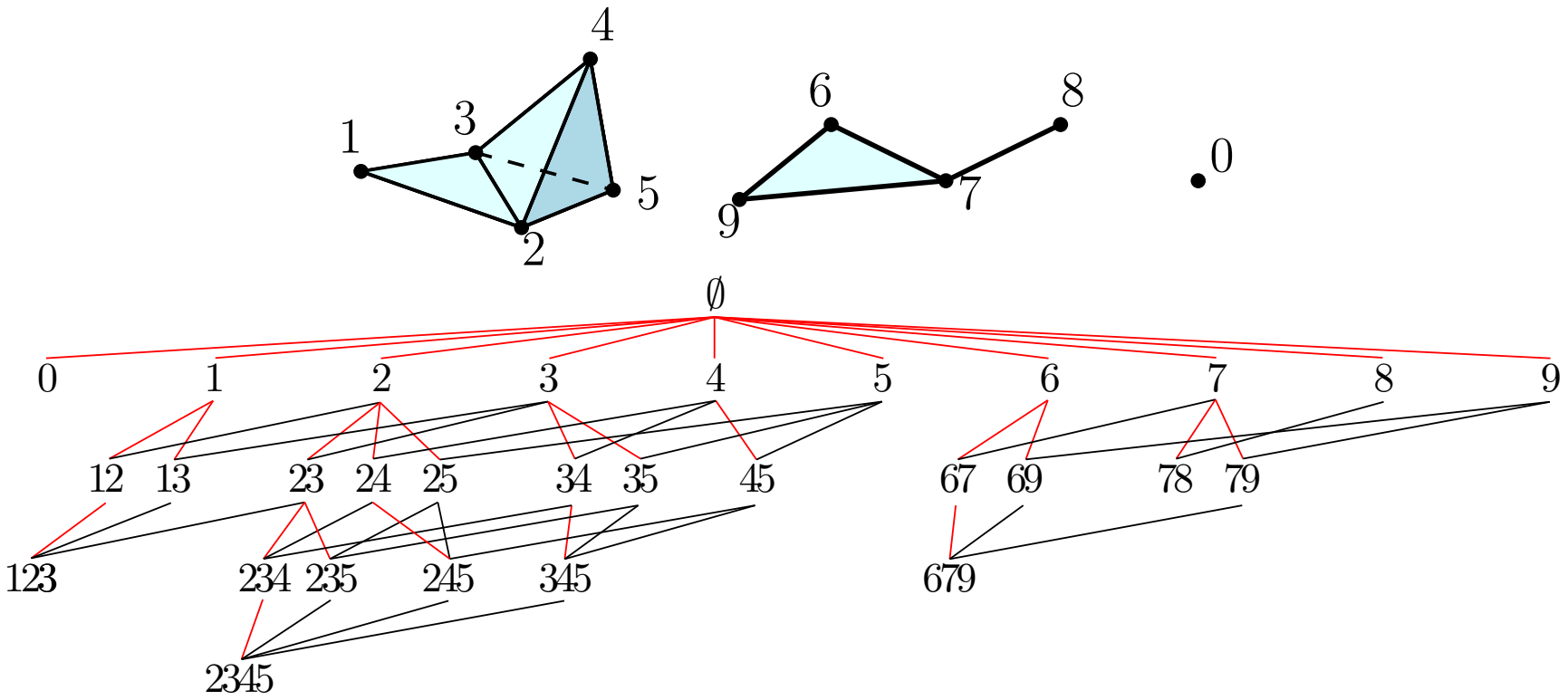
The Simplex Tree

Only incidences from an element to the smallest bigger elements are represented in the Hasse diagram:



The Simplex Tree

We select a specific spanning tree of the Hasse diagram. The choosen incidences respect also the lexicographic order:



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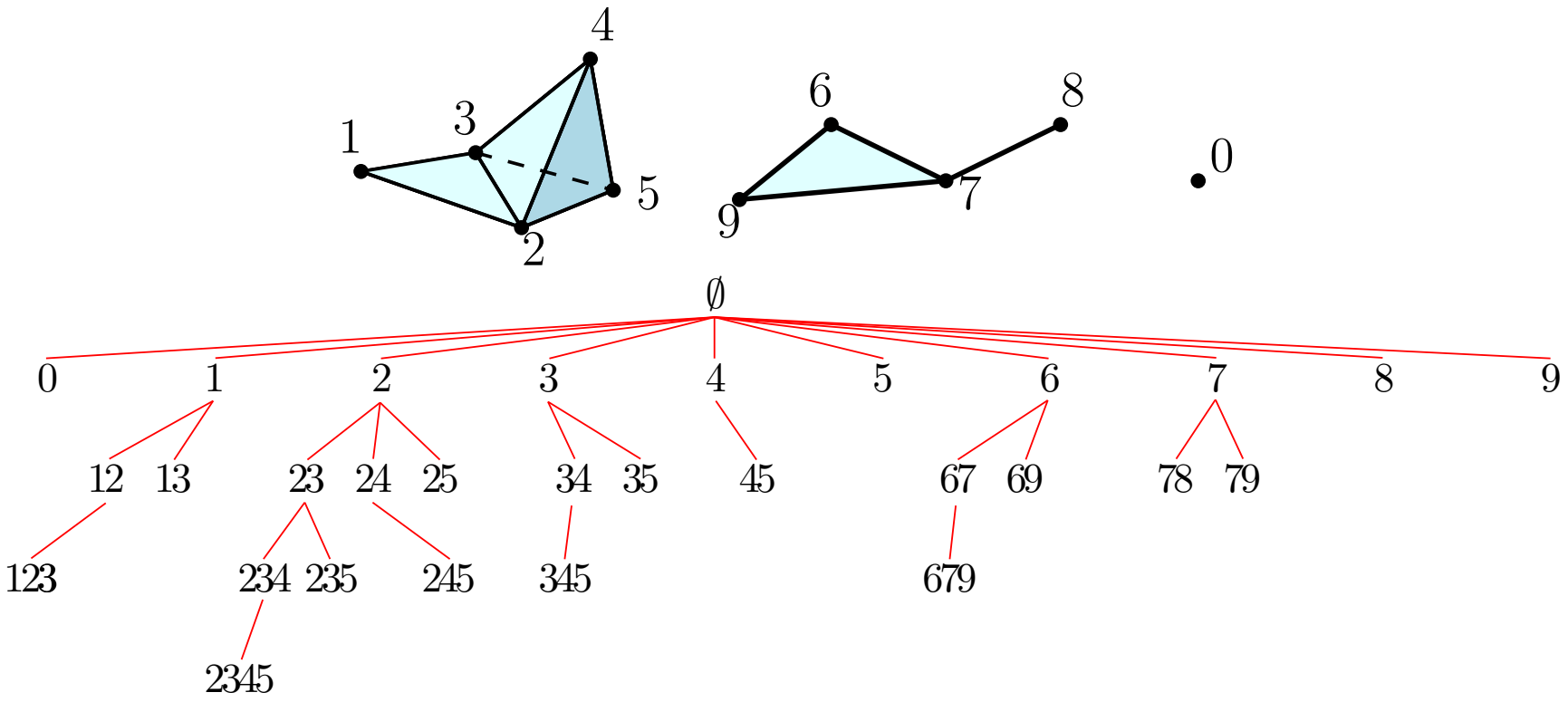
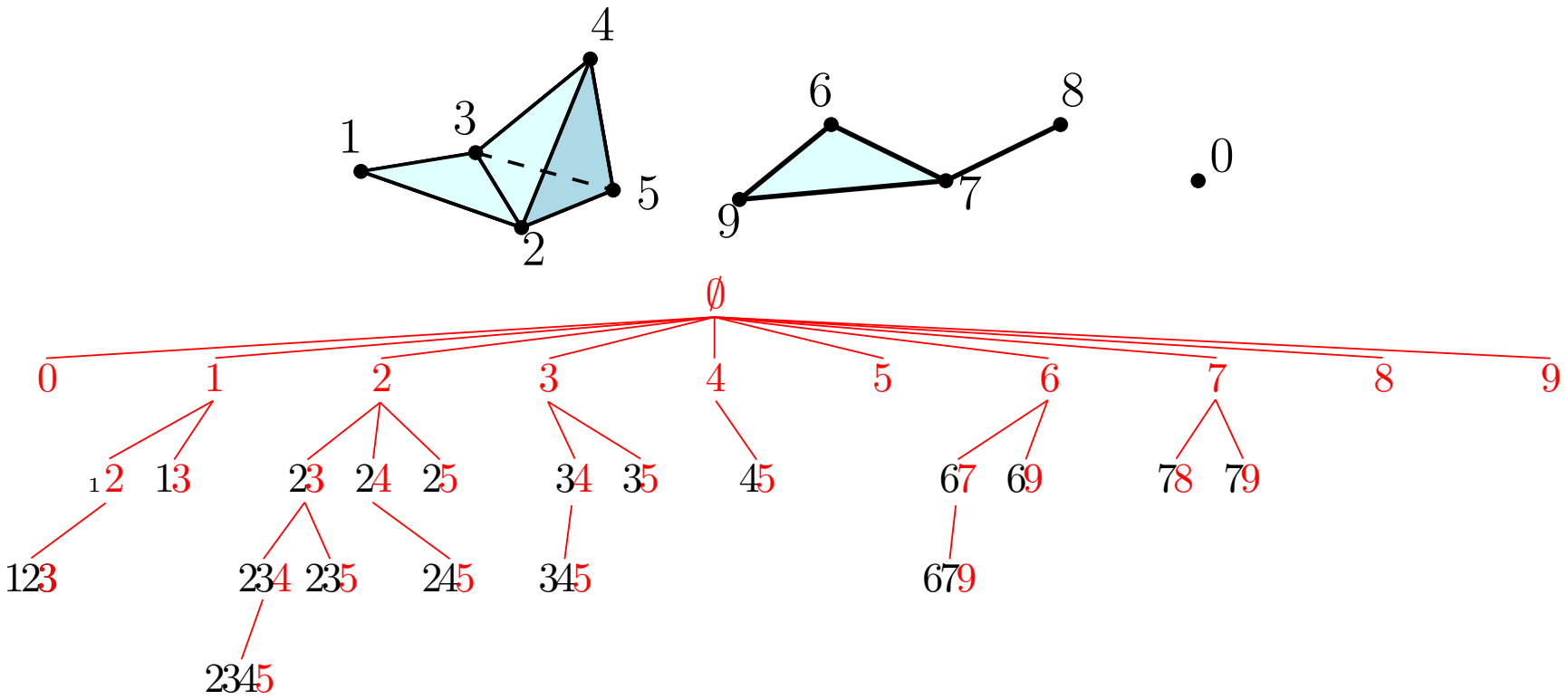


The Simplex Tree

We keep only the biggest vertex in each simplex. The vertices of a simplex are encountered in the path from the root to its node:



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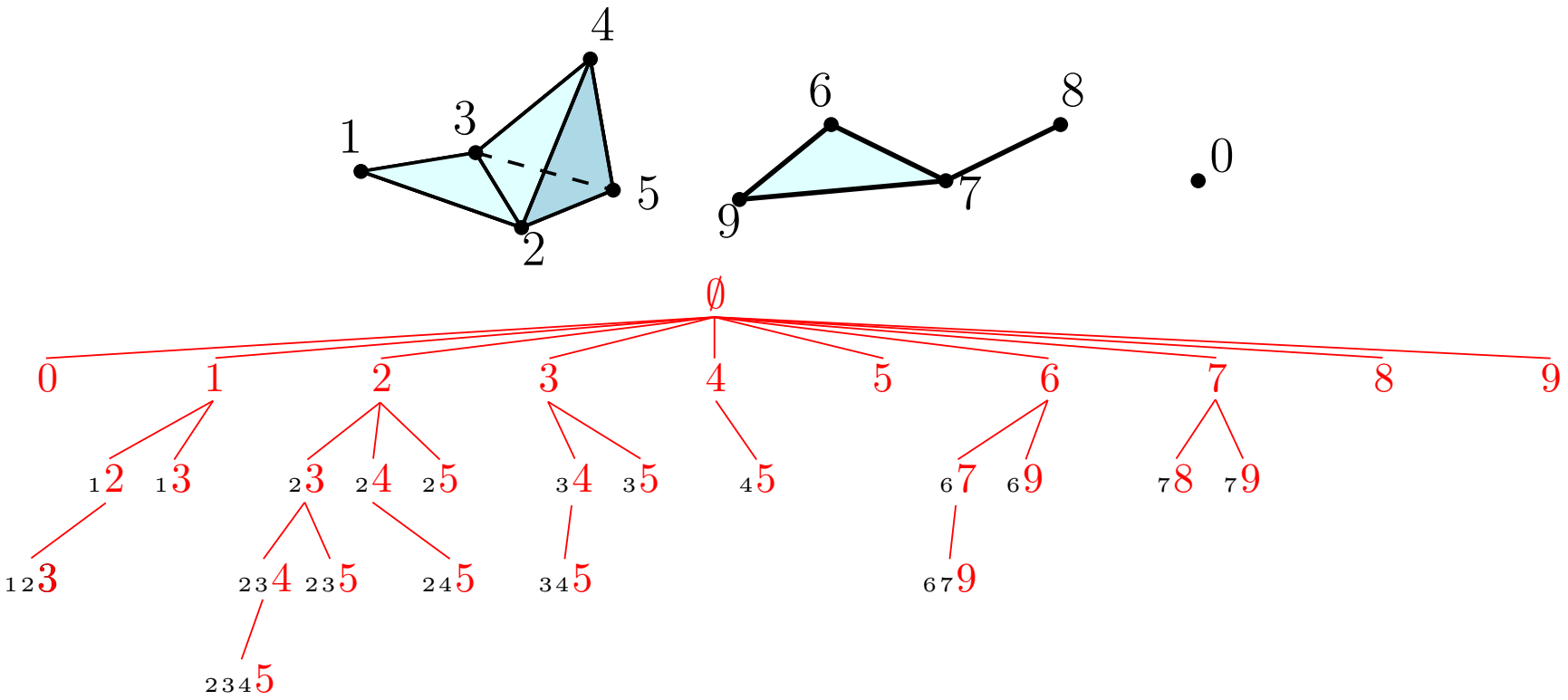
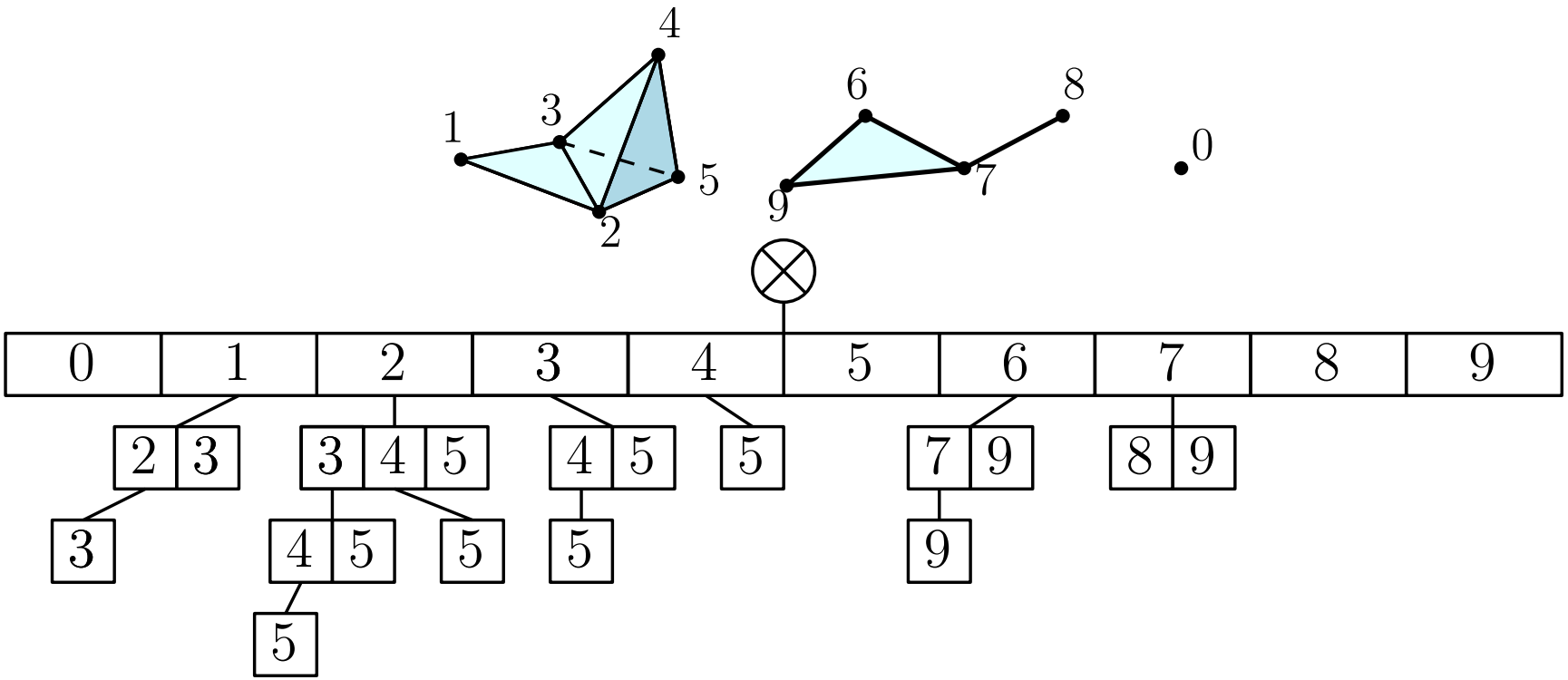


The Simplex Tree

[Boissonnat, M. '12]

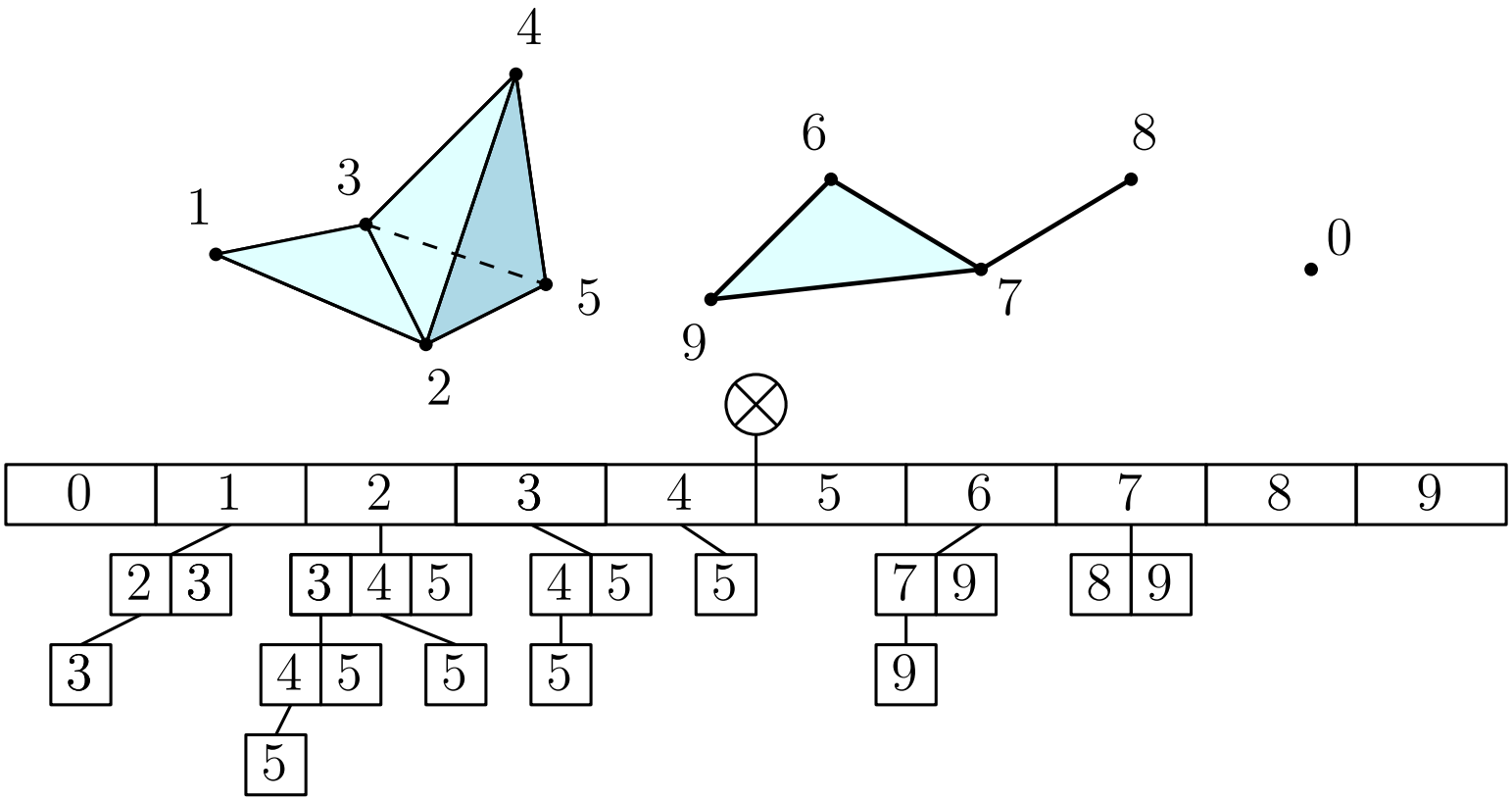
We call this structure a *Simplex Tree*.

Memory complexity: $O(1)$ per simplex.



The Simplex Tree

EQUIVALENTLY: to each simplex $\sigma \in \mathcal{K}$ we associate the ordered list of its vertices, and store it in a *trie*.

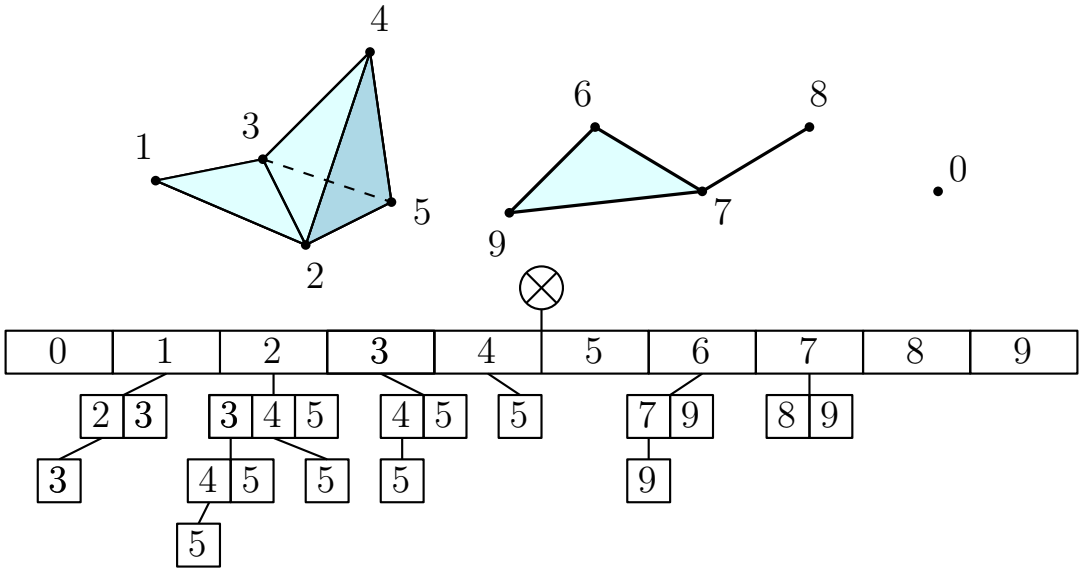


The Simplex Tree

Memory complexity: $O(1)$ per simplex.

Some properties:

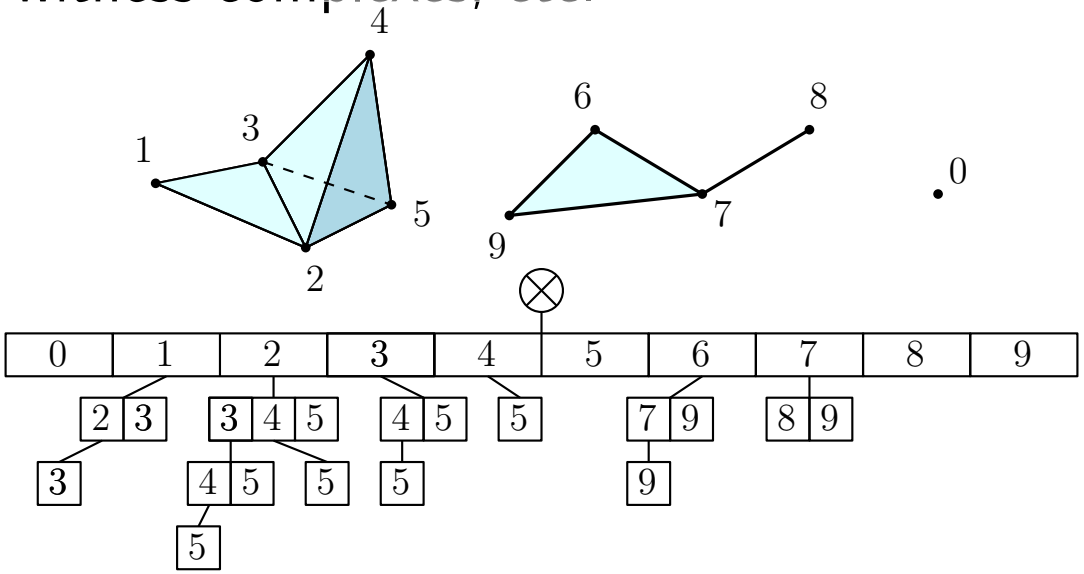
Simplex Tree		Simplicial Complex
#nodes	$=$	$\#\mathcal{K}$
depth	$=$	$\dim(\mathcal{K})+1$
#children(σ)	$\leq$	$\deg(\sigma)$



Simplex tree: Atomic operations

The Simplex Tree allows to compute efficiently:

- **Look-up/Insertion/Deletion** of a simplex
- The **facets** and **subfaces** of a simplex
- The **cofaces** of a simplex
- **Edge contractions**
- **Elementary collapses**
- **Fast construction** of Flag complexes, witness complexes, relaxed witness complexes, etc.



Facets/Boundary Computation

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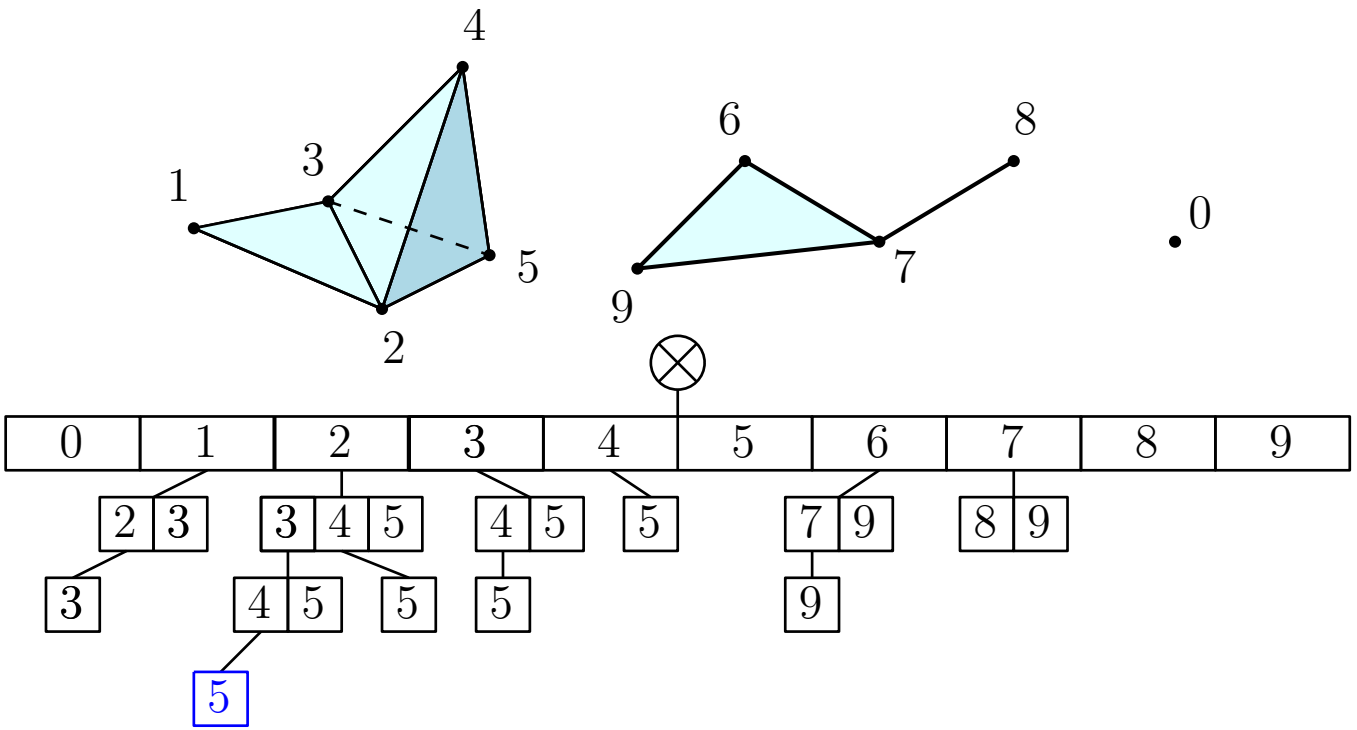
Given a simplex σ we find its $|\sigma|$ codimension 1 subfaces.



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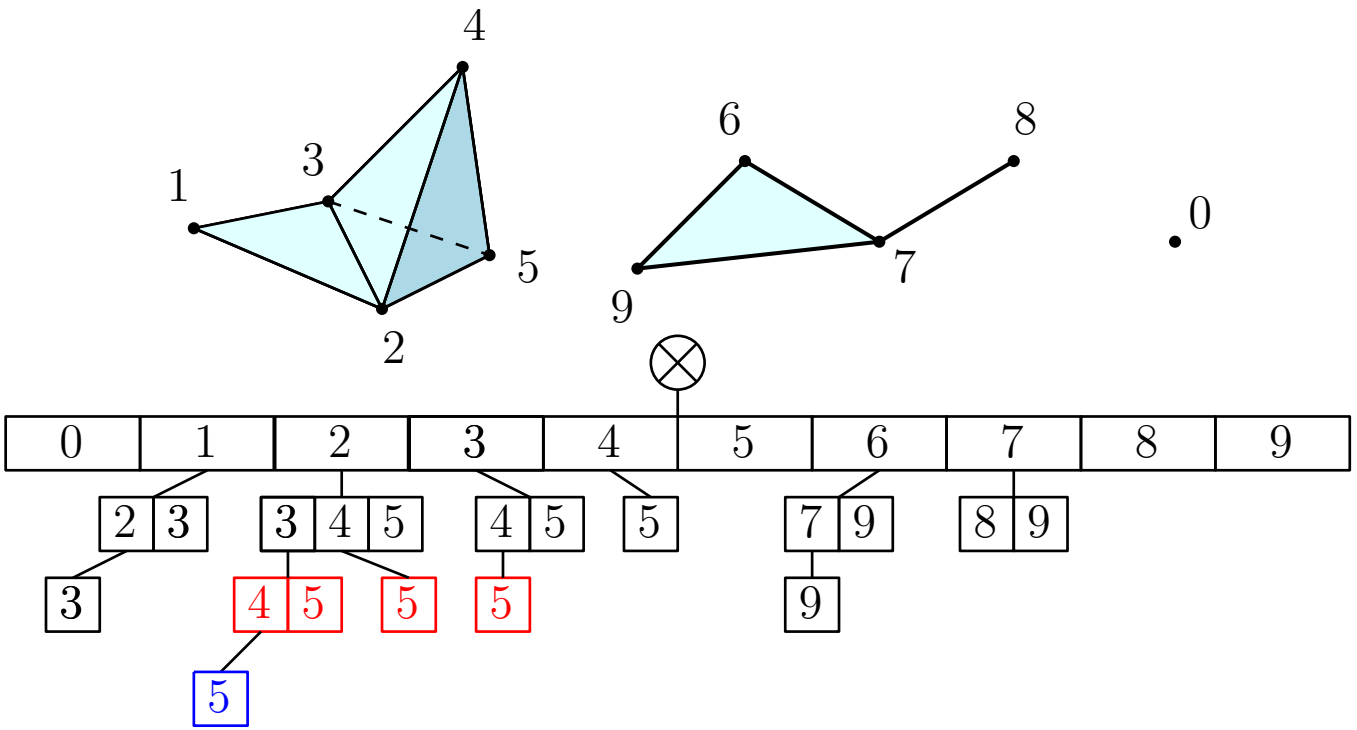

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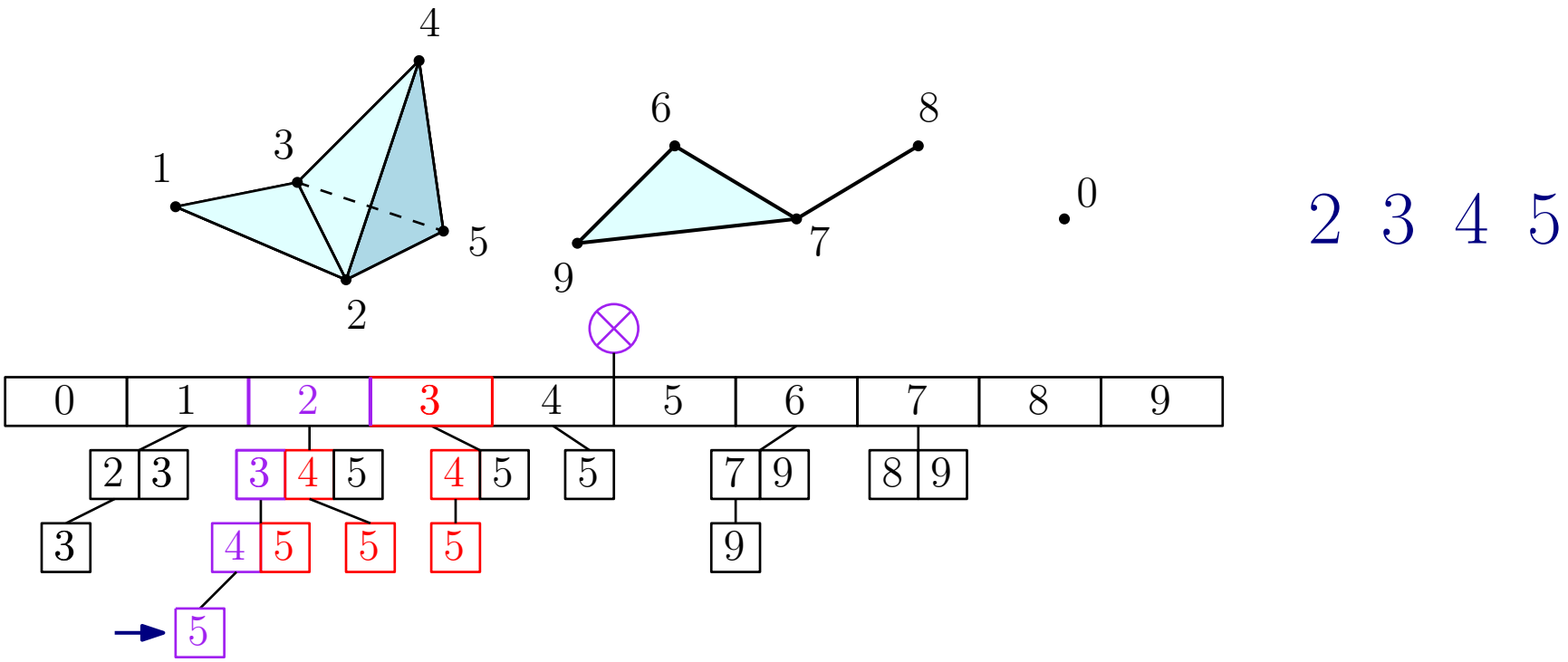

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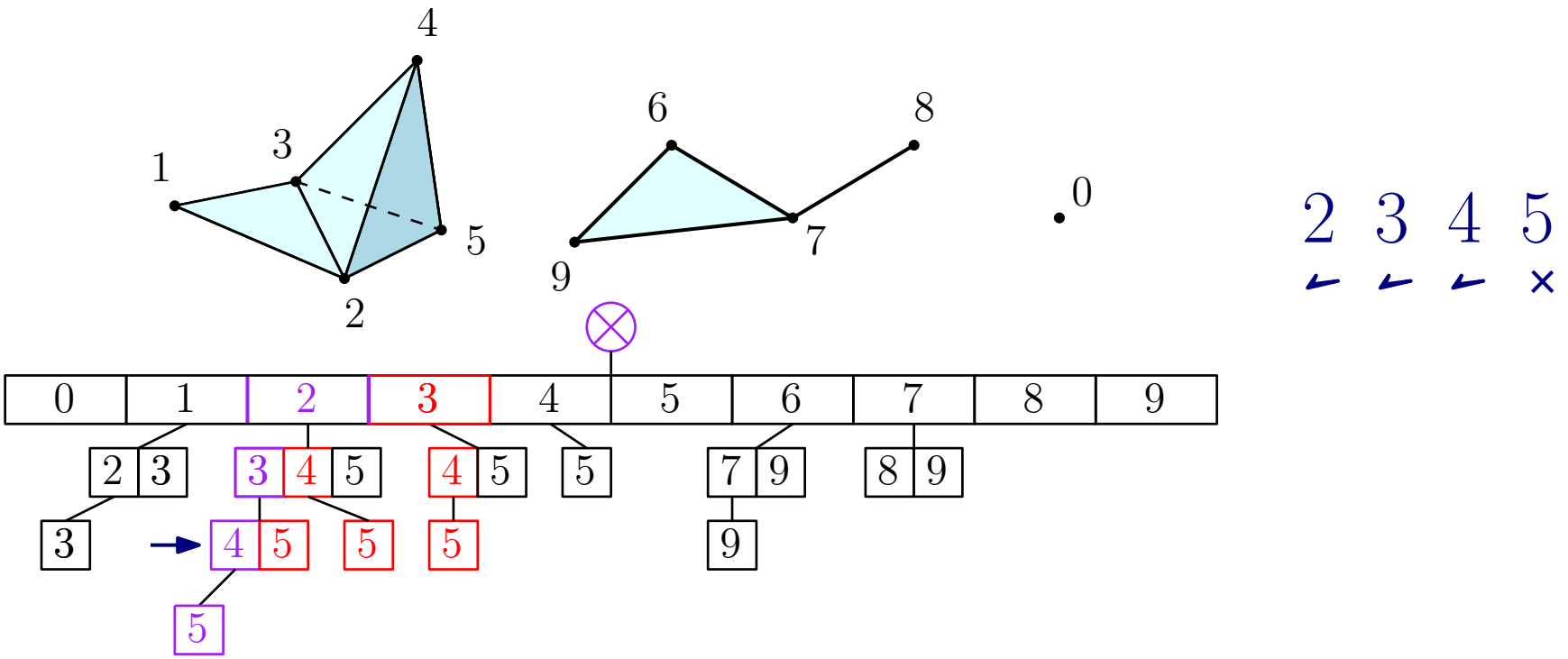

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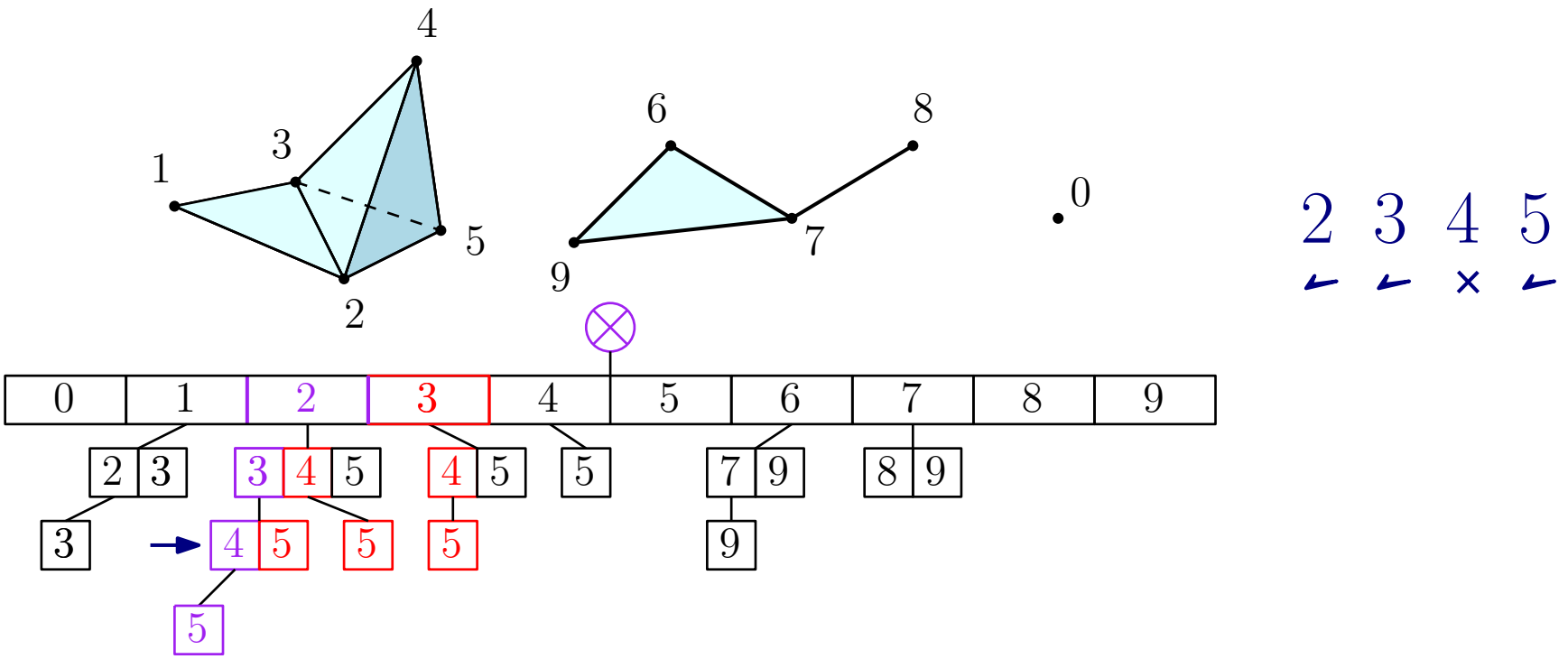

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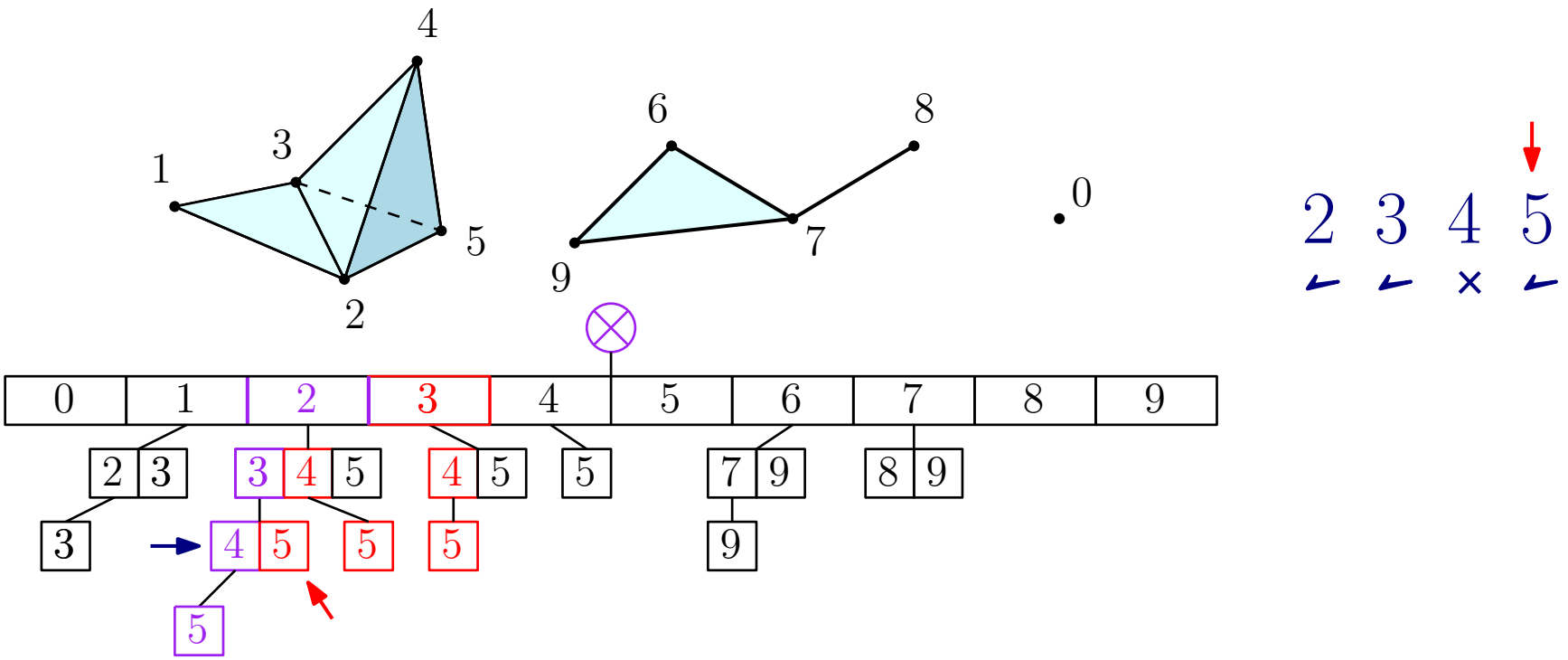

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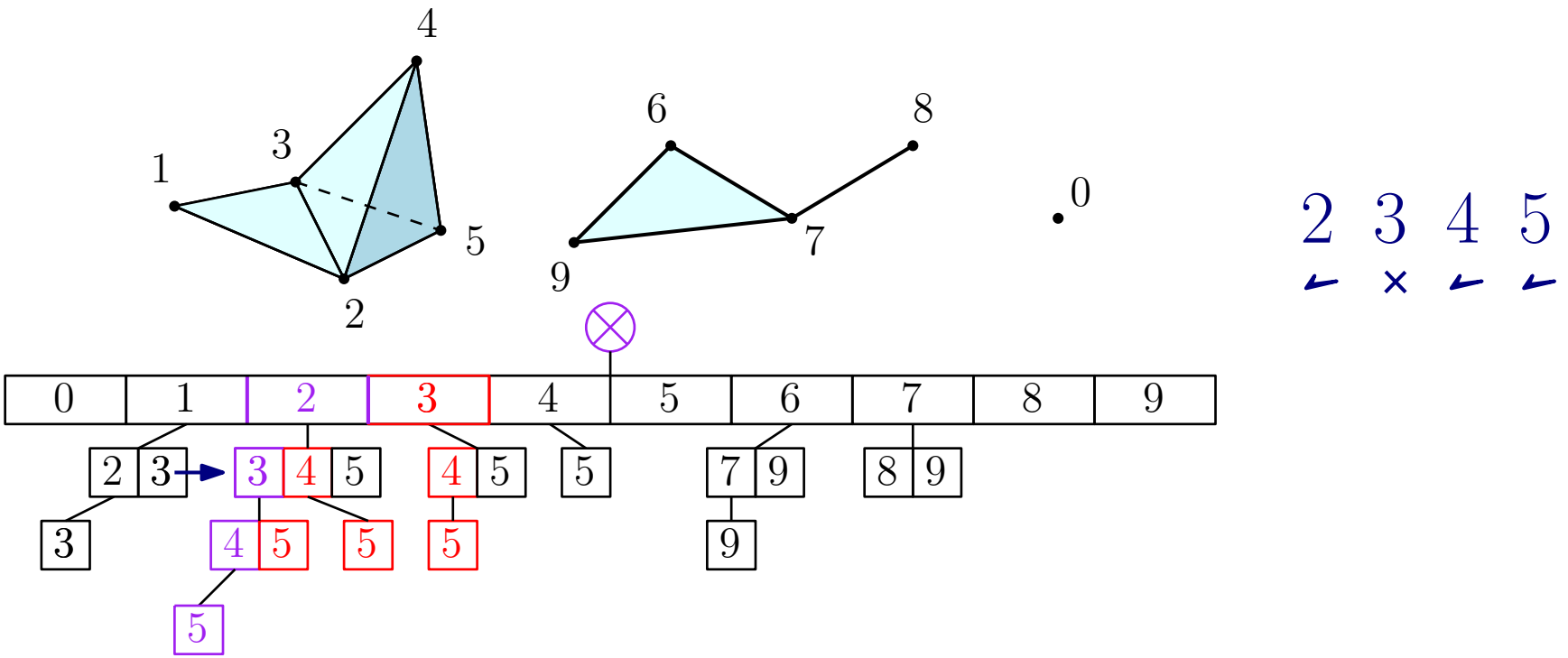

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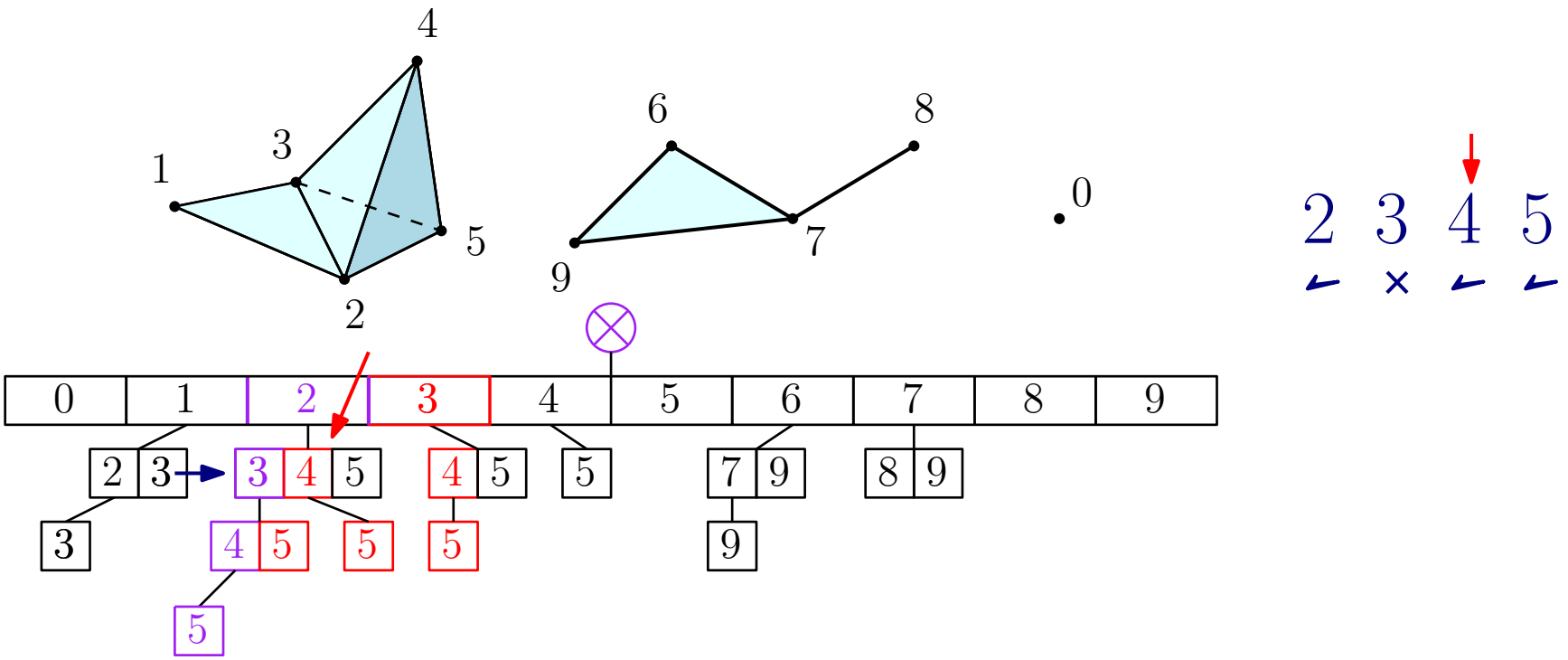

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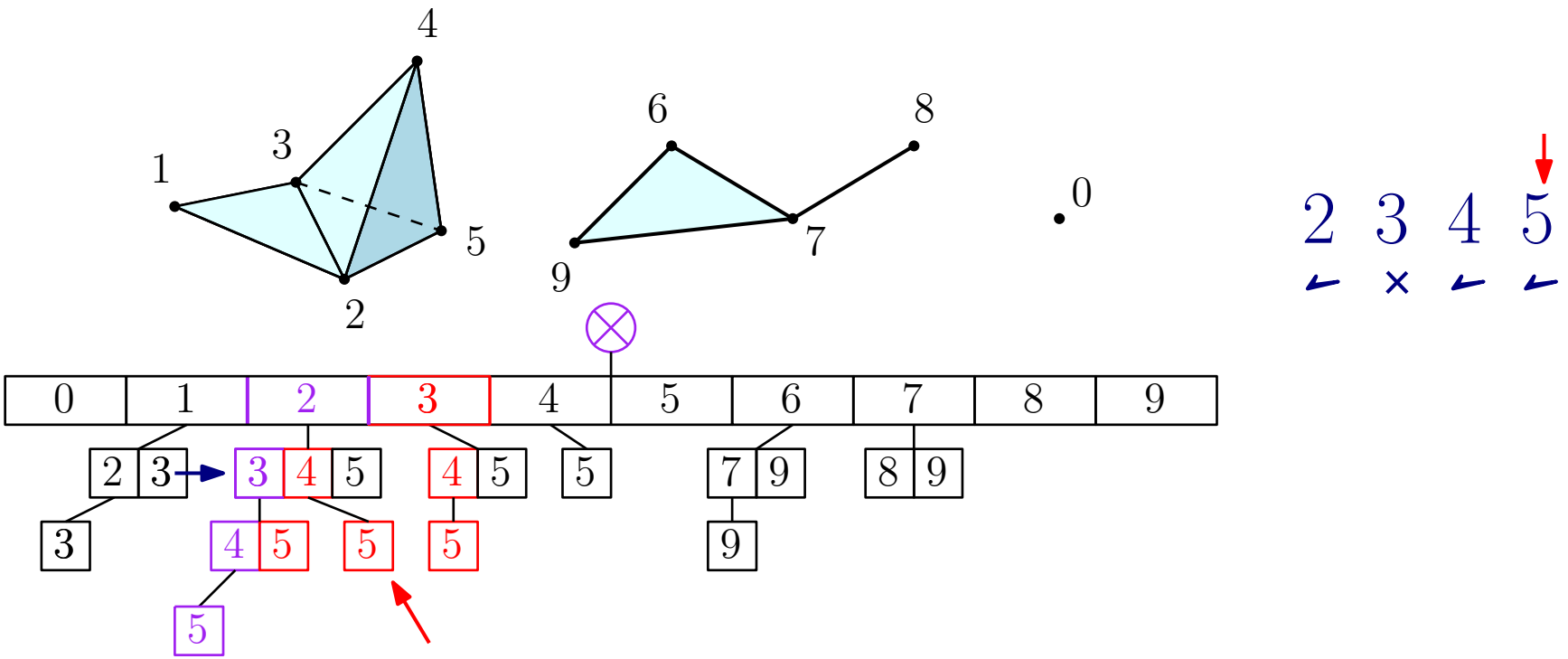

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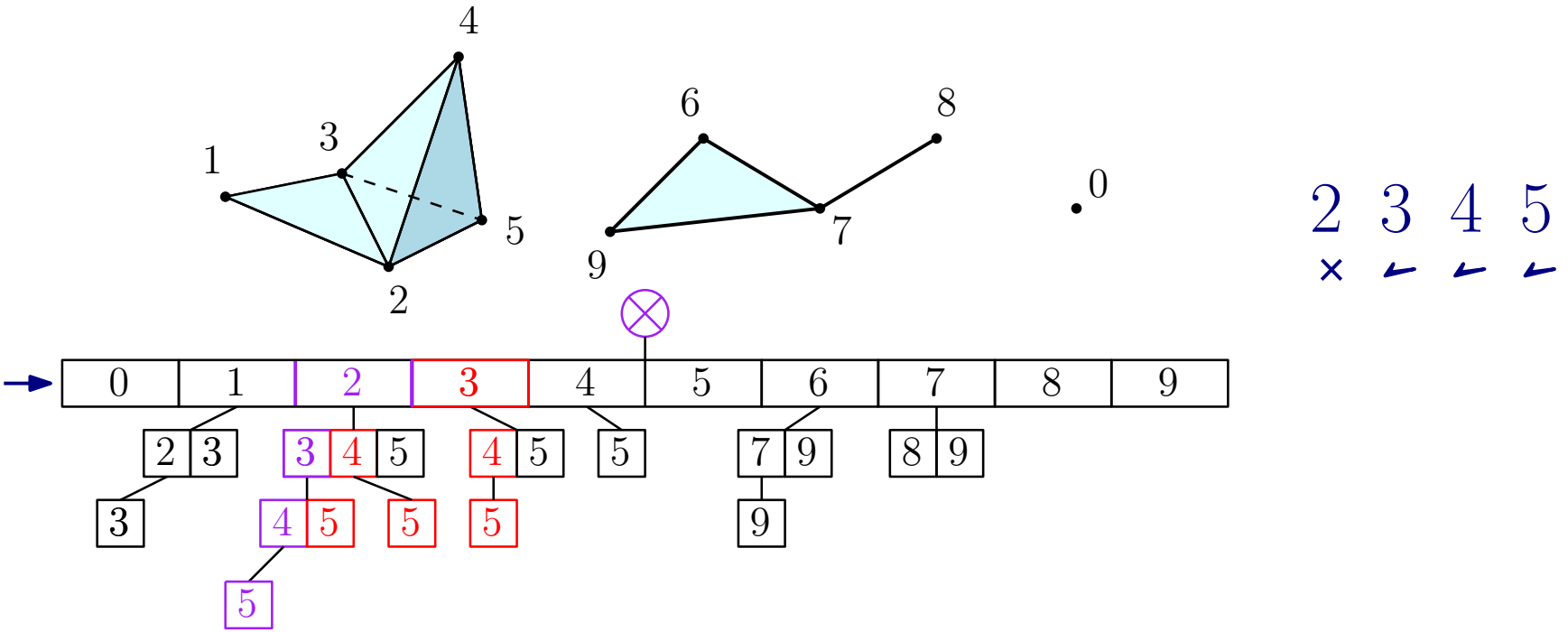

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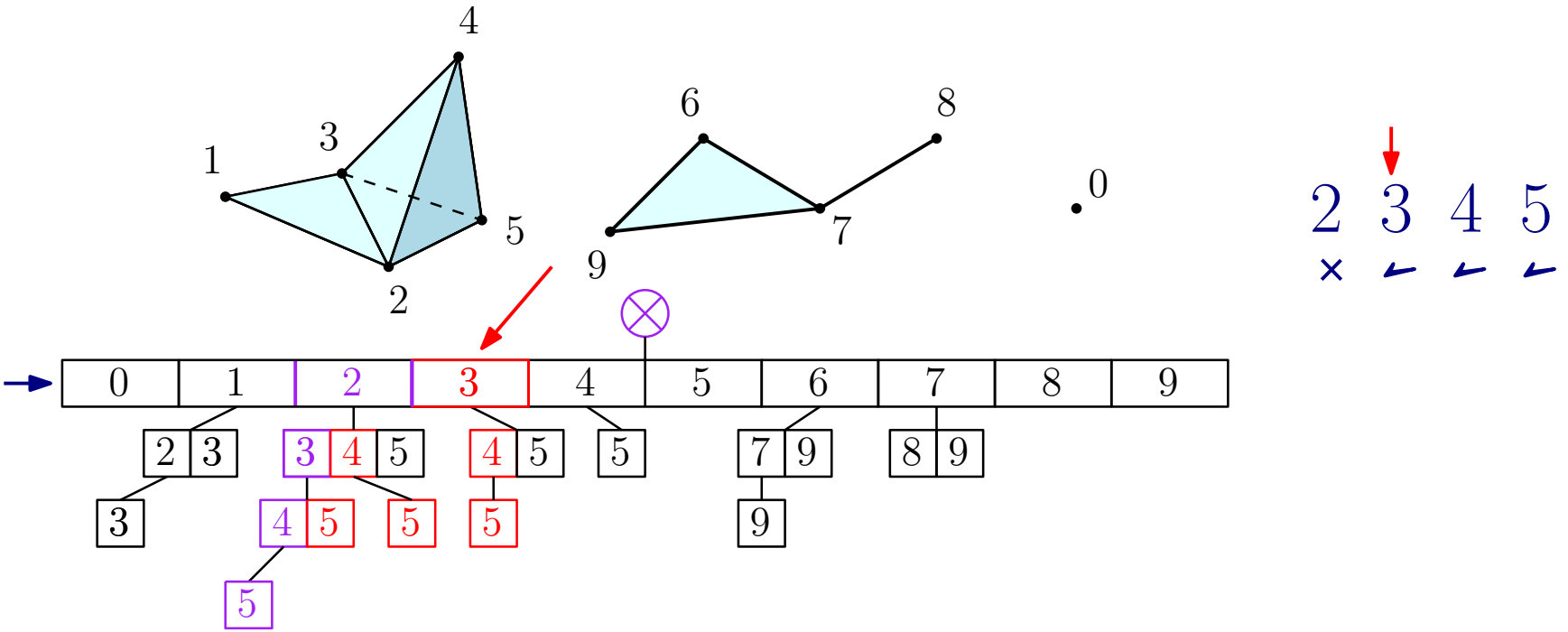

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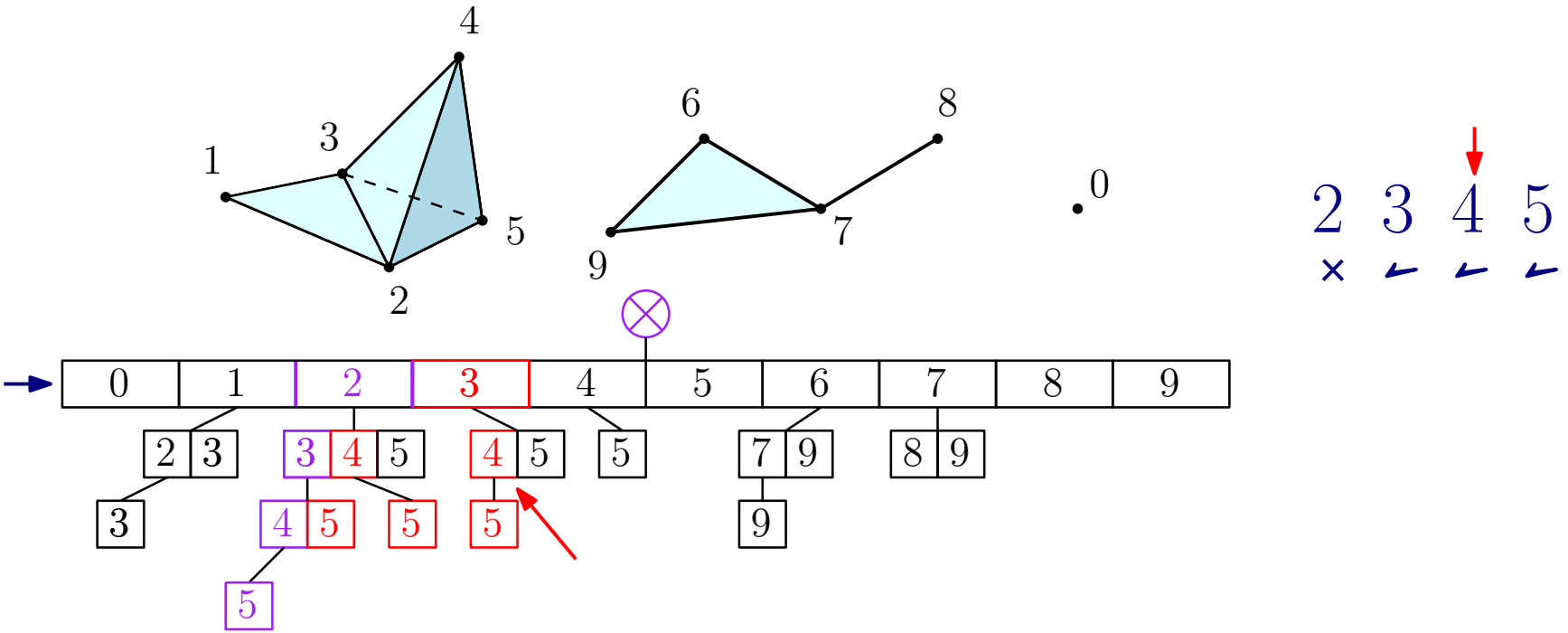

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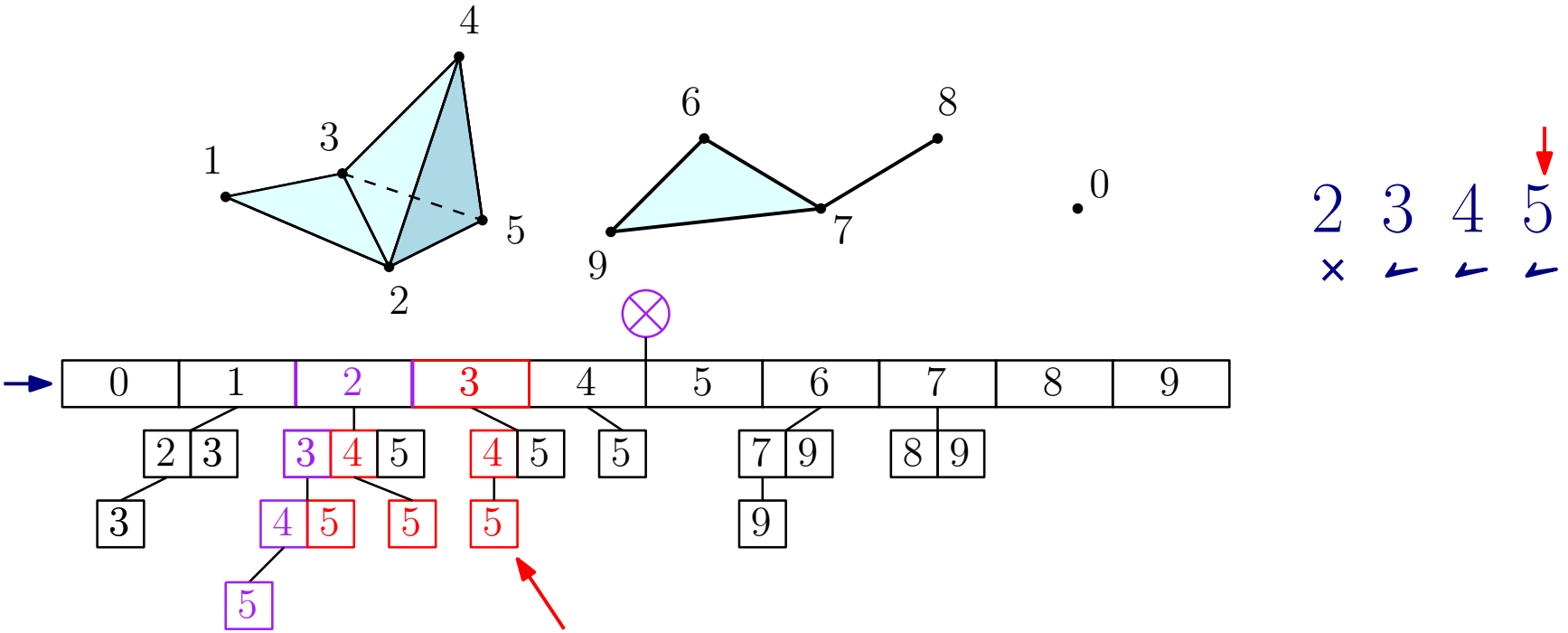


3
Persistent Cohomology and Annotations

Annotations

[Dey,Fan,Wang]

Given a simplicial complex $\mathcal{K}$, let $\mathcal{K}^p$ denote the set of p-simplices in $\mathcal{K}$.

Definition

An *annotation* for $\mathcal{K}^p$ is an assignement $\mathrm{a}^p : \mathcal{K}^p \to \mathbb{Z}_2^g$ of a binary vector $\mathrm{a}_\sigma = \mathrm{a}^p(\sigma)$ of length g. Linear extension to C_p.

Definition

An annotation $\mathrm{a} : \mathcal{K}^p \to \mathbb{Z}_2^g$ is *valid* if:

1. $g = \operatorname{rank} H_p(K)$, and
2. two p-cycles z_1 and z_2 have $\mathrm{a}_{z_1} = \mathrm{a}_{z_2}$ iff their homology classes $[z_1]$ and $[z_2]$ are identical.

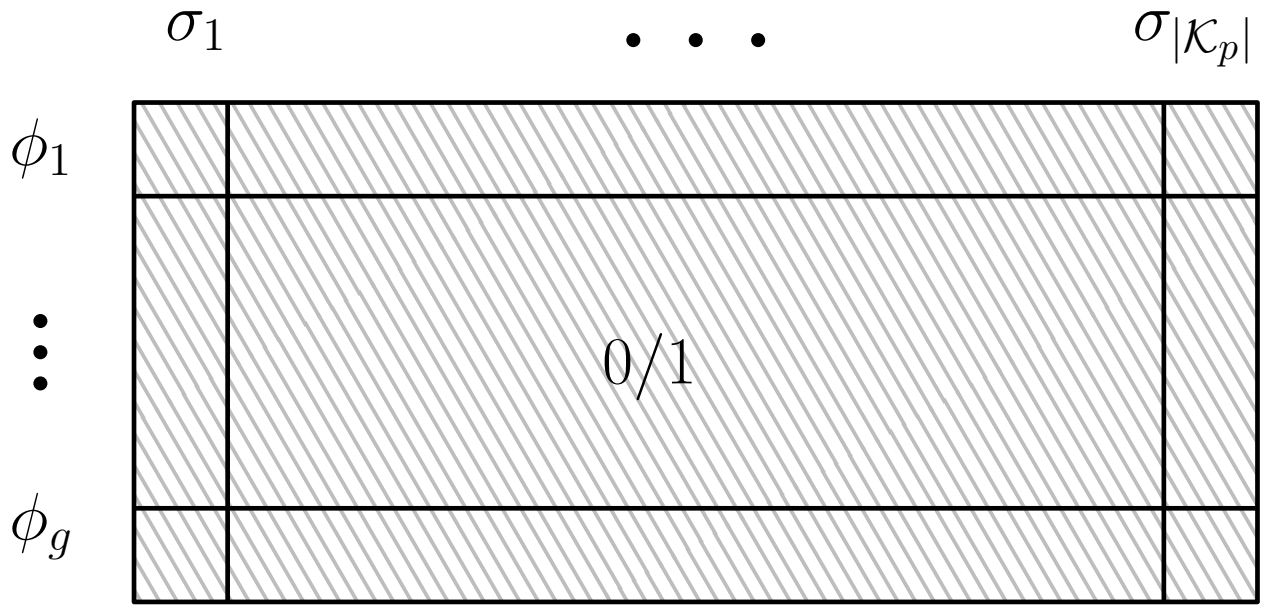
Annotations

[Dey,Fan,Wang]

Theorem

The following two statements are equivalent

1. *An annotation* $\mathsf{a} : \mathcal{K}^p \to \mathbb{Z}_2^g$ *is valid*
2. *The cochains* $\{\phi_j\}_{j=1\cdots g}$ *given by* $\phi_j(\sigma) = \mathsf{a}_\sigma[j]$ *for all* $\sigma \in \mathcal{K}^p$ *are cocycles whose cohomology classes* $\{[\phi_j]\}_{j=1\cdots g}$ *constitute a basis of* $H^p(\mathcal{K})$.

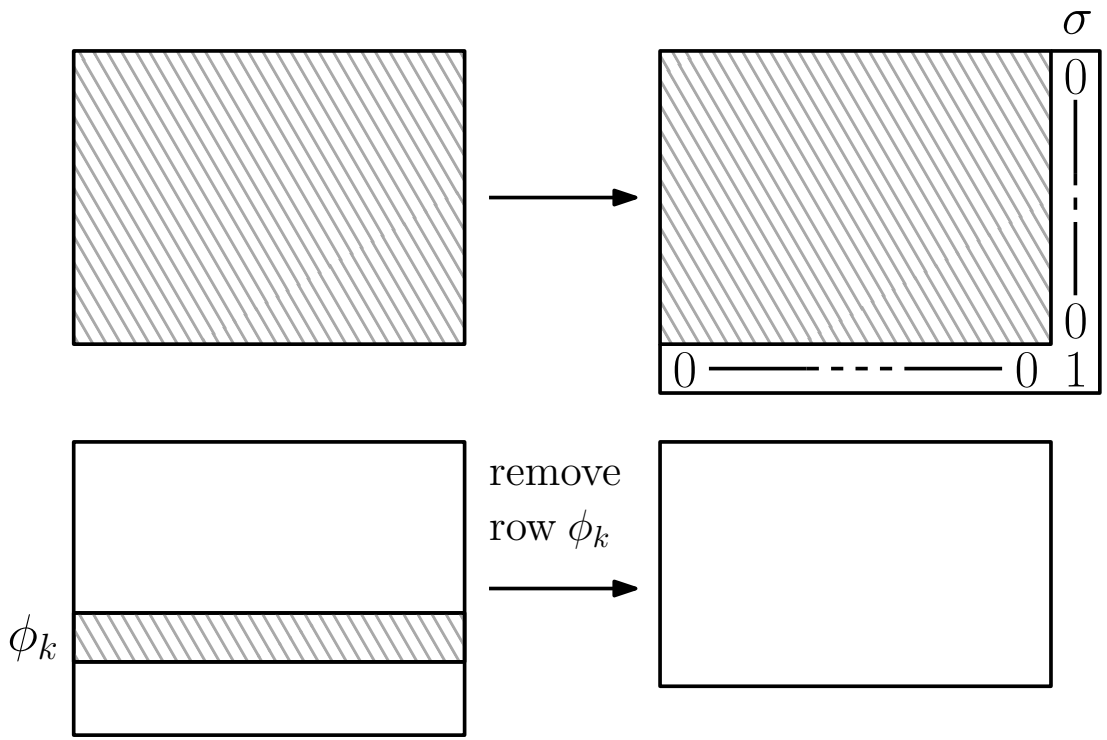


Persistent coHomology Algorithm

[de Silva, Morozov, Vejdemo-Johansson '11]; [Dey,Fan,Wang]

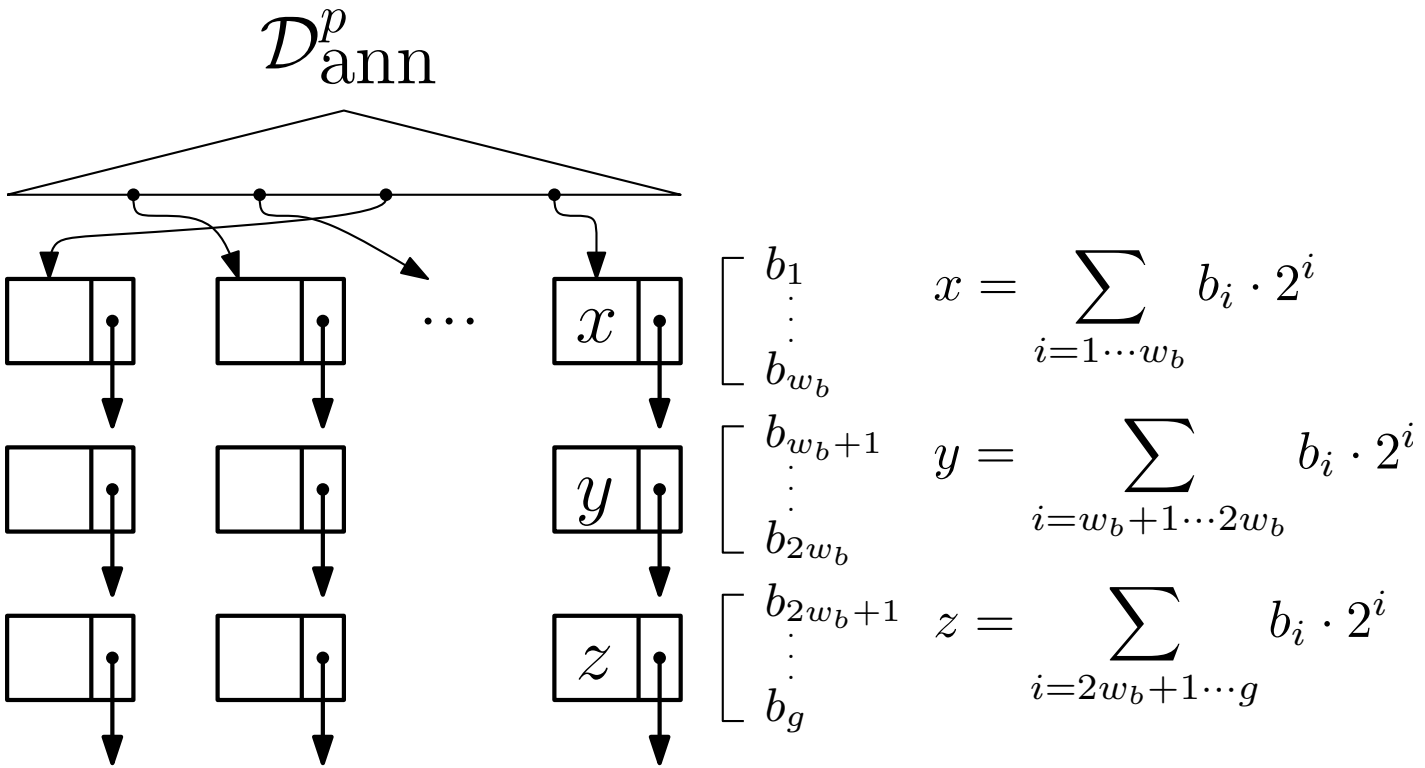
Insert $\sigma = \mathcal{K}_{i+1} \setminus \mathcal{K}_i$; compute $a_{\partial\sigma}$

- if $a_{\partial\sigma} = 0$, create a class
- else kills a class ϕ_k by adding $a_{\partial\sigma}$ to all columns with a 1 at index k



Representation of the Annotation [Boissonnat, Dey, M.]

- No duplicate vector
- Bits are "packed" into integers



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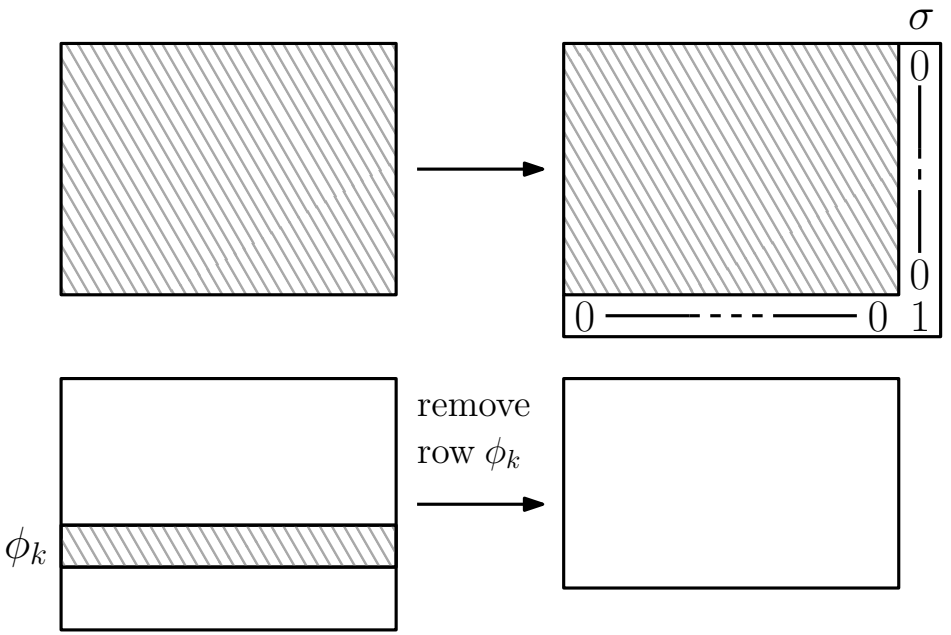
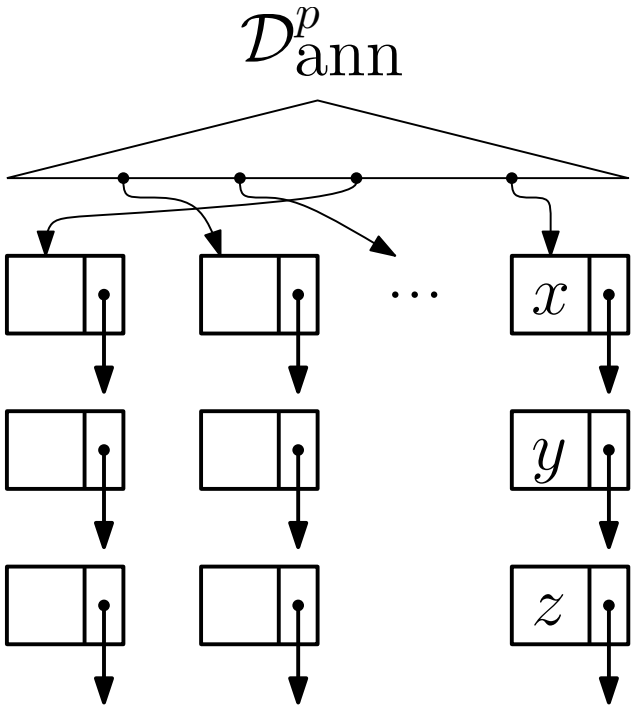


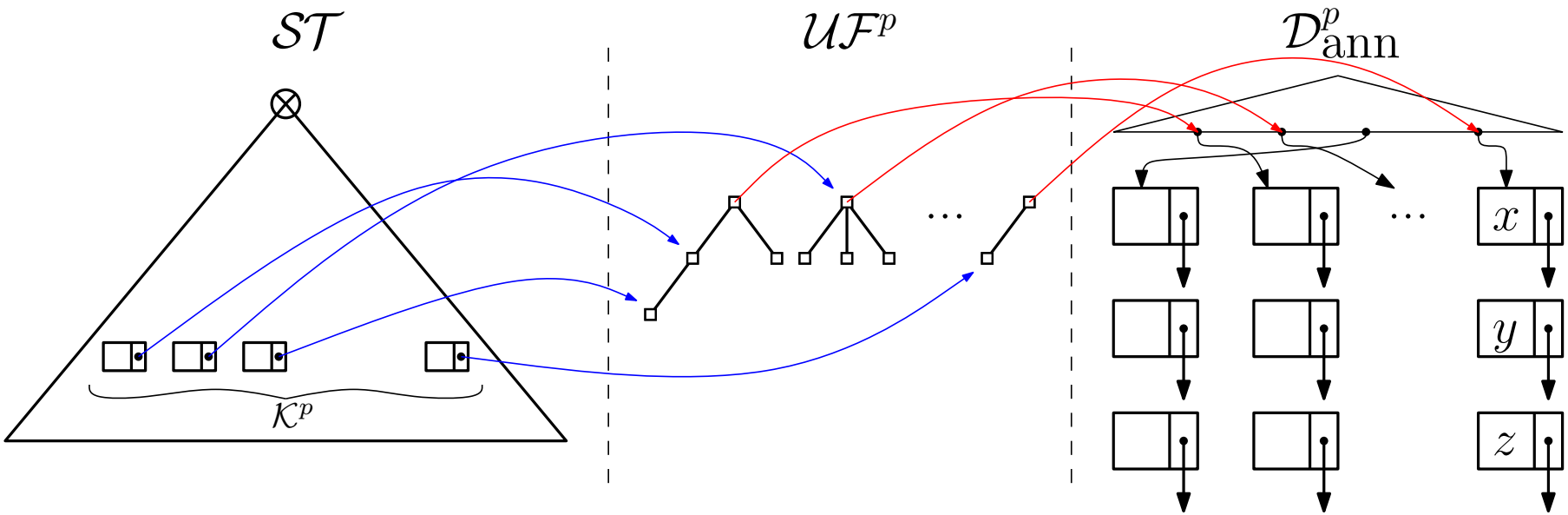


4
The Implementation

[Boissonnat, Dey, M.]

The Data Structure

We connect simplicial complex and annotations with a union-find:



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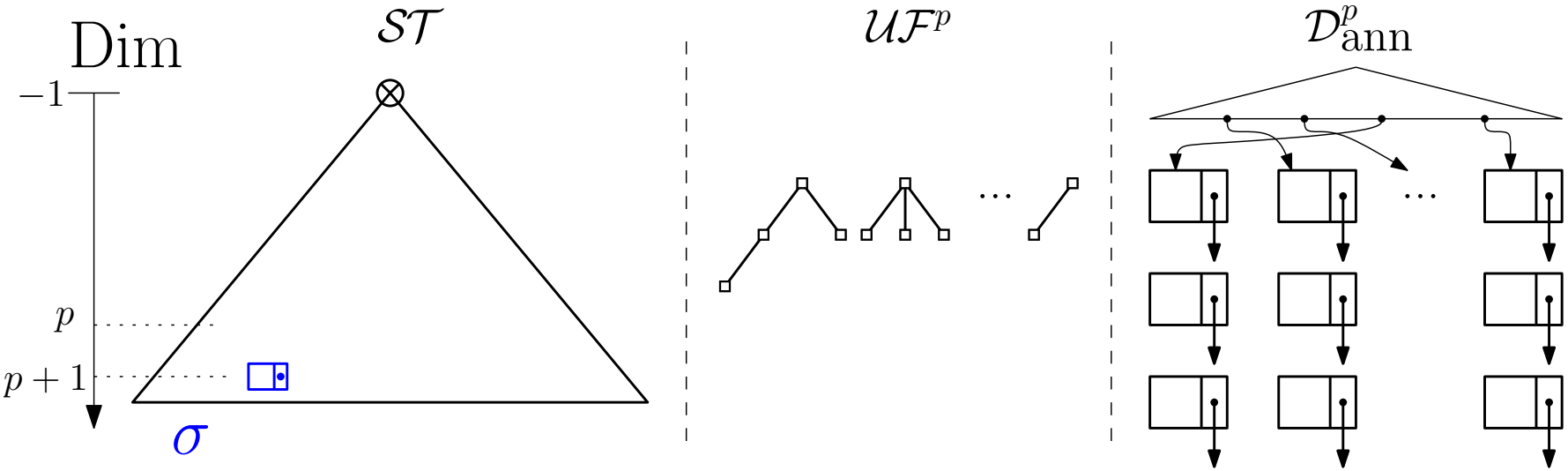

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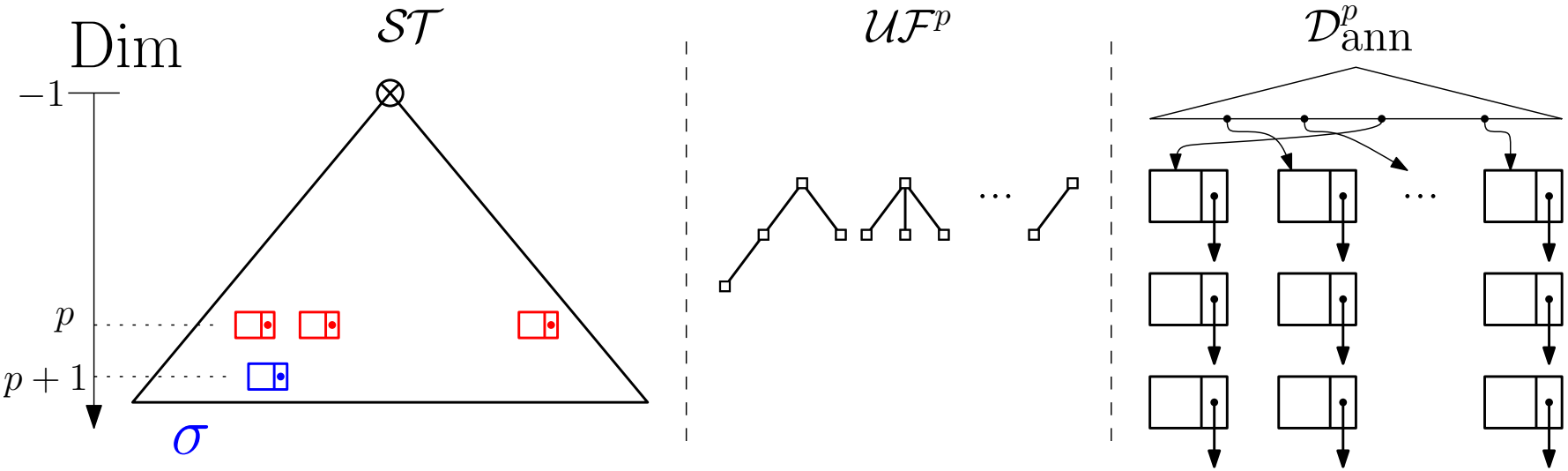

Implementation of the Algorithm

Insert $\sigma = \mathcal{K}_{i+1} \setminus \mathcal{K}_i$; compute $a_{\partial\sigma}$

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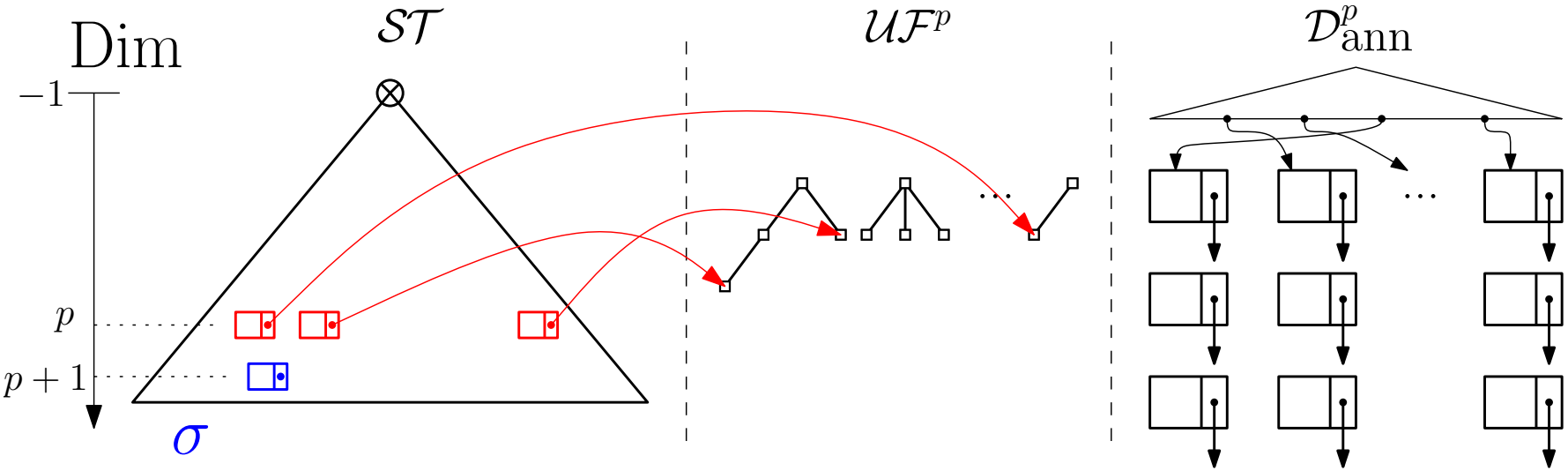

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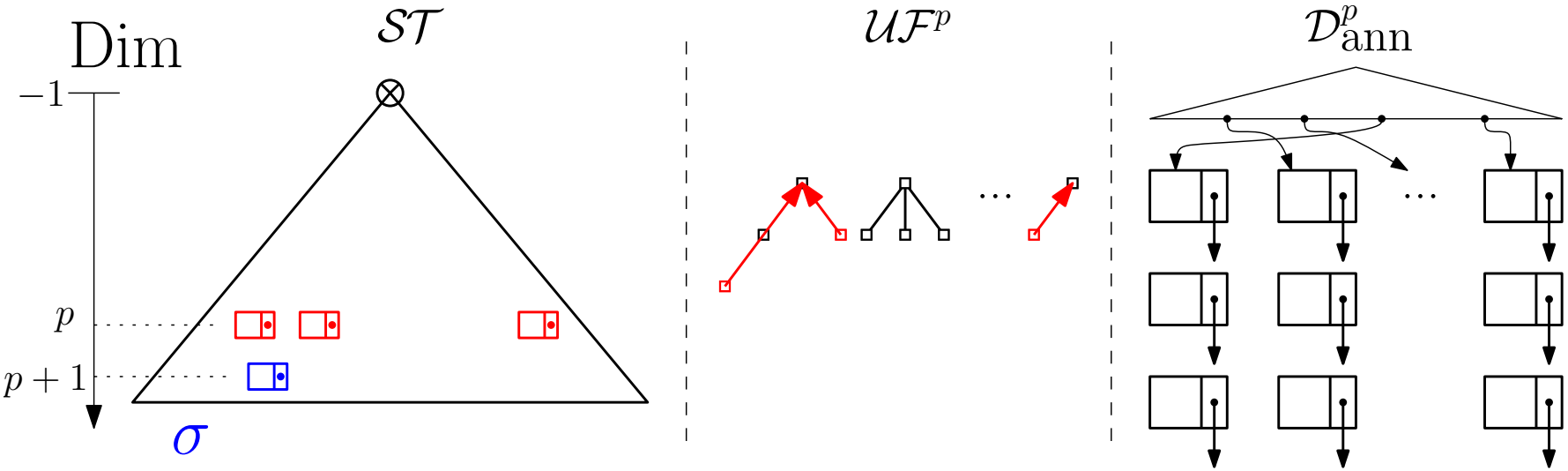

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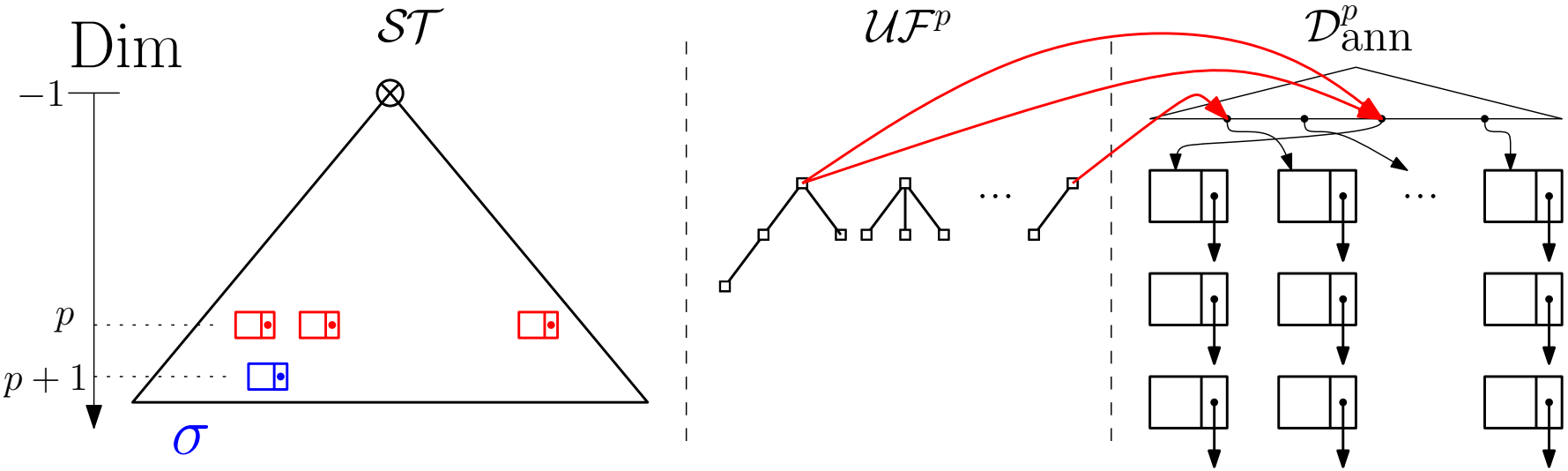

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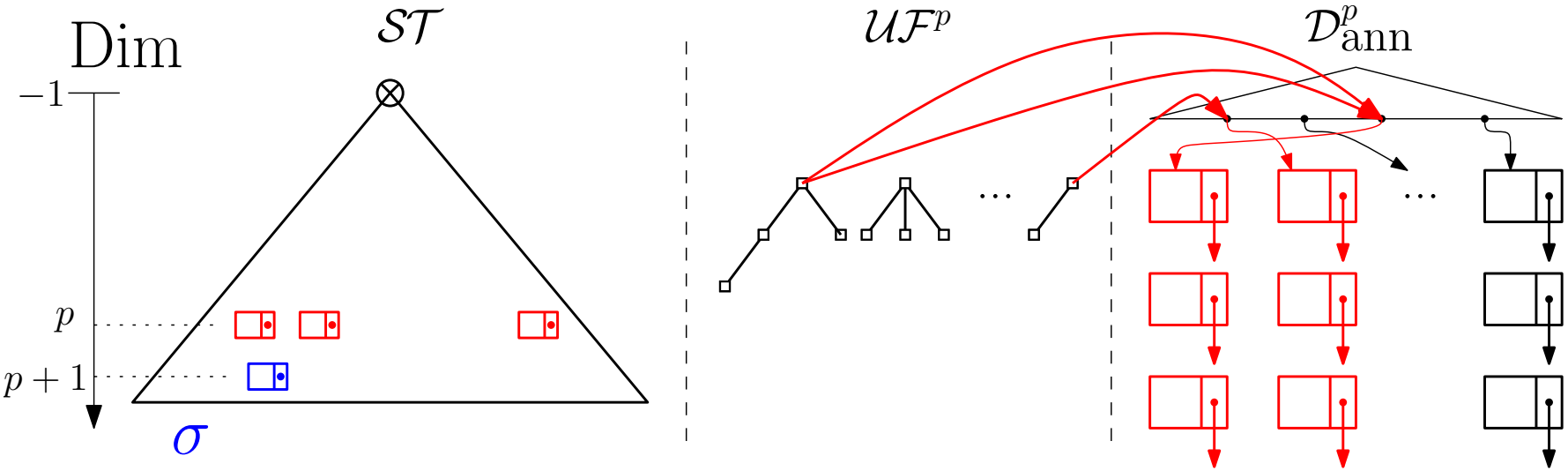


Complexity

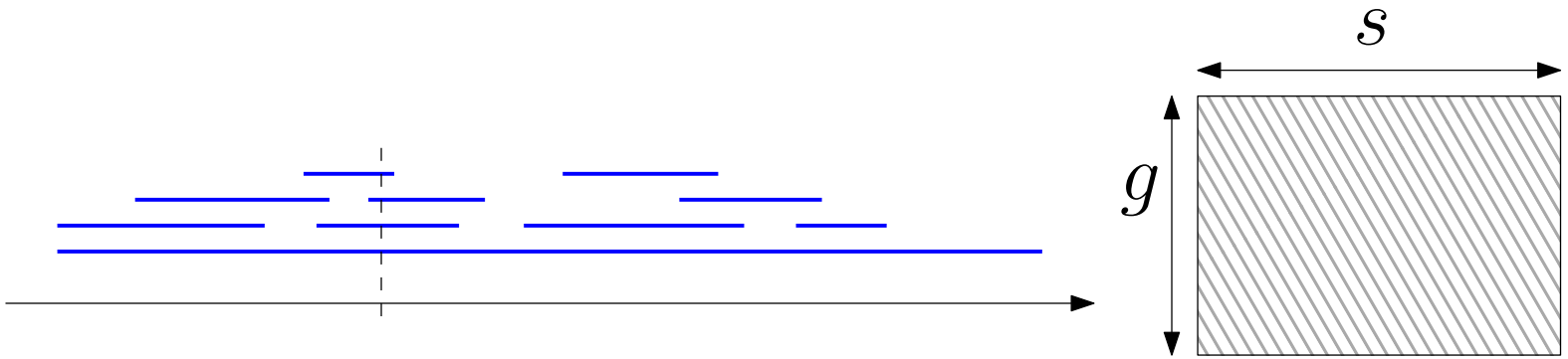
Space:

$$O\left(|\mathcal{K}| + k\frac{g_m s_m}{w_b}\right)$$

Time:

$$O\left(|\mathcal{K}|\left[k\left(\alpha(|\mathcal{K}|) + \left\lceil\frac{g_m}{w_b}\right\rceil + kD_m\right) + s_m\left(\left\lceil\frac{g_m}{w_b}\right\rceil \log(s_m) + \alpha(|\mathcal{K}|)\right)\right]\right)$$

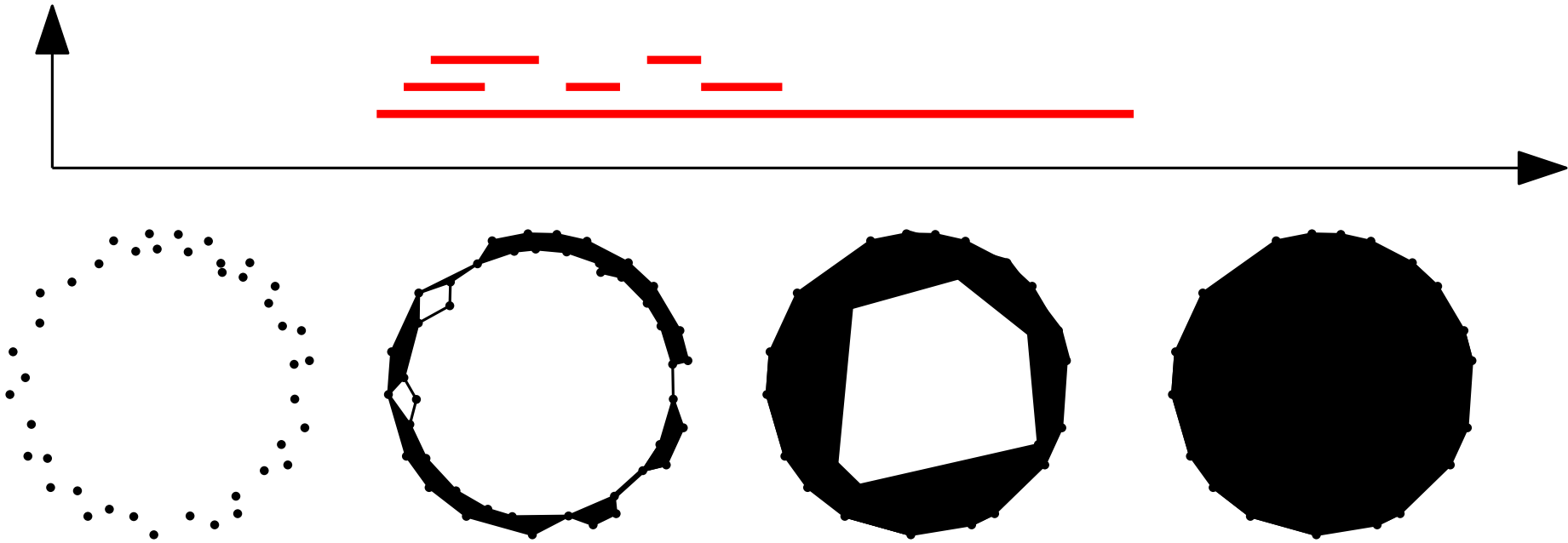
intuitively...



Lazy Evalutation of Simplices

Lazy Evalutation of Simplices

We minimize the number of “alive bars” living in parallel.



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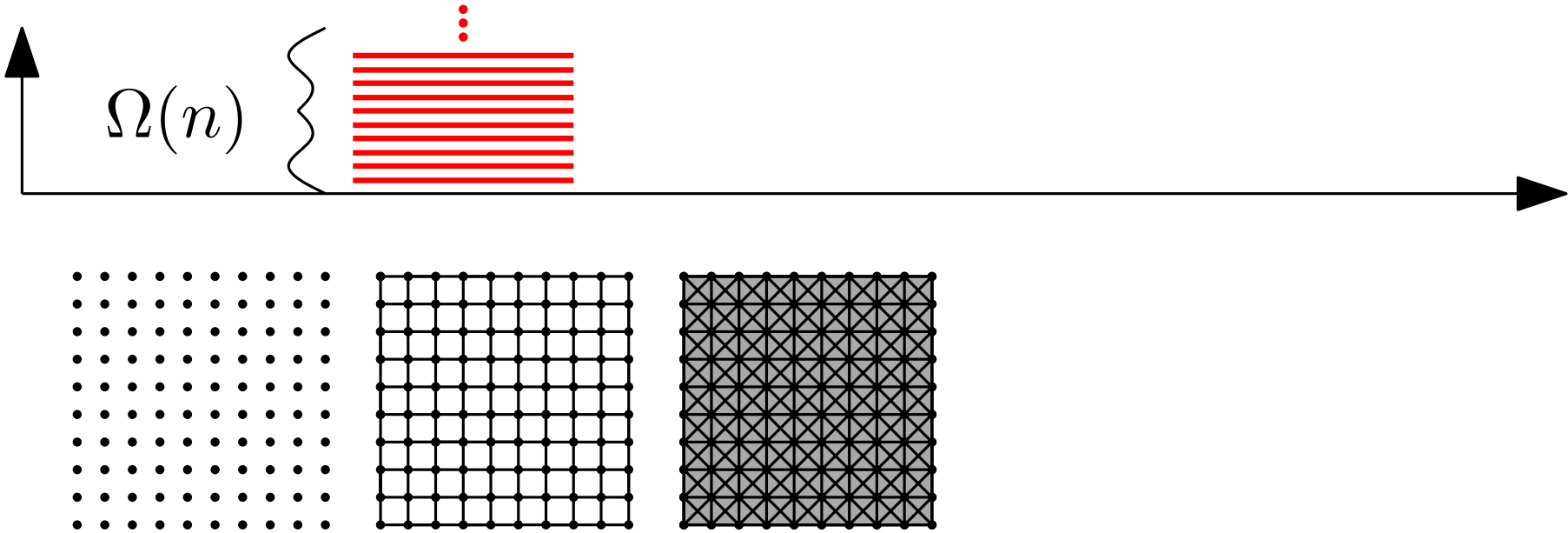
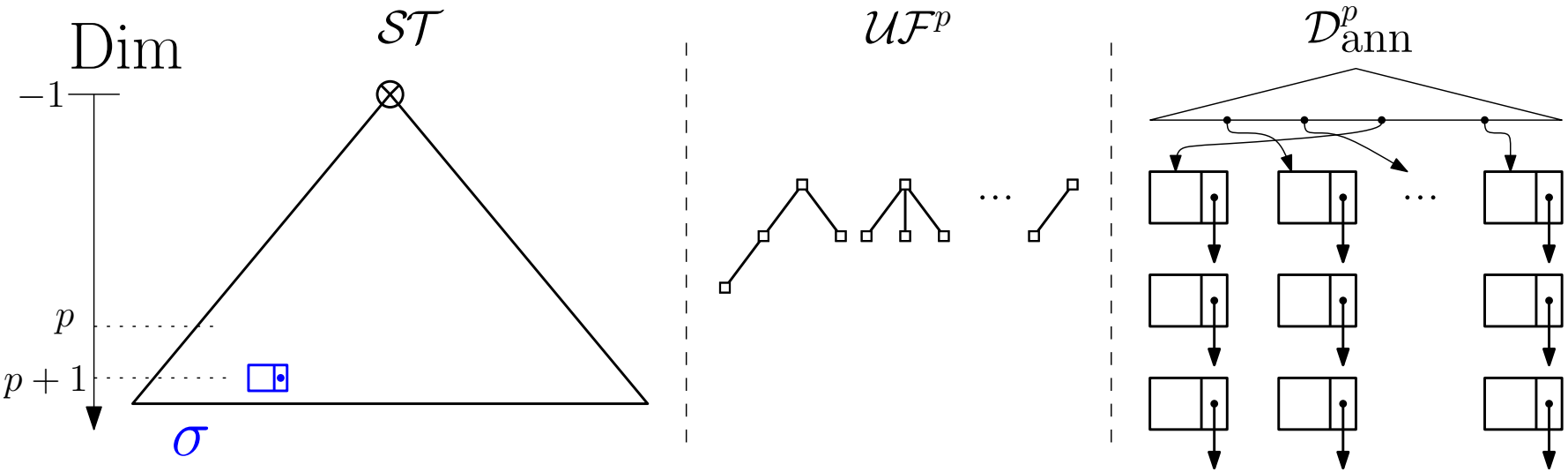


Lazy Evalutation of Simplices

$$\emptyset = \mathcal{K}_{\rho_0} \subset \mathcal{K}_{\rho_1} \subset \cdots \subset \mathcal{K}_{\rho_{m-1}} \subset \mathcal{K}_{\rho_m} = \mathcal{K}$$
$$\sigma_0 \quad \sigma_1 \quad \sigma_2 \quad \cdots \quad \sigma_{m-2} \quad \sigma_{m-1} \quad \sigma_m$$

- we insert killers as soon as we encounter them
- we postpone the insertion of a creator σ until we encounter one of its cofaces

We mark the simplices whose insertion has been postponed. When considering σ in the filtration:



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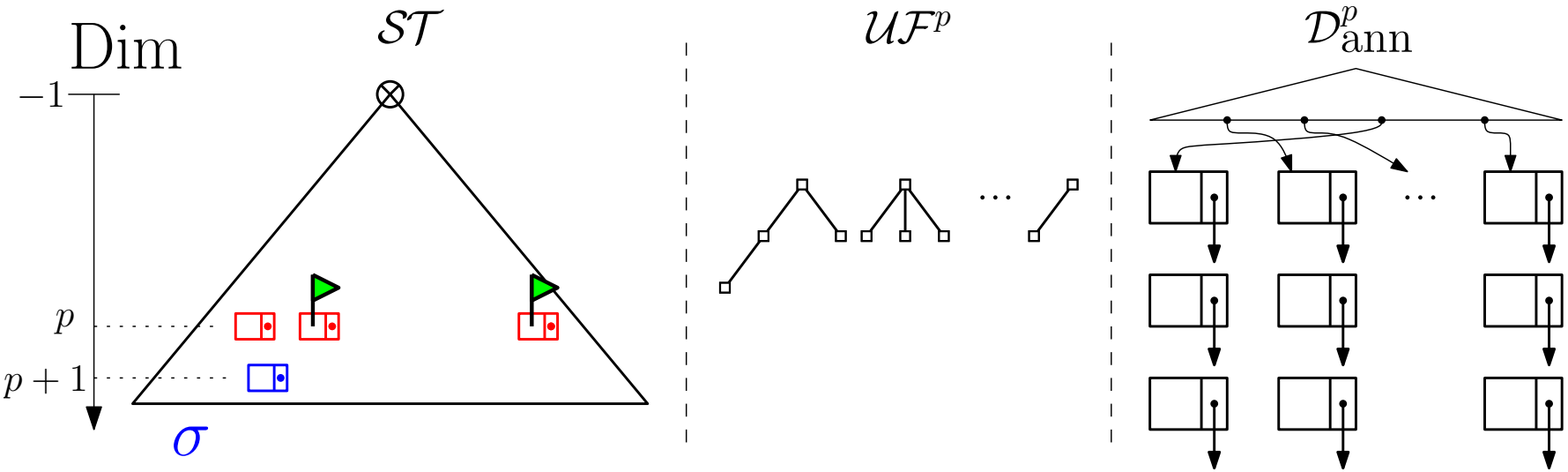

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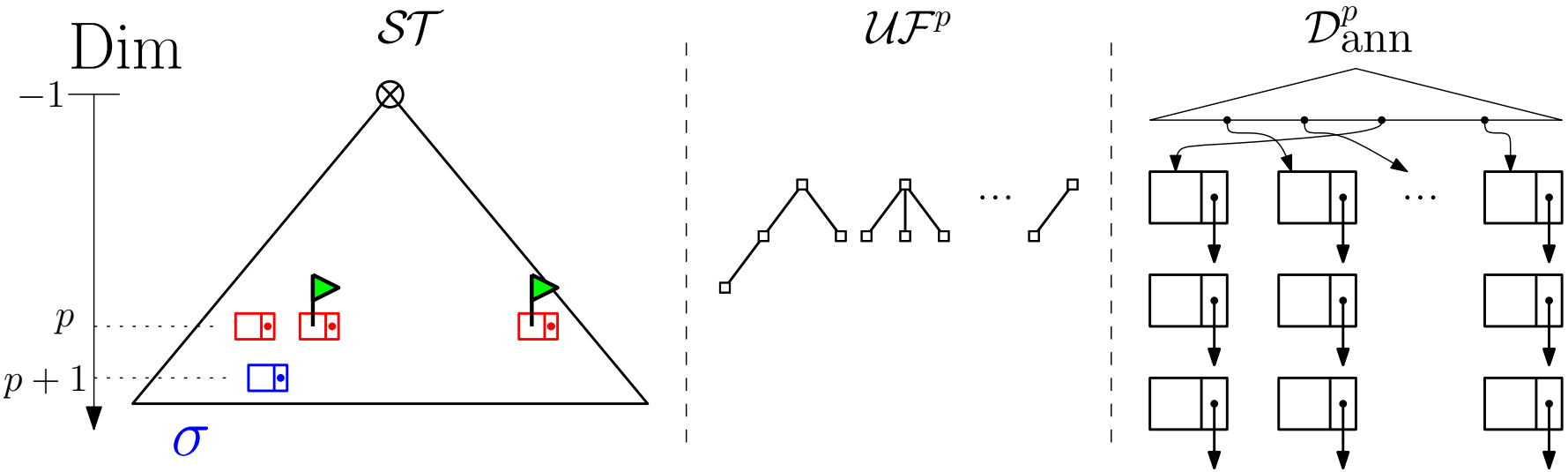
- we postpone the insertion of a creator σ until we encounter one of its cofaces

No additional complexity!
Same persistence diagram!



5
Experiments

Performance

Data	$\lvert\mathcal{P}\rvert$	D	d	r	k	$\lvert\mathcal{K}\rvert$	T_{ann}	$T_{\text{ann}}/\lvert\mathcal{K}\rvert$(s.)
S4	507	5	4	0.75	5	$191 \cdot 10^6$	$\sim$ 32min	$1.0 \cdot 10^{-5}$
Bud	1000	3	2	2.4	3	$283 \cdot 10^6$	$\sim$ 10min	$2.2 \cdot 10^{-6}$
Bro	500	25	?	0.8	16	$38 \cdot 10^6$	$\sim$ 181min	$2.8 \cdot 10^{-4}$
Cy8	500	24	2	1.3	17	$18 \cdot 10^6$	$\sim$ 9min	$3.1 \cdot 10^{-5}$
KI	4900	5	2	0.415	5	$218 \cdot 10^6$	$\sim$ 29min	$7.9 \cdot 10^{-6}$

Figure: Data, timings and statistics

$$O\left(|\mathcal{K}| + k\frac{g_{\text{m}}s_{\text{m}}}{w_b}\right)$$

$$O\left(|\mathcal{K}|\left[k\left(\alpha(|\mathcal{K}|) + \left\lceil\frac{g_{\text{m}}}{w_{\text{b}}}\right\rceil + kD_{\text{m}}\right) + s_{\text{m}}\left(\left\lceil\frac{g_{\text{m}}}{w_{\text{b}}}\right\rceil \log(s_{\text{m}}) + \alpha(|\mathcal{K}|)\right)\right]\right)$$

Homology vs coHomology

Comparison with JPLEX and DIONYSUS: Persistent Homology vs Persistent coHomology

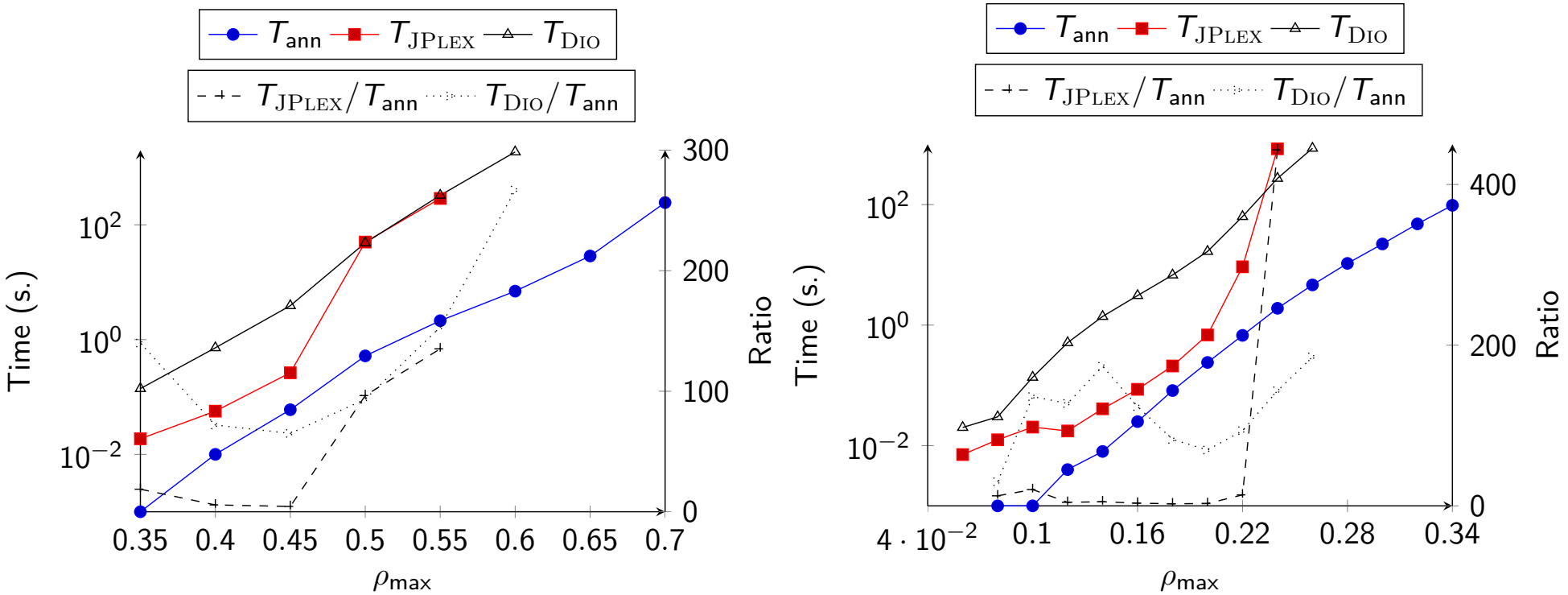
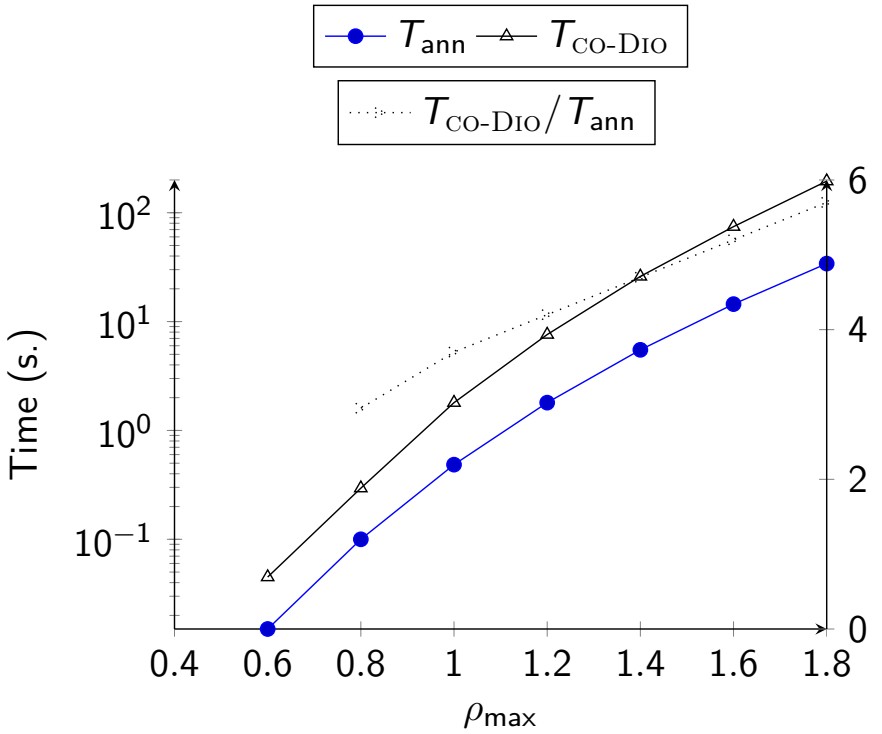


Figure: **S4** and **KI**

coHomology vs coHomology

Comparison with DIONYSUS: coHomology vs coHomology



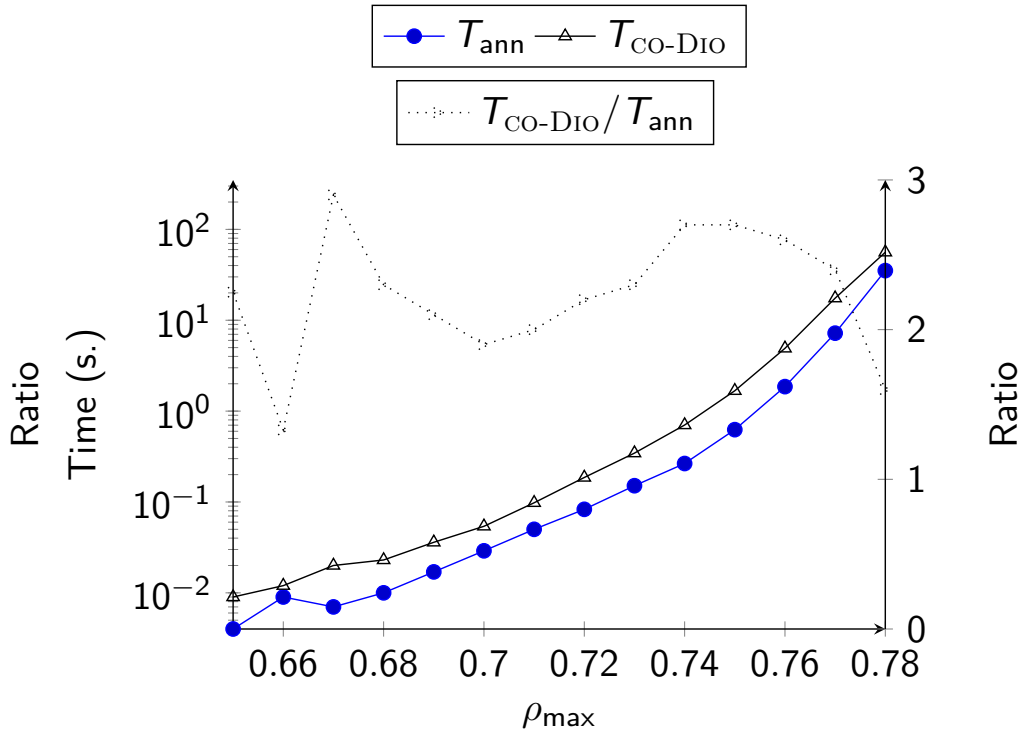
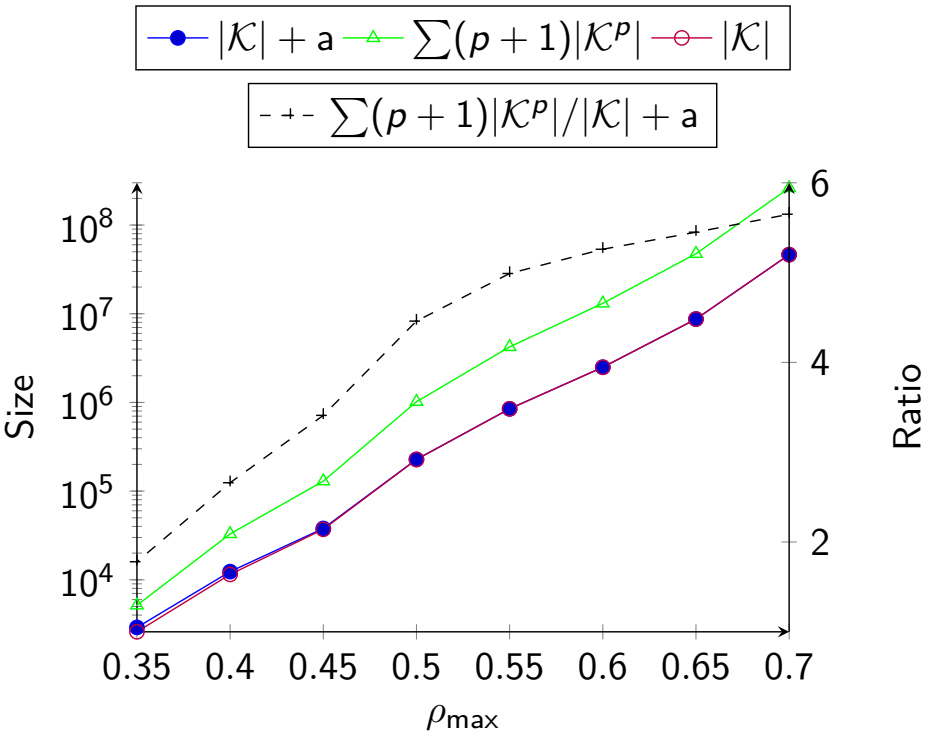


Figure: **Bud** and **Bro**

Memory



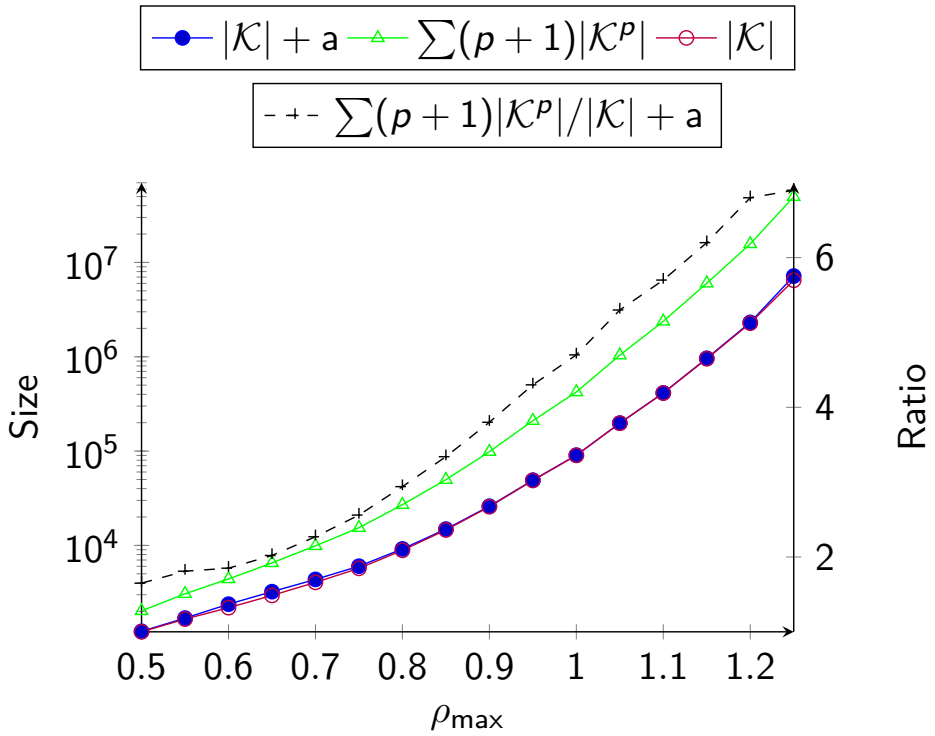


Figure: **S4** and **Cy8**

Numbers!

Dim:	**S4**: 1	2	3	4	**Bud**: 1	2	**Kl**: 1	2	3	4
G_m/g_m	4.9	1.2	6.2	6.1	2.1	8.4	11.8	10.3	10.3	8.9
$\lvert\mathcal{K}^p\rvert/s_m$	10^2	10^3	10^4	10^3	10^3	10^5	10^3	10^4	10^4	10^4
$\lceil g_m/w_b \rceil$	5	4	10	86	5	2	4	1	11	87

Dim:	**Bro**: 1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
G_m/g_m	2.1	1.8	5.4	5.7	5.2	5.6	4.0	4.2	3.0	3.7	3.7	2.9	3.0	3.7	3.0
$\lvert\mathcal{K}^p\rvert/s_m$	10^1	10^3	10^3	10^3	10^2	10^2	10^2	10^2	10^2	10^2	10^2	10^2	10^2	10^2	10^2
$\lceil g_m/w_b \rceil$	6	6	6	36	150	330	703	694	726	343	133	46	8	228	342

Dim:	**Cy8**: 1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
G_m/g_m	2.3	1.7	3.9	3.8	4.1	4.1	3.5	3.5	3.9	2.7	2.6	3.0	2.8	1.9	2.7	1
$\lvert\mathcal{K}^p\rvert/s_m$	10^3	10^3	10^3	10^3	10^3	10^3	10^2	10^2	10^2	10^2	10^2	10^2	10^2	10^2	10^2	10^2
$\lceil g_m/w_b \rceil$	3	1	3	12	33	74	147	186	160	168	93	33	10	3	1	1

Figure: Statistics about the evolution of the dimension of the homology groups we maintain during the computation.

Conclusion

Future Work

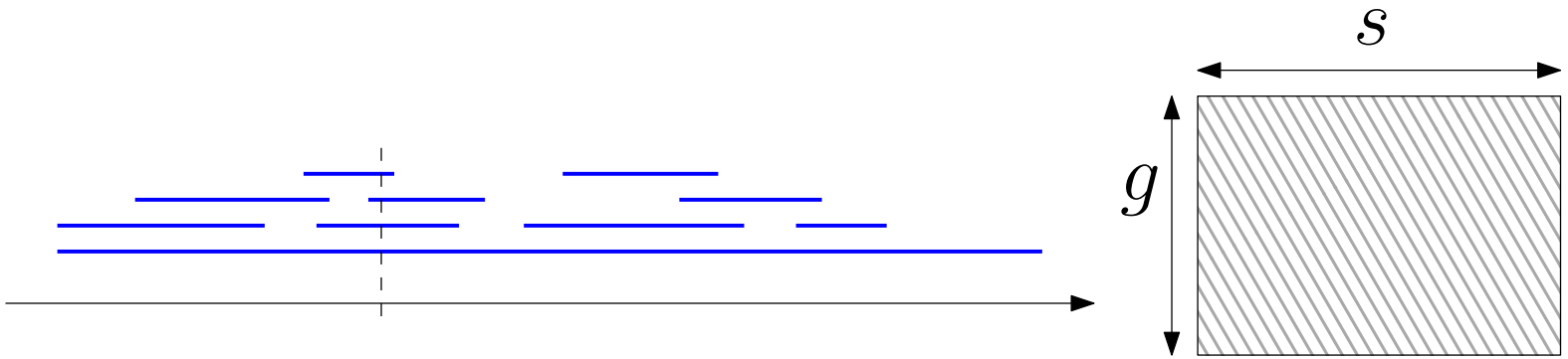
Space:

$$O\left(|\mathcal{K}| + k\frac{g_m s_m}{w_b}\right)$$

Time:

$$O\left(|\mathcal{K}|\left[k\left(\alpha(|\mathcal{K}|) + \left\lceil\frac{g_m}{w_b}\right\rceil + kD_m\right) + s_m\left(\left\lceil\frac{g_m}{w_b}\right\rceil \log(s_m) + \alpha(|\mathcal{K}|)\right)\right]\right)$$

intuitively...



Thank you!

Question?