Persistent Homology: Formalization

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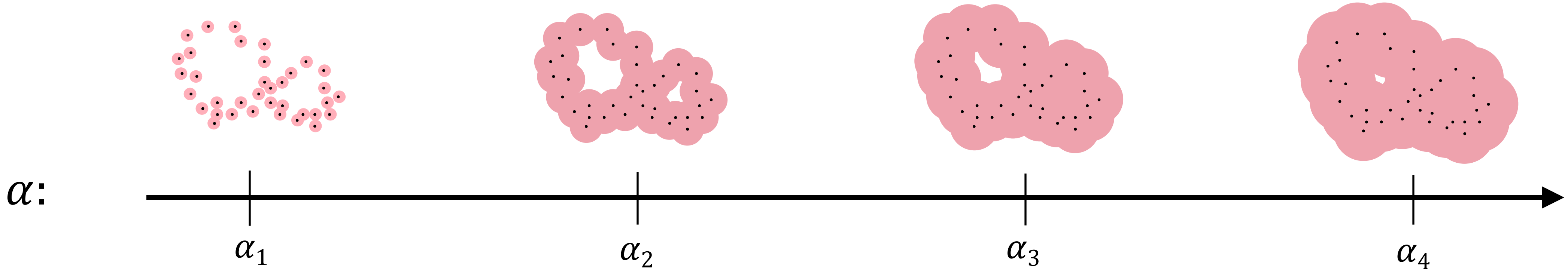
Outline for studying persistent homology

1. Intro to persistent homology
    - Build intuitions of persistent homology: what it does, what it produces
2. Formalizing persistent homology
    - Introduce its input (filtration) and study an algorithm for computation
3. Different ways for building filtrations
    - Vietoris-Rips filtration, sub-levelset filtration
    - Cubical complexes (for images)
4. Interpretation and stability of persistence diagram

“The growing space”



- Recall the growing space:
  - We have a value α ranging within an interval, say, from 0 to ∞
  - Let each value α corresponds to a topological space so that
  - The topological space grows as α increases from 0 to ∞

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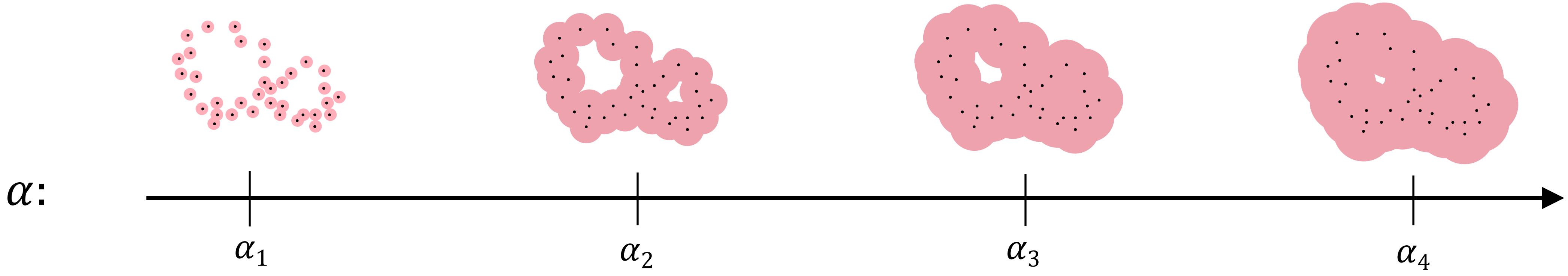
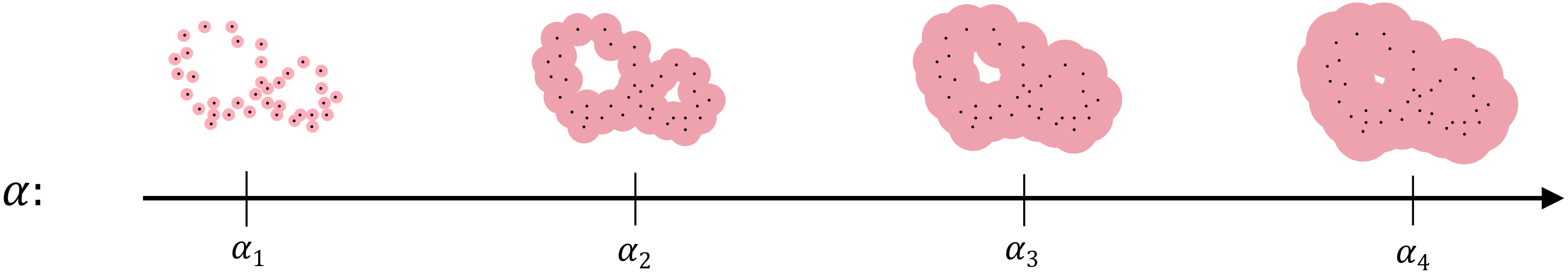


- Recall the growing space:
  - We have a value α ranging within an interval, say, from 0 to ∞
  - Let each value α corresponds to a topological space so that
  - The topological space grows as α increases from 0 to ∞
- Suppose I ask you to represent such a growing space in the computer, can you think of any problems?

“The growing space”



- Problem 1:
  - When α ranges within an interval $[s, f]$, no matter how small the interval is, there are always infinitely many values within the interval

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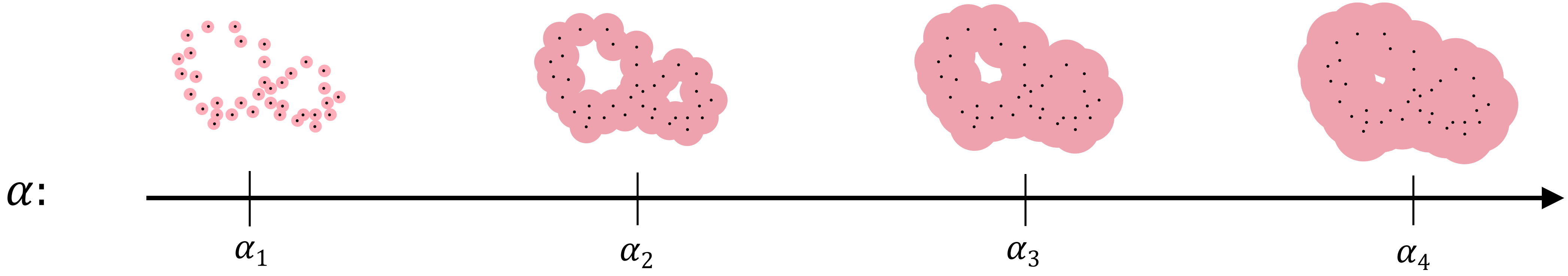

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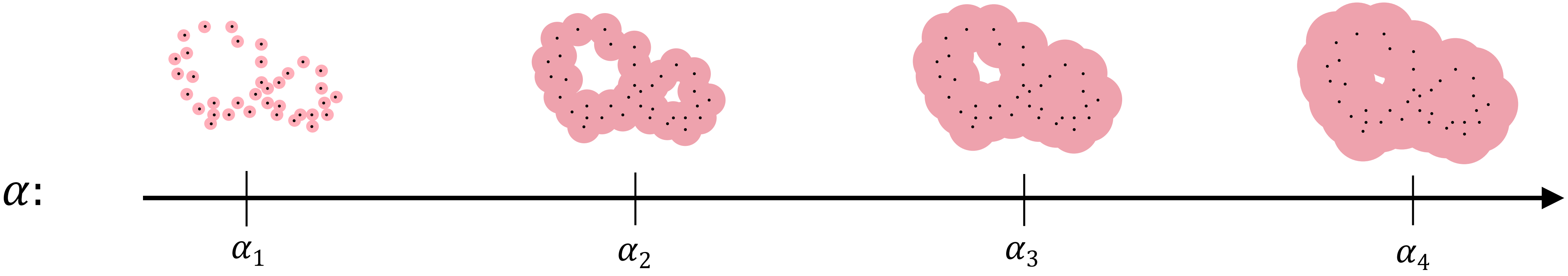

- Problem 1:
  - When α ranges within an interval $[s, f]$, no matter how small the interval is, there are always infinitely many values within the interval
  - Each α value may correspond to a possibly different space
  - This means there could be infinitely many spaces that we need to store in the computer, which is impossible

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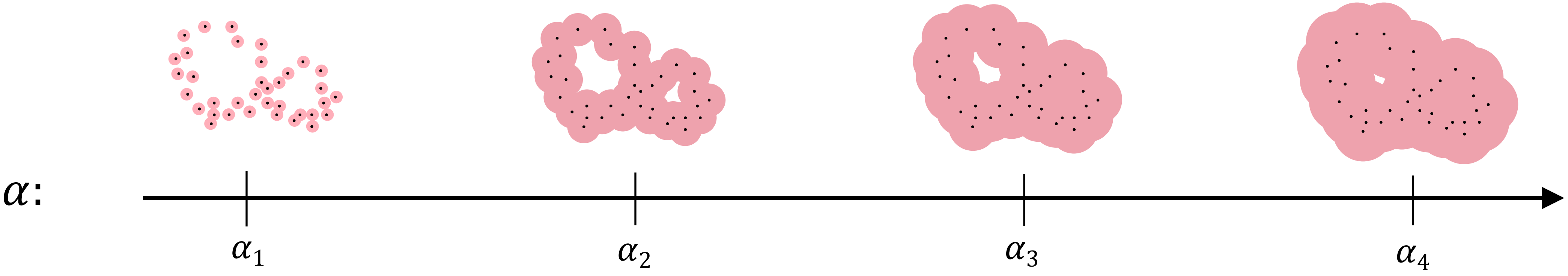

- Solution:
  - While there are infinitely many values for α, our data is still “finite” (e.g., the above point cloud contains finitely many points)

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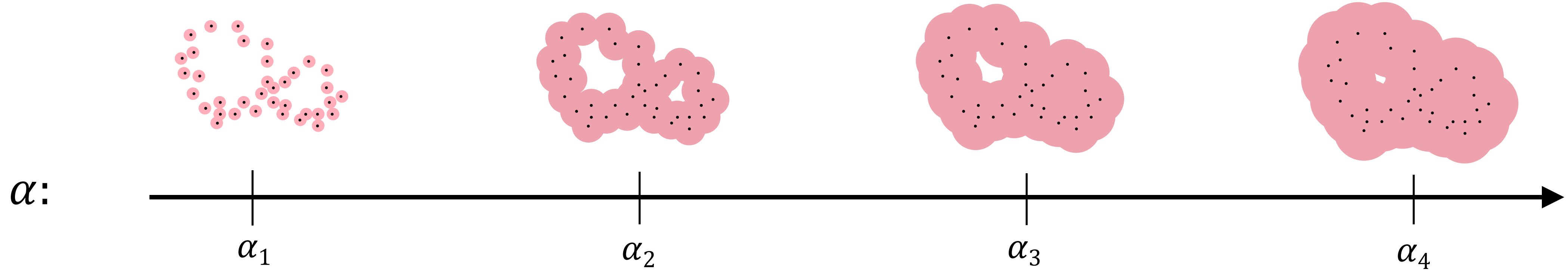

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  - This means that there are only finitely many values of α where the topological space “essentially changes”

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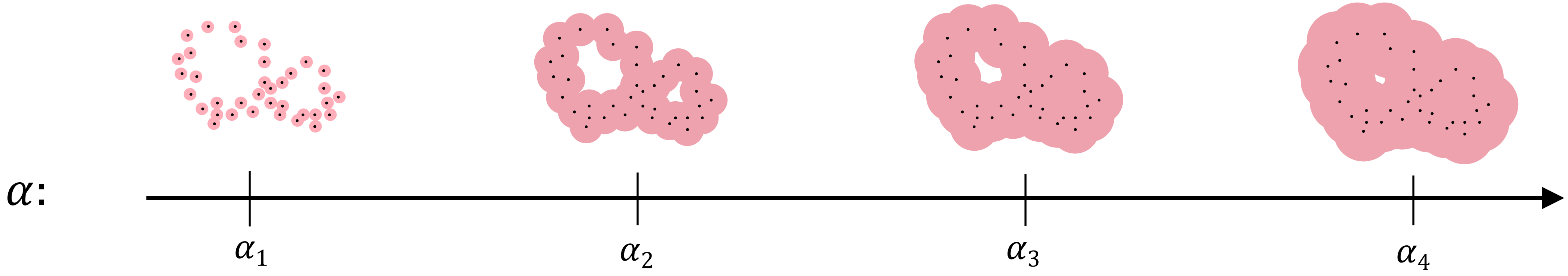
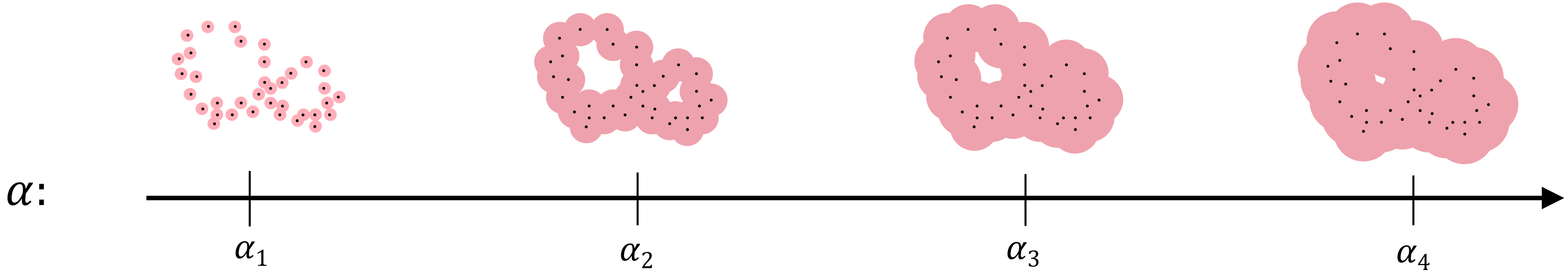


- Solution:
  - While there are infinitely many values for α, our data is still “finite” (e.g., the above point cloud contains finitely many points)
  - This means that there are only finitely many values of α where the topological space “essentially changes”
  - So we only need to record finitely many spaces in computer

“The growing space”



- Remark
  - We will not be very accurate on what the “essential changes” mean here (should be clearer later)

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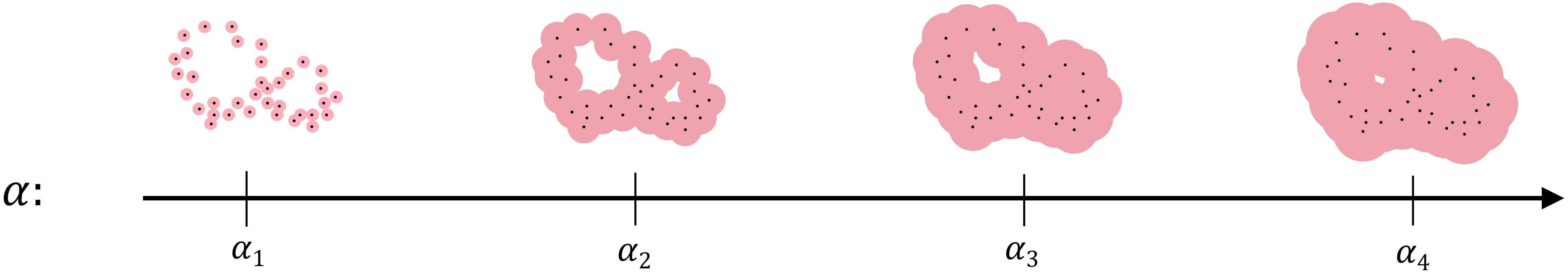

- Remark
  - We will not be very accurate on what the “essential changes” mean here (should be clearer later)
  - BTW, these values where topological space “essentially changes” are called critical values
  - Critical values are important concepts in “Morse theory”, but we will not go very deep on it in this course

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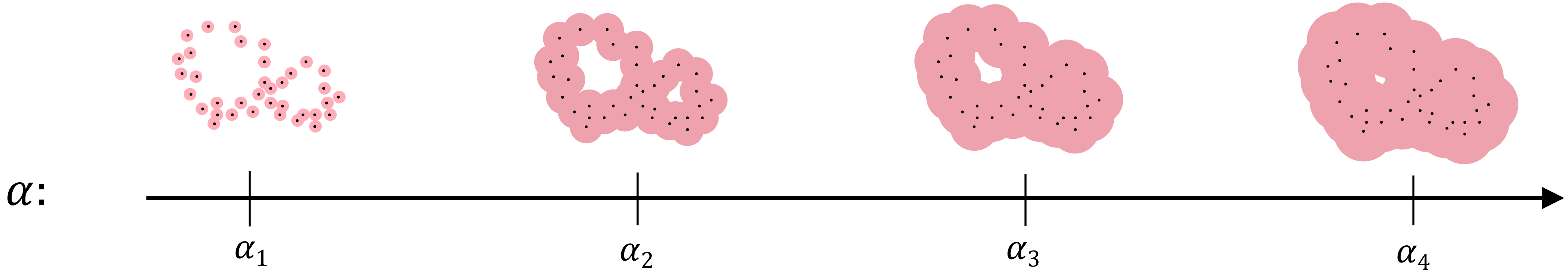
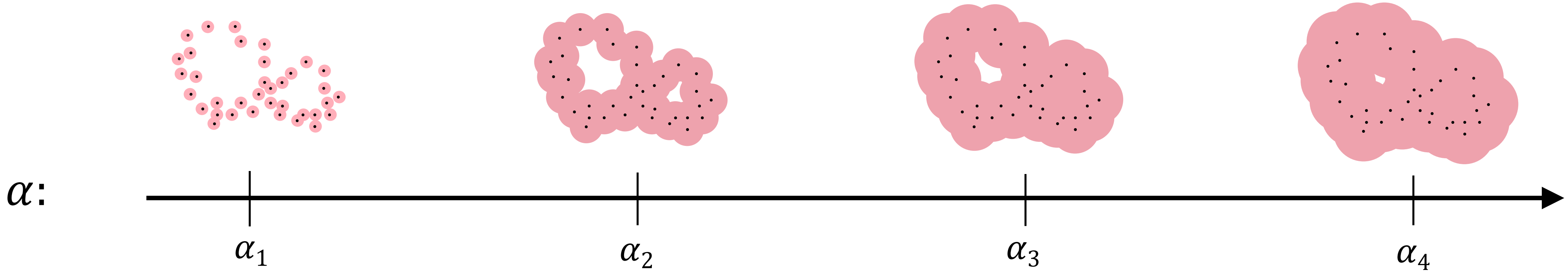


- Problem 2:

“The growing space”



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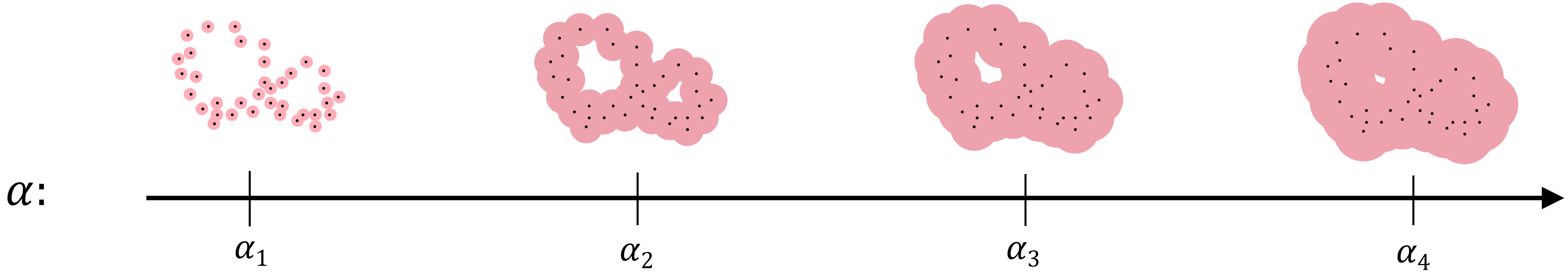

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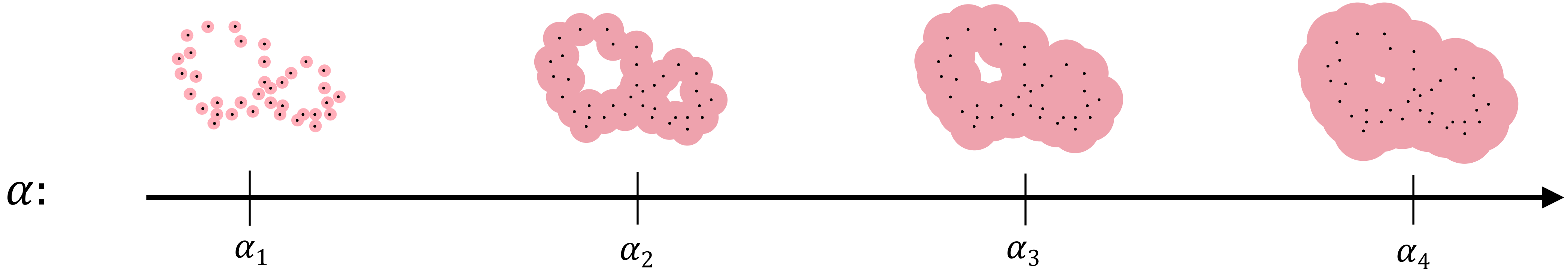
    - Even there are finitely many spaces to record, we still need a way to represent each topological space in computer
- Solution:
    - Using simplicial complexes!

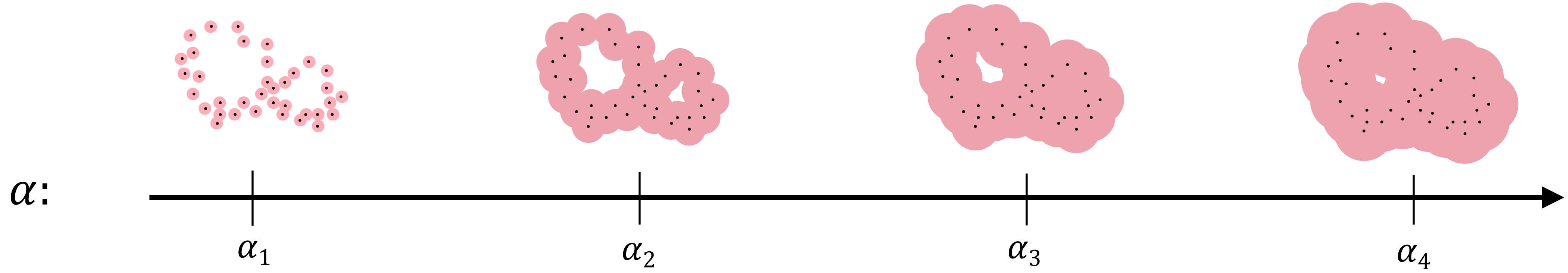
Filtration



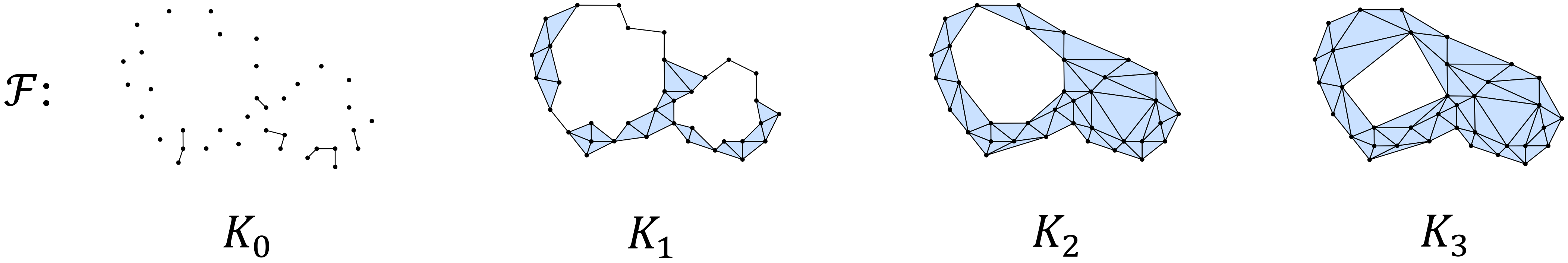
- Hence, the "growing space" in computer is represented by a finite sequence of simplicial complexes, called a **filtration**, which is typically denoted by a calligraphic letter $\mathcal{F}$,

$$\mathcal{F}:\ K_0, K_1, \ldots, K_m$$

Filtration



- **Below** is an example of a filtration:



Filtration

- Another example:

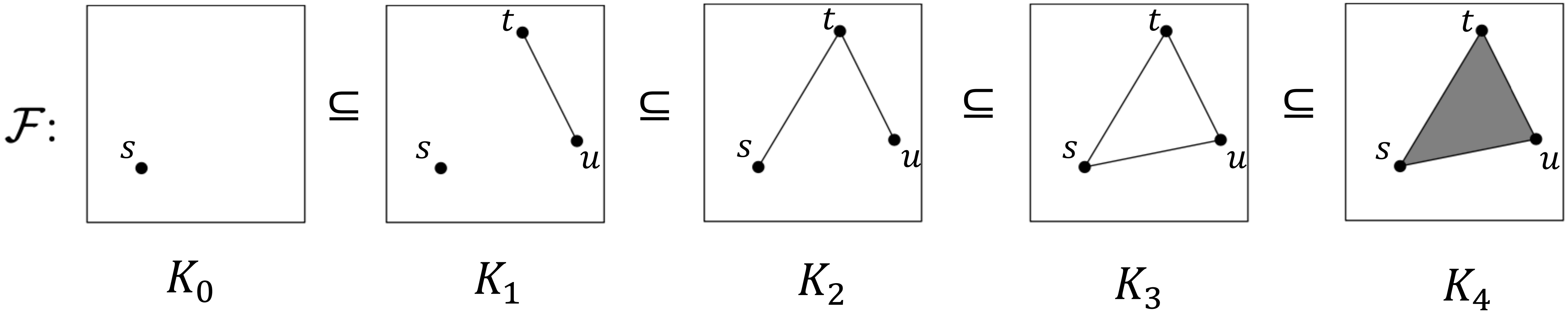


Image source: Patrick Schnider. Introduction to Topological Data Analysis Lecture Notes FS 2023

Filtration

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- How do we account for the fact that the spaces (complexes) grow?
- Answer: We make sure the complexes “grow” by making sure the previous complex is a “subset” (subcomplex) of the next complex.
- **Definition**: A **filtration** is a nested sequence of simplicial complexes

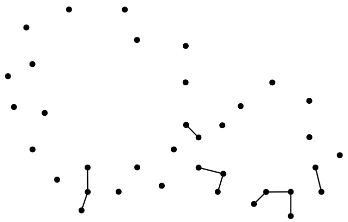
$$\mathcal{F}:\ K_0 \subseteq K_1 \subseteq \cdots \subseteq K_m$$

such that each K_i is a subcomplex of K_{i+1}.

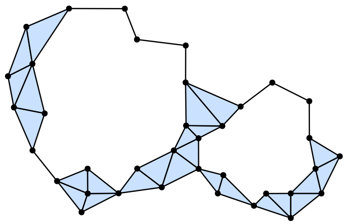
Filtration

- Example:

$\mathcal{F}:$



$\subseteq$



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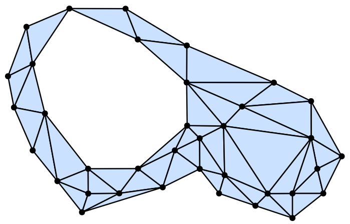

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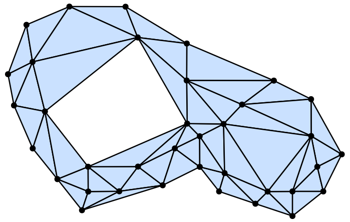

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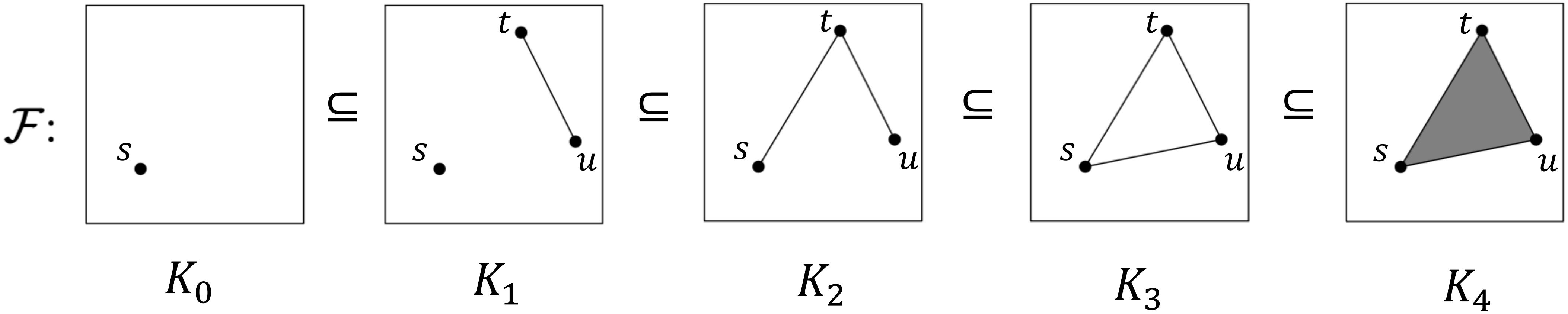

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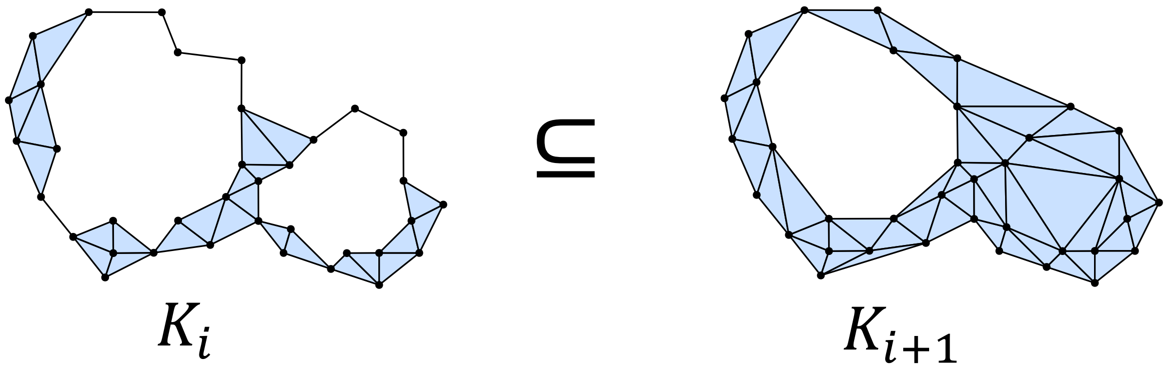
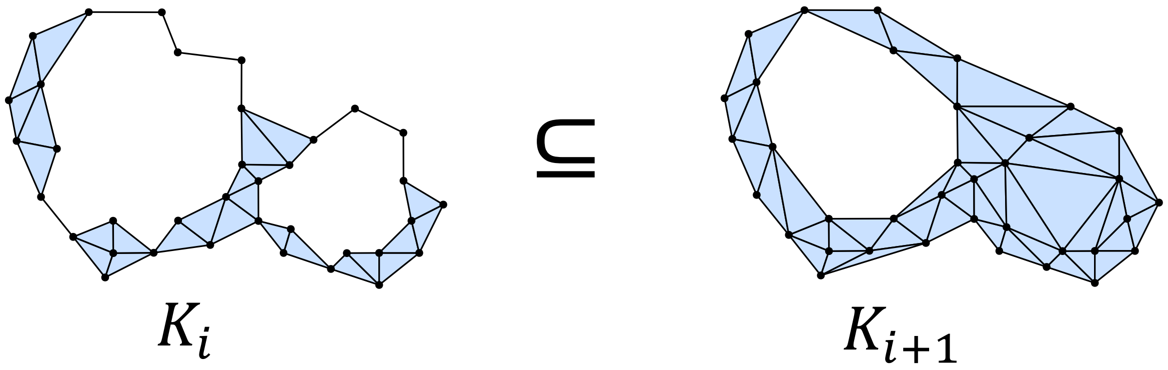


- Now we want to further interpret a filtration
- For this, we focus on a single inclusion in a filtration

Filtration



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- Since it’s an inclusion, the difference of the two complexes is that K_{i+1} has some additional simplices than K_i

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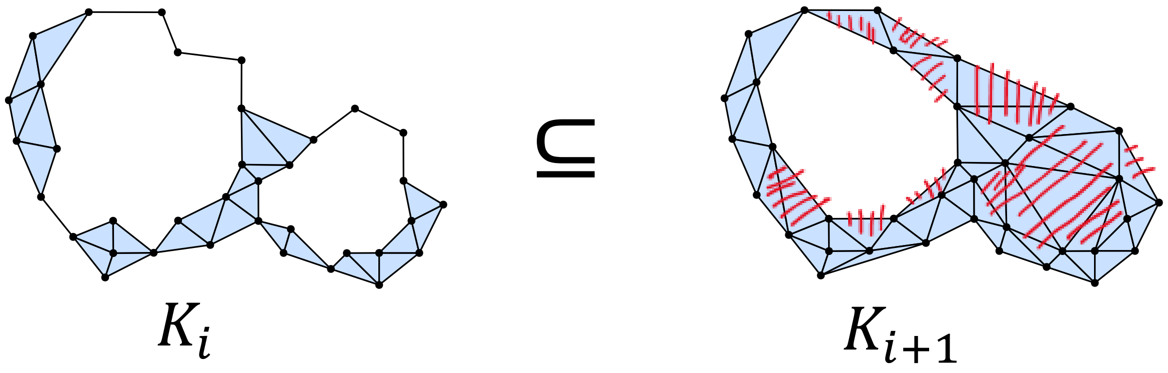

$K_i \subseteq K_{i+1}$

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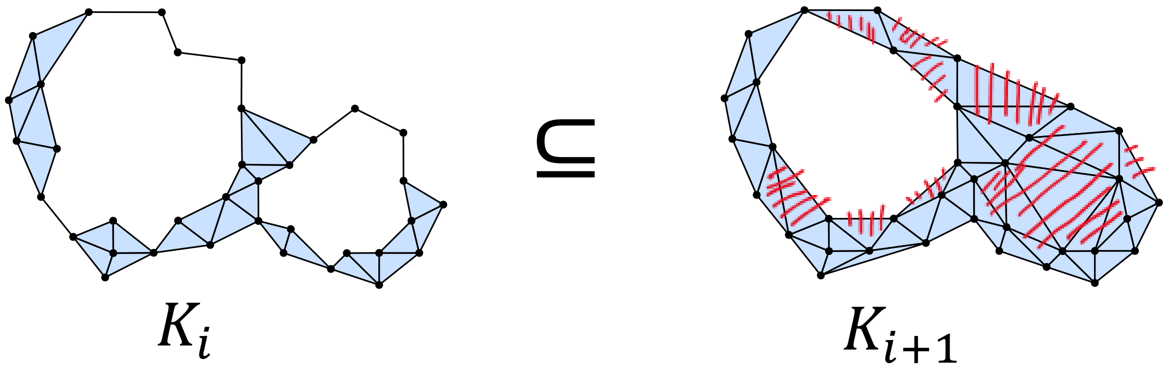

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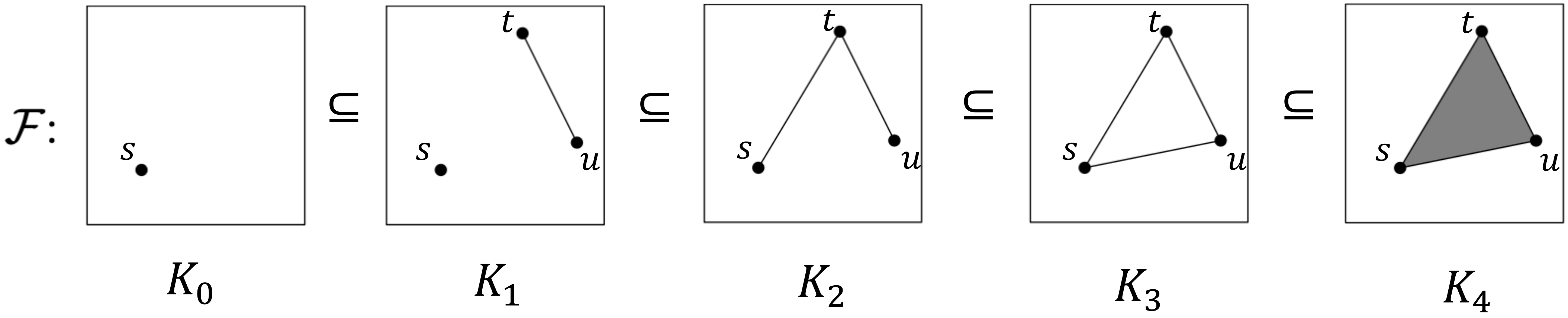
- For this, we focus on a single inclusion in a filtration
- Since it’s an inclusion, the difference of the two complexes is that K_{i+1} has some additional simplices than K_i
- So we can consider each inclusion $K_i \subseteq K_{i+1}$ in a filtration

$$\mathcal{F}\colon\ K_0 \subseteq K_1 \subseteq \cdots \subseteq K_m$$

as an insertion of a bunch of simplices

Filtration

For the example:



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Filtration

- More **regulations:** For a filtration

$$\mathcal{F}:\ K_0 \subseteq K_1 \subseteq \cdots \subseteq K_m$$

we typically let the first complex K_0 be empty, and call the last complex K_m the "total complex" (because it contains all simplices) and denote it as K.

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- (1) is easy to see. To see (2), suppose that σ is added later than τ. Then at a certain time, τ is already added to a complex K_i but σ is not in K_i yet. This contradicts the fact that any face of a simplex in the complex is also in the complex.

PD for Filtration

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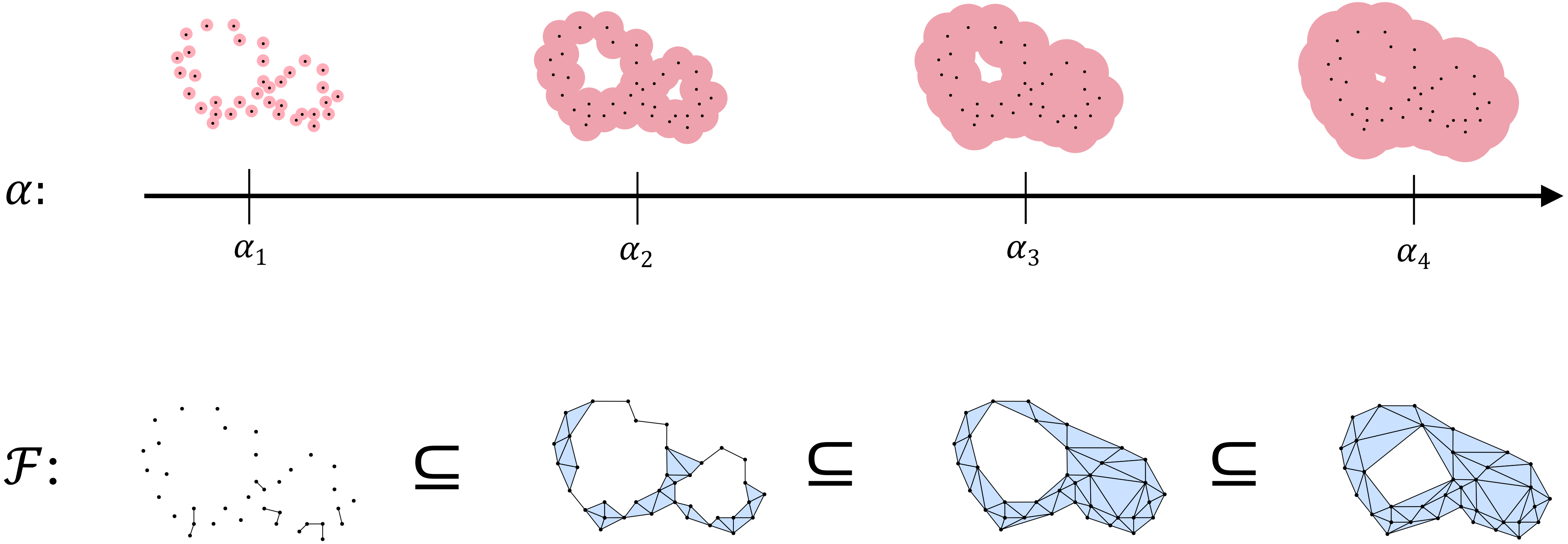
- Filtrations are inputs to the persistent homology pipeline that we want to formalize
- But still we need to formally define a PD on a filtration of simplicial complexes
- Previously, we only saw some examples of PD on a sequence of “growing spaces”, which are not exactly a filtration of complexes.
- Moreover, we haven’t really formally defined a PD on a growing space other than showing some examples

PD for Filtration

- Eventually, we will show that, PDs can be formally defined on both a “growing space” (which is continuous) and a “filtration of complexes” (which is discrete).



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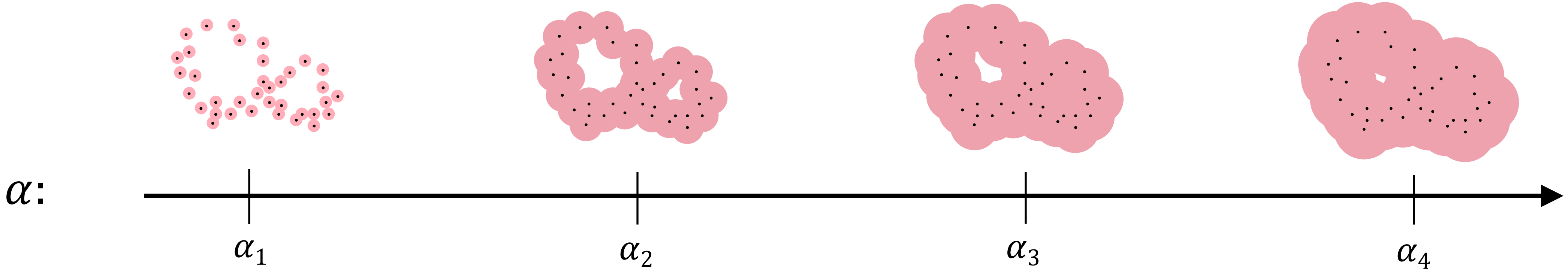
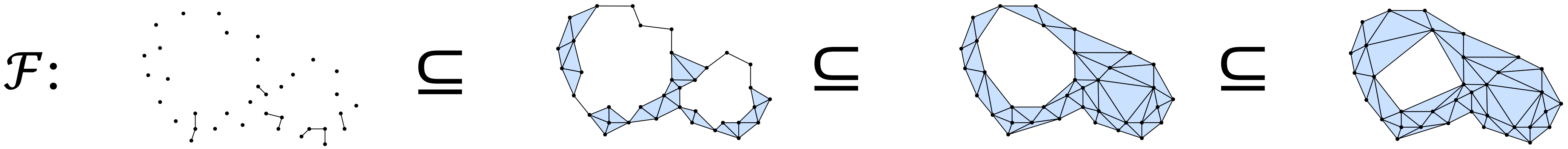
- Eventually, we will show that, PDs can be formally defined on both a "growing space" (which is continuous) and a "filtration of complexes" (which is discrete).
- We sometimes call the former one a "continuous" filtration and latter a "discrete" filtration (by default, a "filtration" without modifiers is always a discrete one).



"Continuous" filtration



"Discrete" filtration

PD for Filtration

- However, formally defining PD on a continuous or a discrete filtration needs a lot of mathematics (a lot of algebra, category theory, or quiver theory), which is beyond the scope of the course.
- So to understand the definition of a PD, we shall see how to compute a PD on a discrete filtration.
- Things can get a bit technical from now on, but I want to stress that this course is trying to focus on applications. So these technical contents are mainly supposed to help build solids skills on applying persistent homology.

Simplex-wise Filtration

- For computing persistence diagram, we focus on a special type of filtration.
- **Definition**: A **simplex-wise filtration** is a filtration such that each consecutive complexes differ by only a single simplex, i.e., in

$$\mathcal{F}:\ \emptyset = K_0 \subseteq K_1 \subseteq \cdots \subseteq K_m = K$$

for each inclusion $K_{i-1} \subseteq K_i$, we have that K_i is derived from K_{i-1} by inserting a single simplex typically denoted σ_i.

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- Because of the constructions, we can also consider a simplex-wise filtration

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as a sequence of simplices $\sigma_0, \sigma_1, \dots, \sigma_{m-1}$ inserted one by one following the order.

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as a sequence of simplices $\sigma_0, \sigma_1, \ldots, \sigma_{m-1}$ inserted one by one following the order.

- **Fact**: Each general filtration (not necessarily simplex-wise) can be made into a simplex-wise one by padding additional complexes (or expanding the inclusions)

Simplex-wise Filtration

- K_0 to K_1: insert vertices t and u and edge tu
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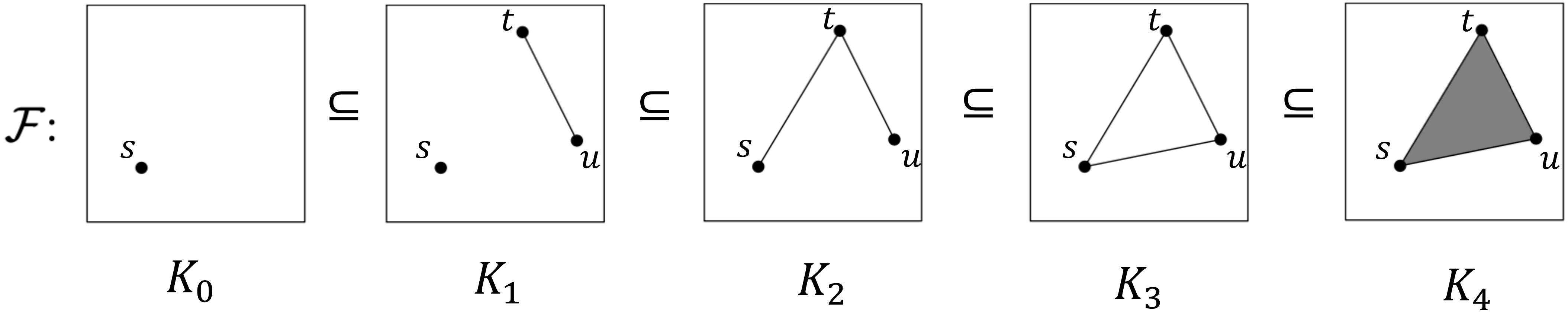

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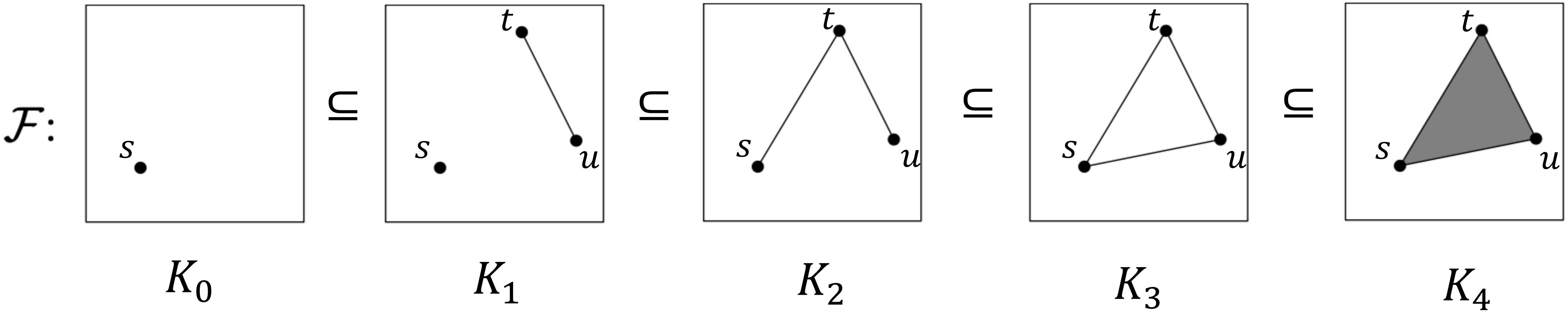


- To convert to simplex-wise, only need to add an empty complex at the beginning and insert two additional complexes between K_0 to K_1.

Image source: Patrick Schnider. Introduction to Topological Data Analysis Lecture Notes FS 2023

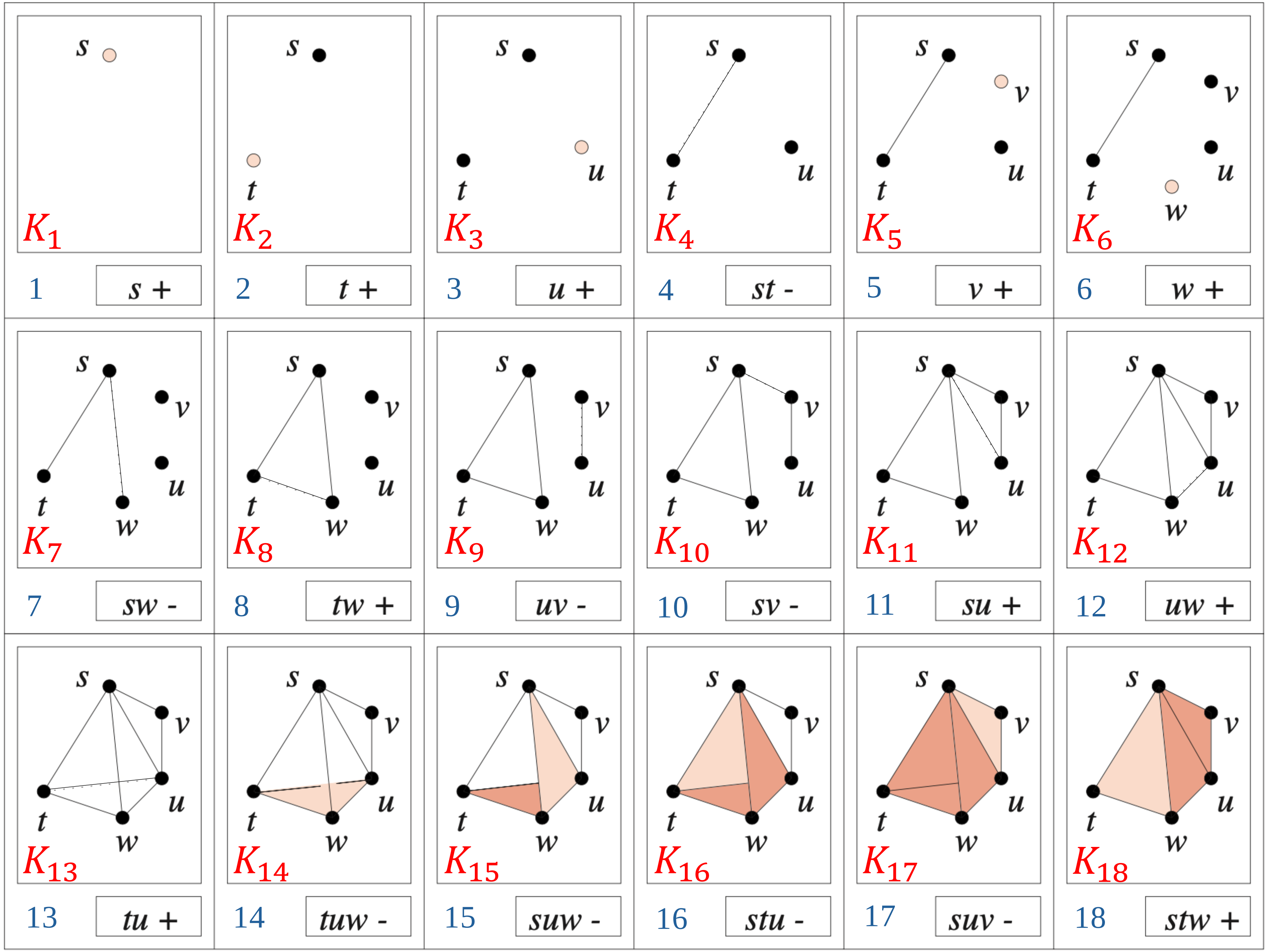
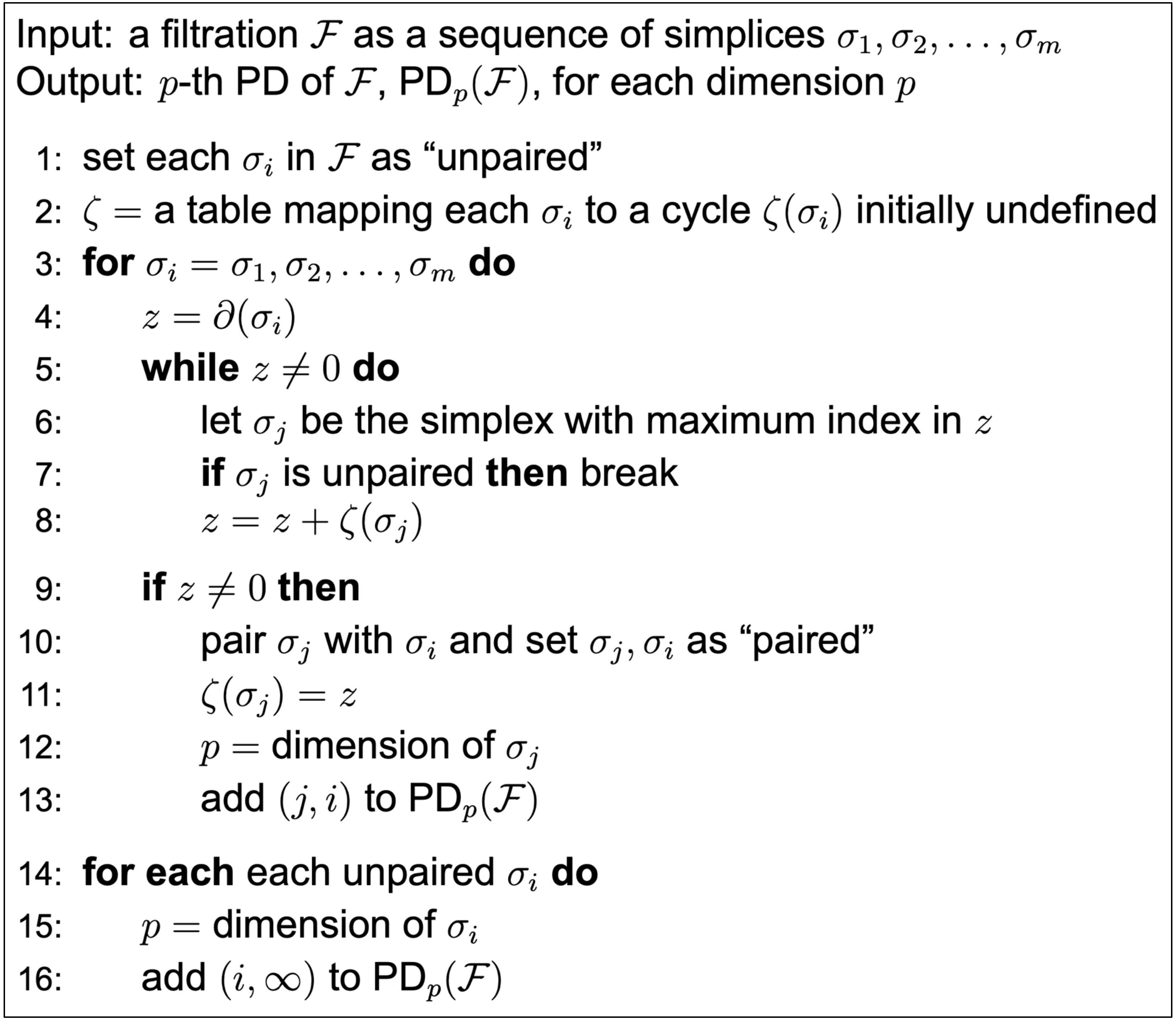


Image source: Edelsbrunner, Letscher, and Zomorodian. Topological persistence and simplification.

Algorithm

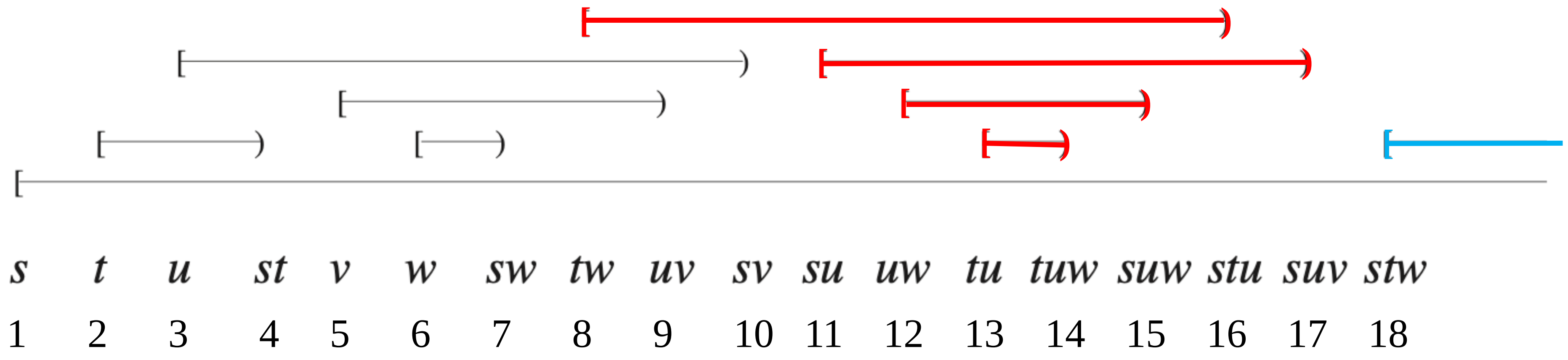
- Notice that the input filtration $\mathcal{F}$ must be simplex-wise



Input: a filtration $\mathcal{F}$ as a sequence of simplices $\sigma_1, \sigma_2, \ldots, \sigma_m$
Output: p-th PD of $\mathcal{F}$, $\mathrm{PD}_p(\mathcal{F})$, for each dimension p

```
set each $\sigma_i$ in $\mathcal{F}$ as “unpaired”
$\zeta$ = a table mapping each $\sigma_i$ to a cycle $\zeta(\sigma_i)$ initially undefined
**for** $\sigma_i = \sigma_1, \sigma_2, \ldots, \sigma_m$ **do**
    $z = \partial(\sigma_i)$
    **while** $z \neq 0$ **do**
        let $\sigma_j$ be the simplex with maximum index in $z$
        **if** $\sigma_j$ is unpaired **then** break
        $z = z + \zeta(\sigma_j)$
    **if** $z \neq 0$ **then**
        pair $\sigma_j$ with $\sigma_i$ and set $\sigma_j, \sigma_i$ as “paired”
        $\zeta(\sigma_j) = z$
        $p$ = dimension of $\sigma_j$
        add $(j, i)$ to $\mathrm{PD}_p(\mathcal{F})$
**for each** each unpaired $\sigma_i$ **do**
    $p$ = dimension of $\sigma_i$
    add $(i, \infty)$ to $\mathrm{PD}_p(\mathcal{F})$
```

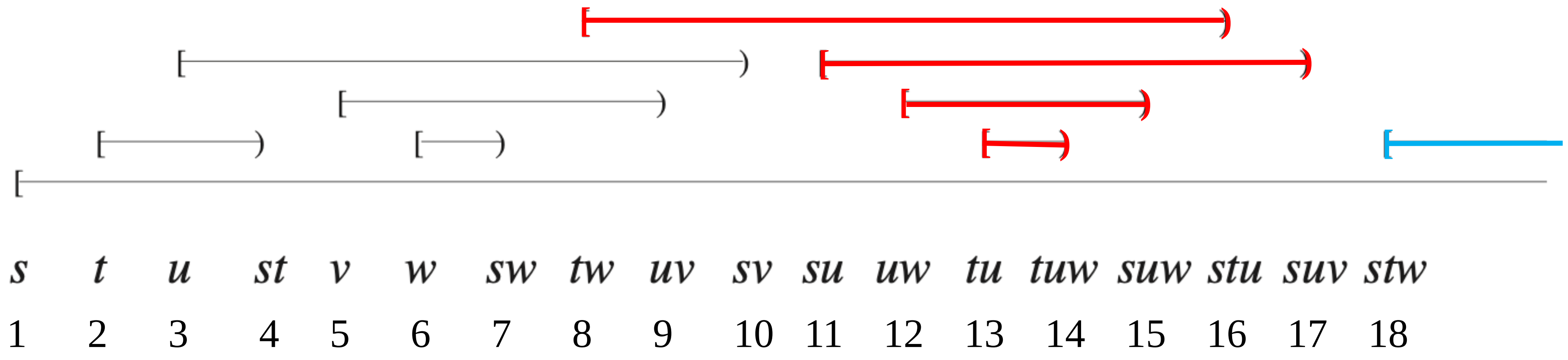
Resulting PD



- Black: PD_0
- Red: PD_1
- Blue: PD_2

Image source: Edelsbrunner, Letscher, and Zomorodian. Topological persistence and simplification.

Resulting PD



- Notice: instead of drawing each pair of birth / death as a point on 2D plane, we just let each pair of birth and death form an interval, indicating the "time" in which a certain homology hole persists (will see examples later)

Image source: Edelsbrunner, Letscher, and Zomorodian. Topological persistence and simplification.

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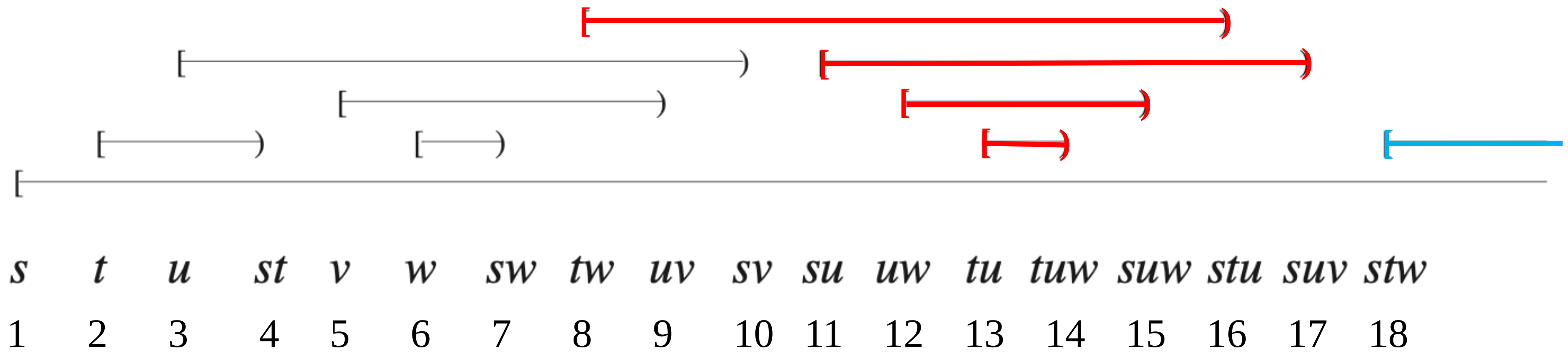

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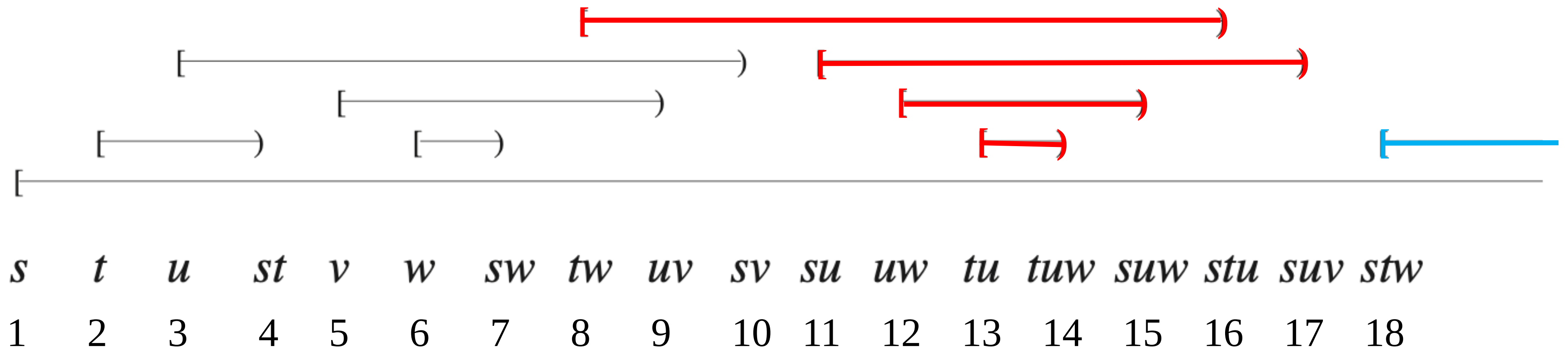

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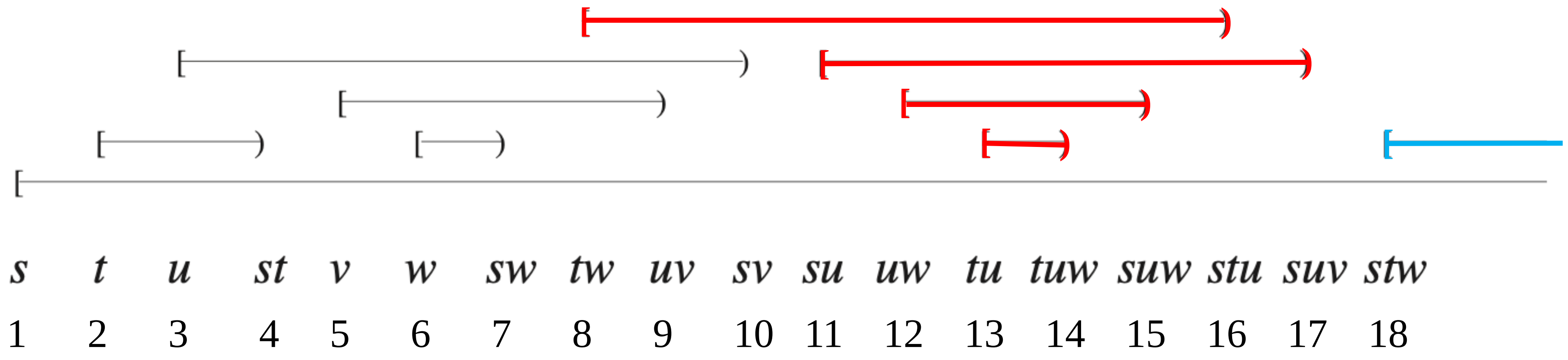

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- The above is also called the **persistence barcode**
- So persistence barcodes and persistence diagrams are just the same things displayed in different ways (we sometimes also use the two terms interchangeably)
- Also notice: In persistence barcode, we always draw each interval as left-closed, right open (there is a technical reason for this but explaining this a little beyond scope)

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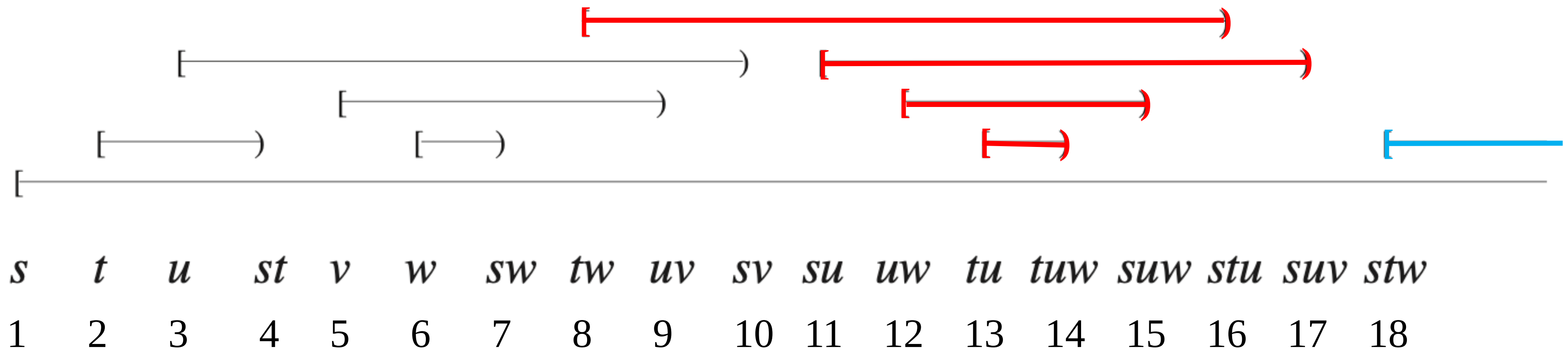

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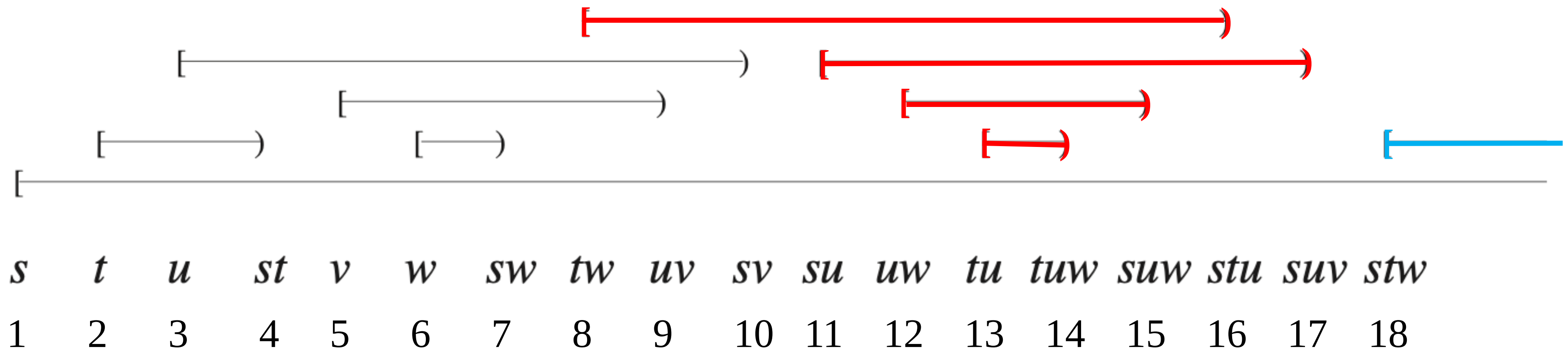

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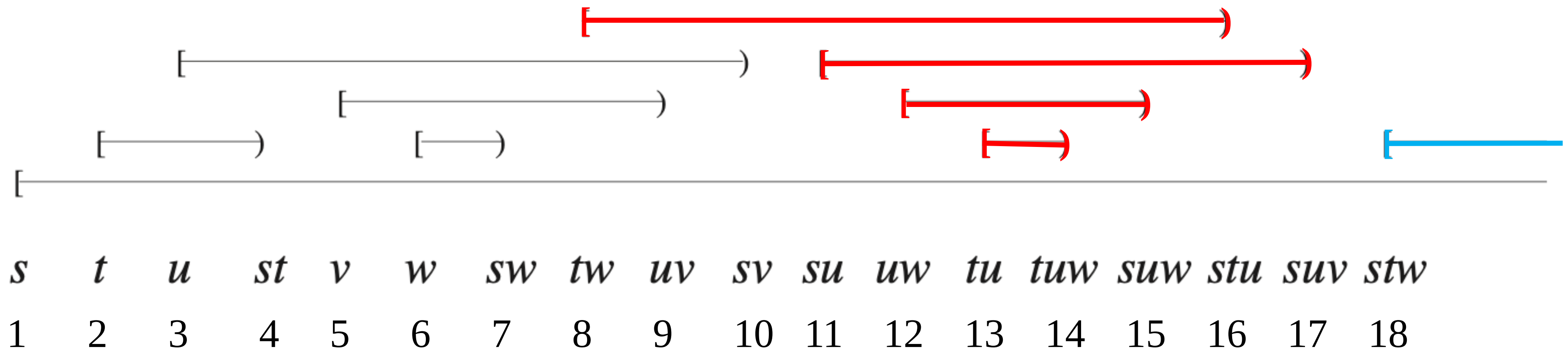

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- This $\zeta[\sigma_b]$ is also called the **representative** for the interval $[b, d)$.

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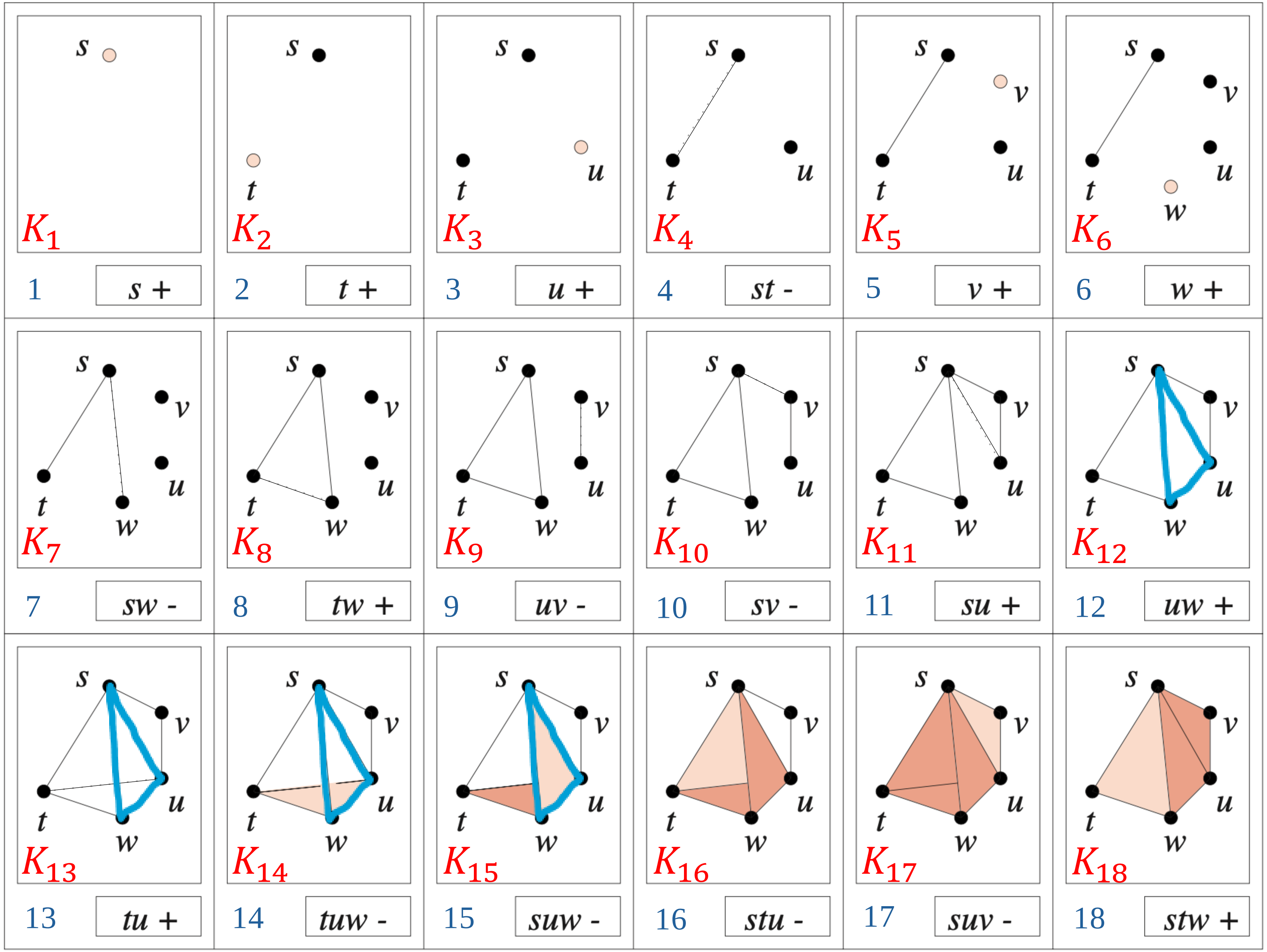

1d hole captured by interval $[12,15) \in PD_1$

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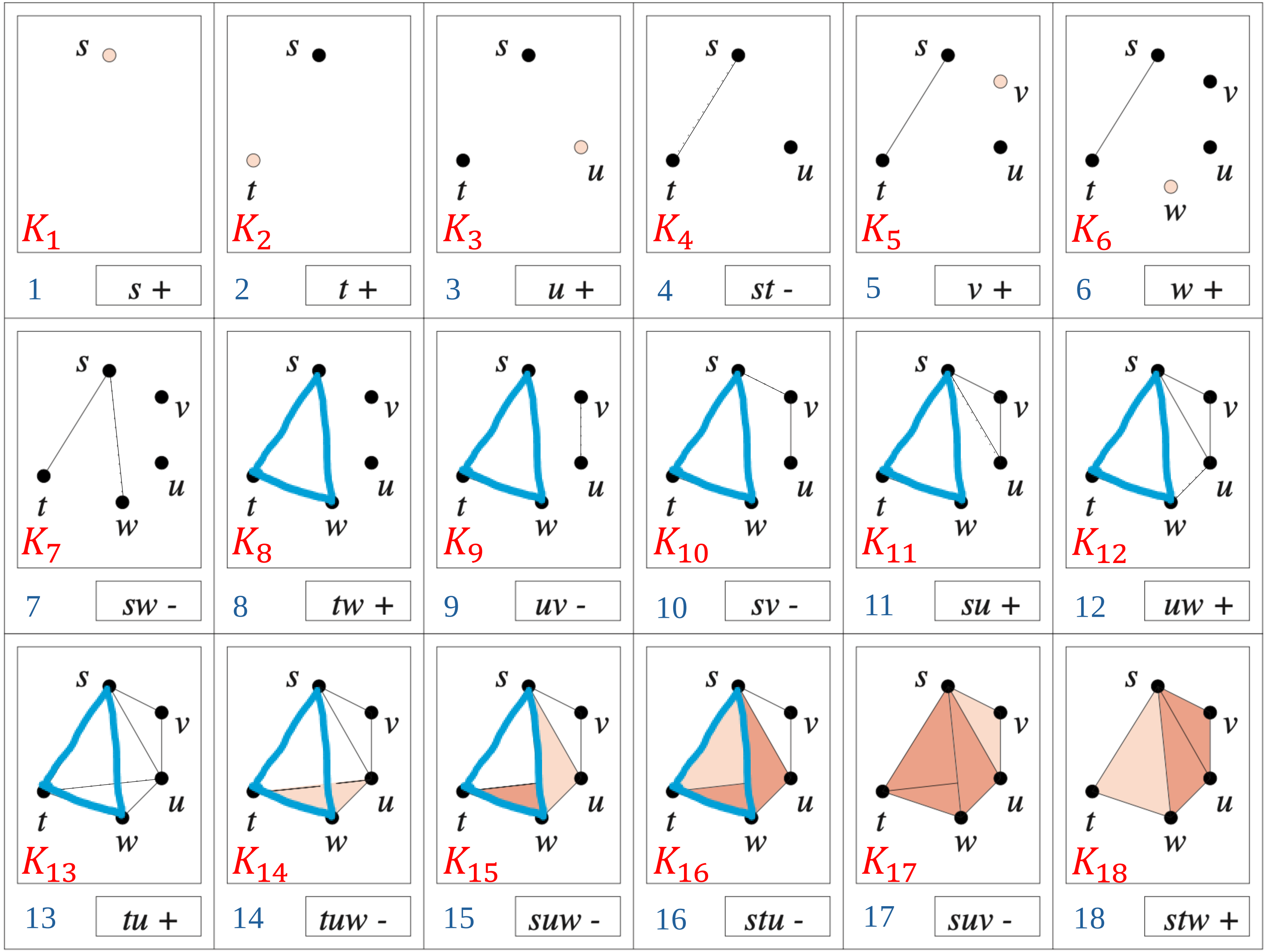

1d hole captured by interval $[8,16) \in PD_1$

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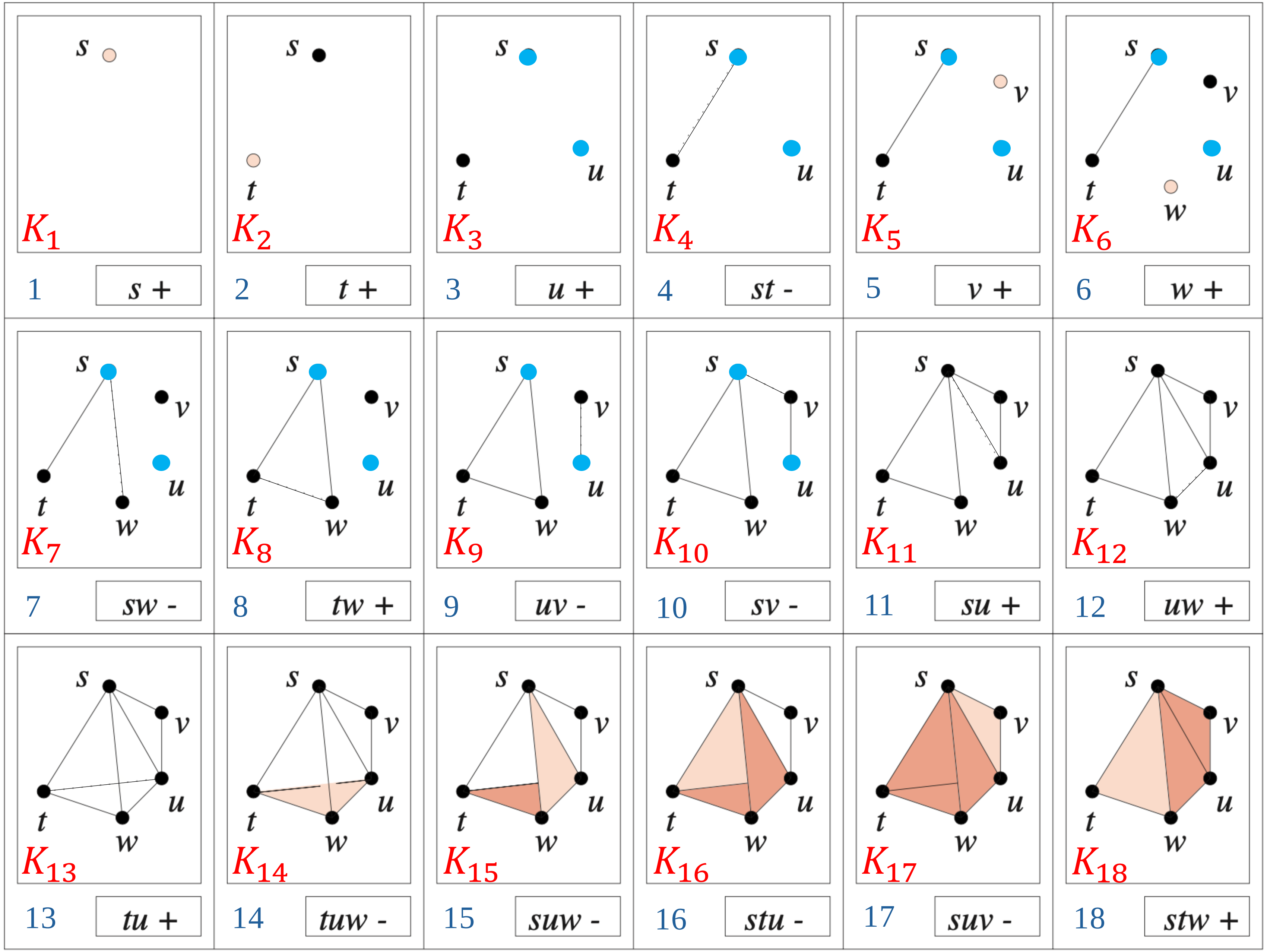

- 0d hole captured by interval $[3,10) \in PD_0$, which is the gap between s and u.
- The gap disappears when the two points become connected

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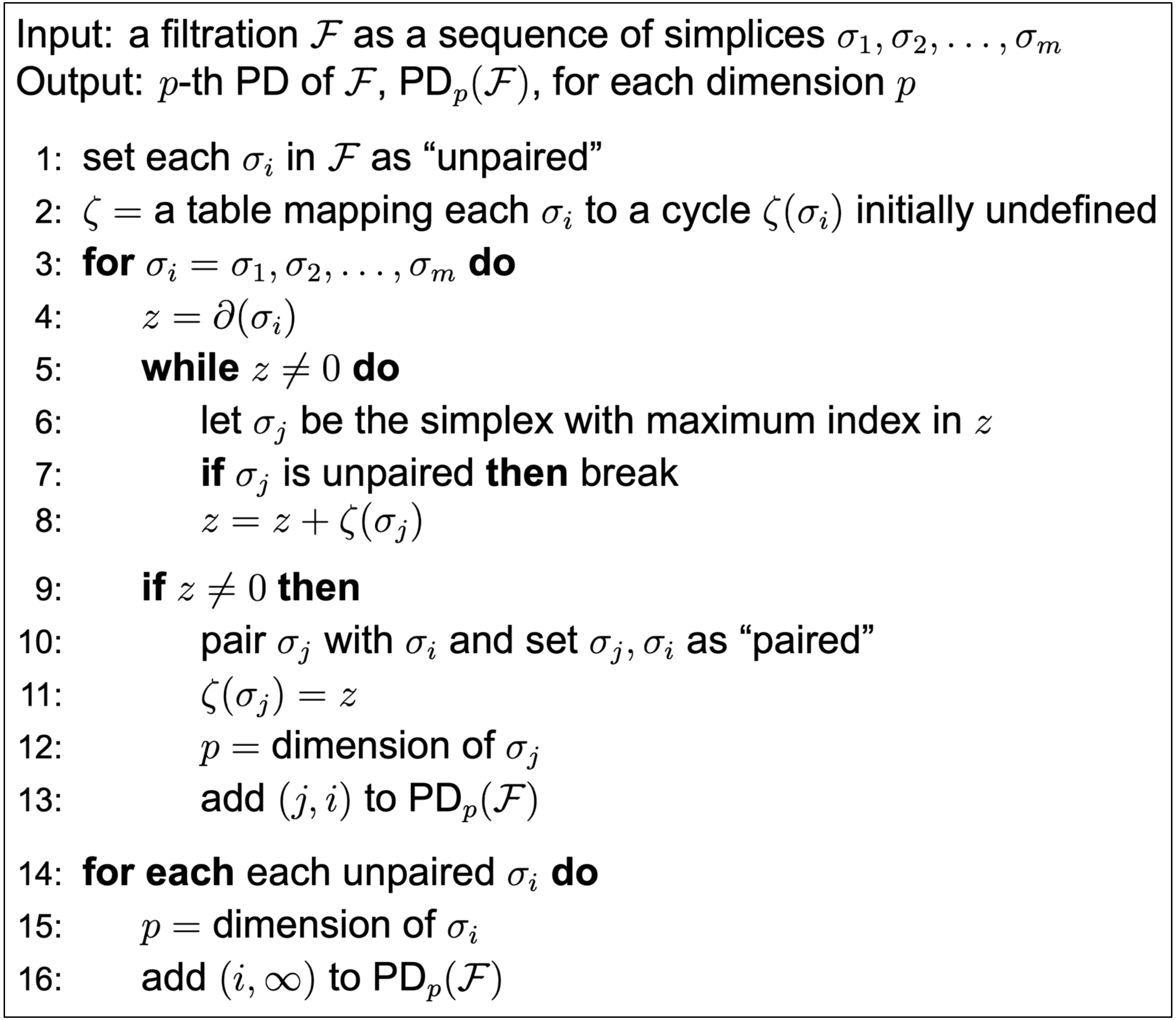
More interpretations of the algorithm:

- When processing each σ_i, if the while loop ends with $z = 0$, then the simplex σ_i is called **positive**



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Output: p-th PD of $\mathcal{F}$, $\mathrm{PD}_p(\mathcal{F})$, for each dimension p

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More interpretations of the algorithm:

- When processing each σ_i, if the while loop ends with $z = 0$, then the simplex σ_i is called **positive**
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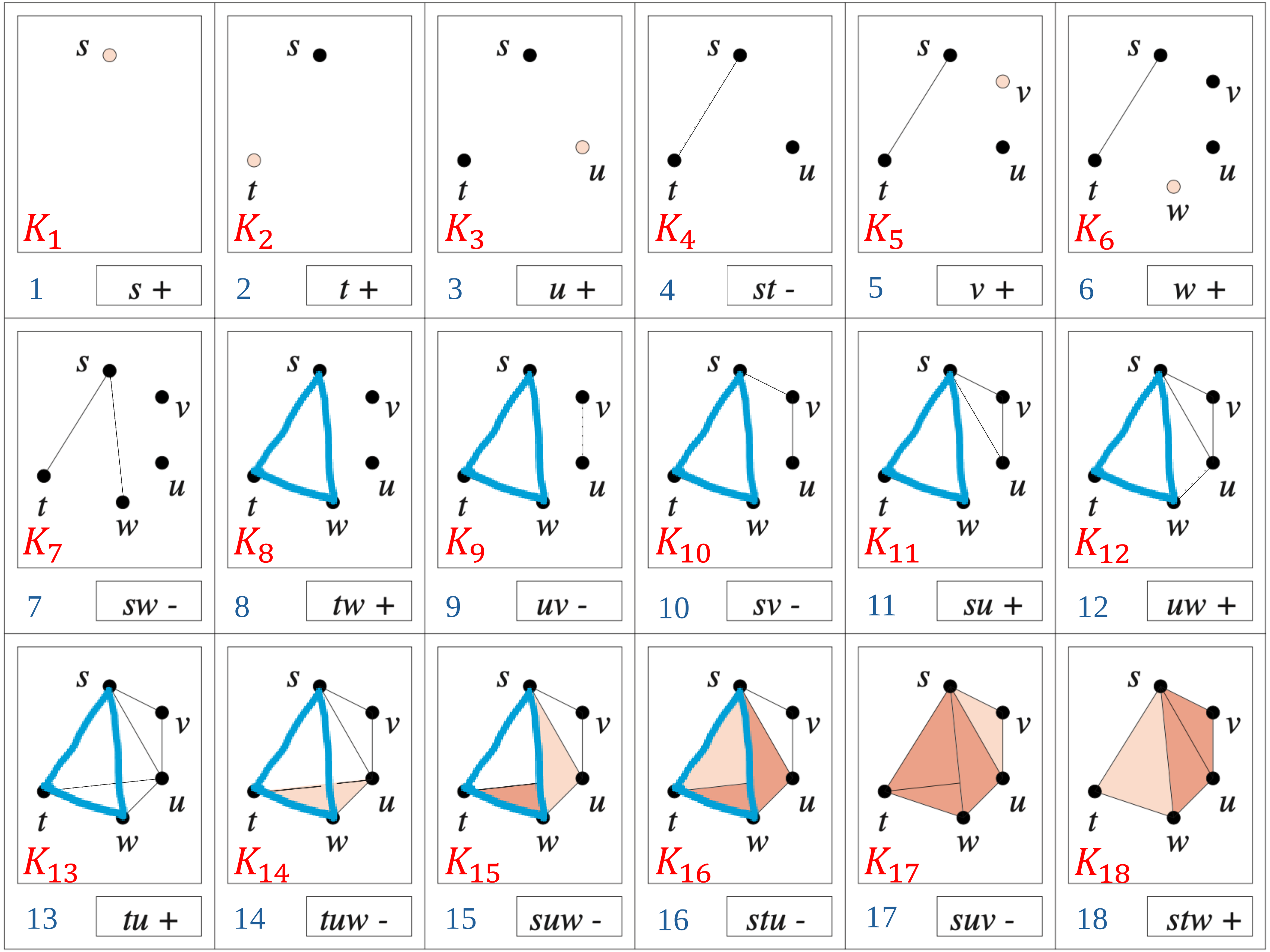
- E.g., inserting $\sigma_8 = tw$ creates the blue 1d hole



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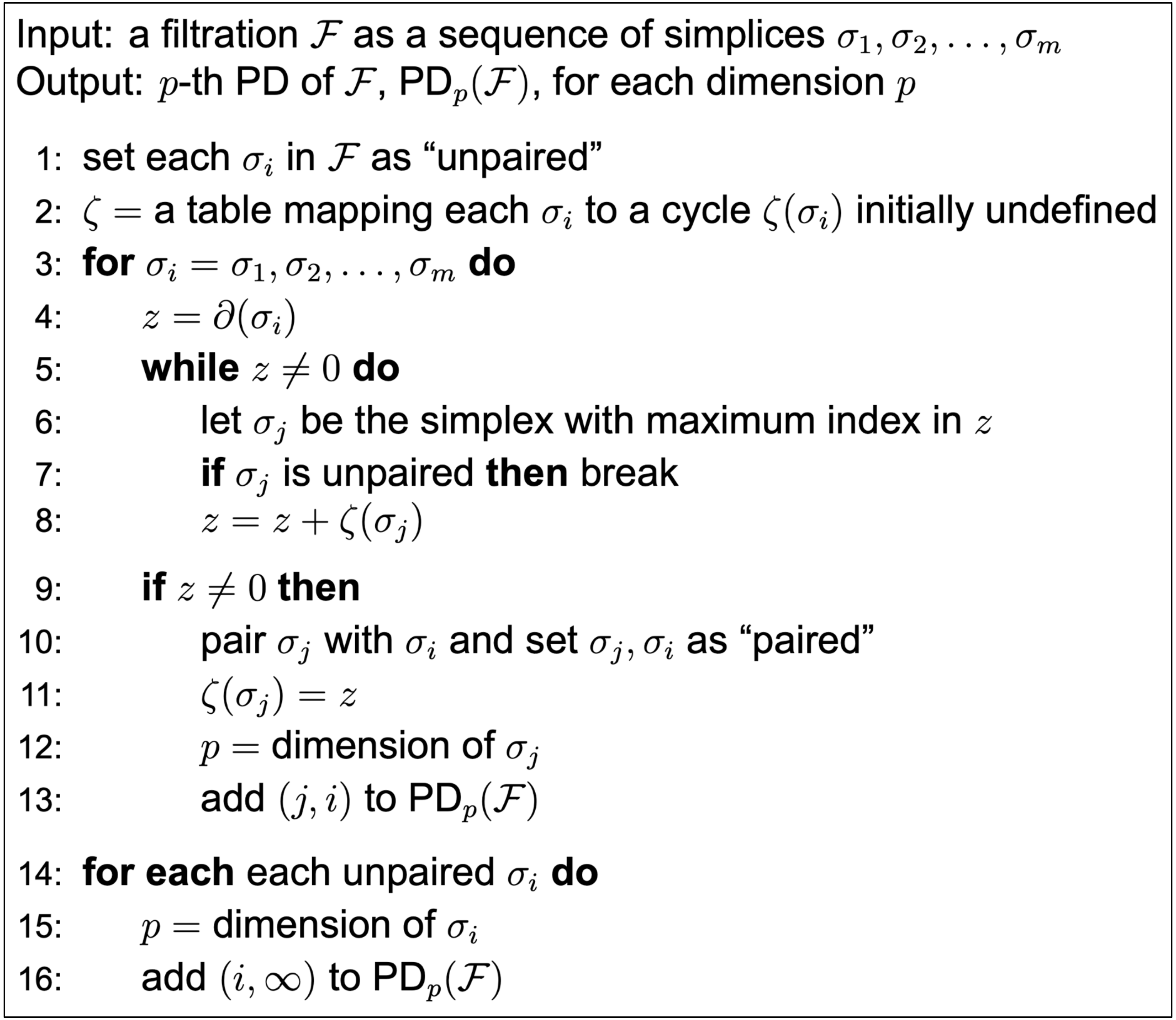
- If the while loop ends with $z \neq 0$, then the simplex σ_i is called **negative**



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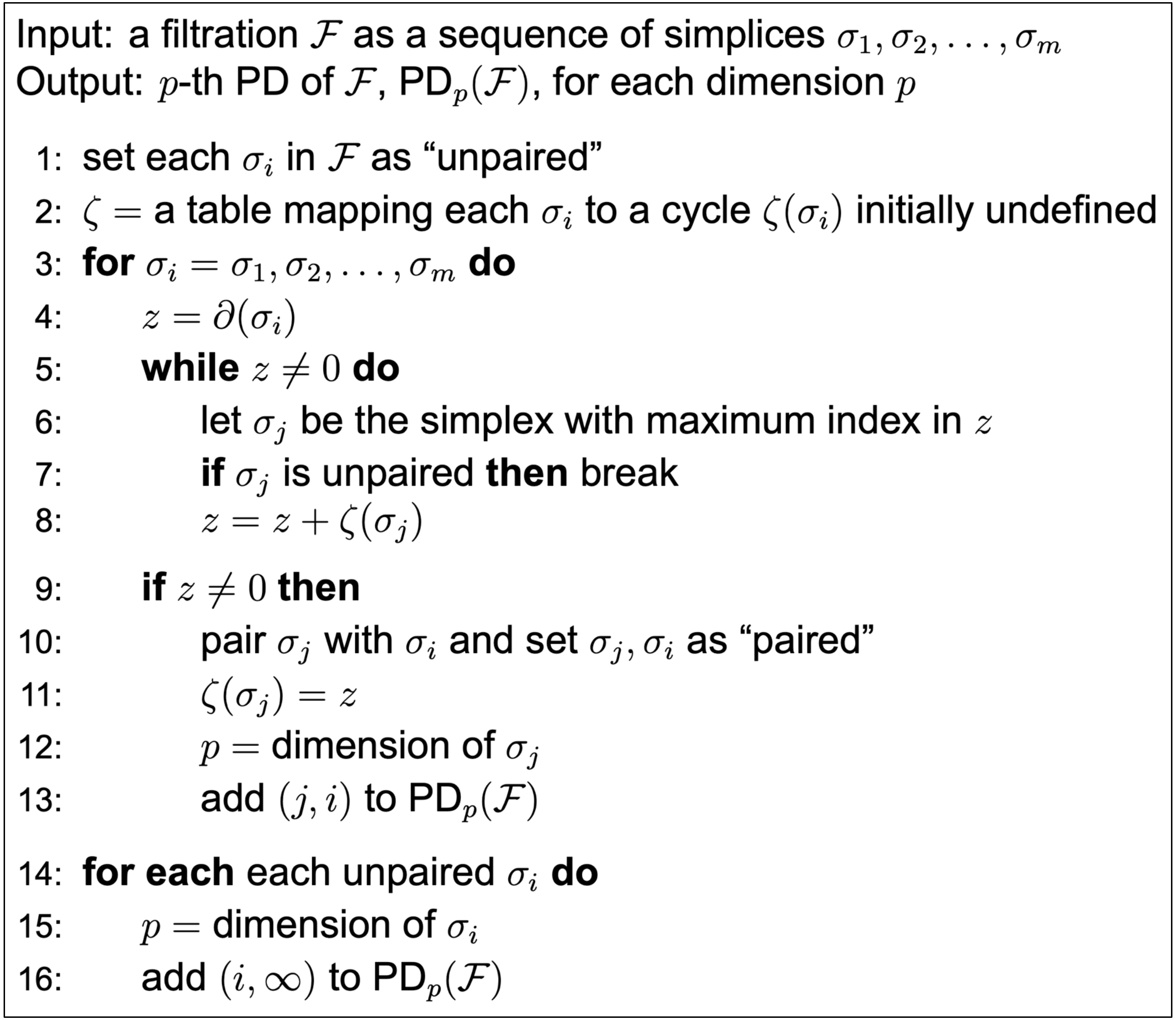
- It means that inserting σ_i creates a homology hole die (becomes trivial)



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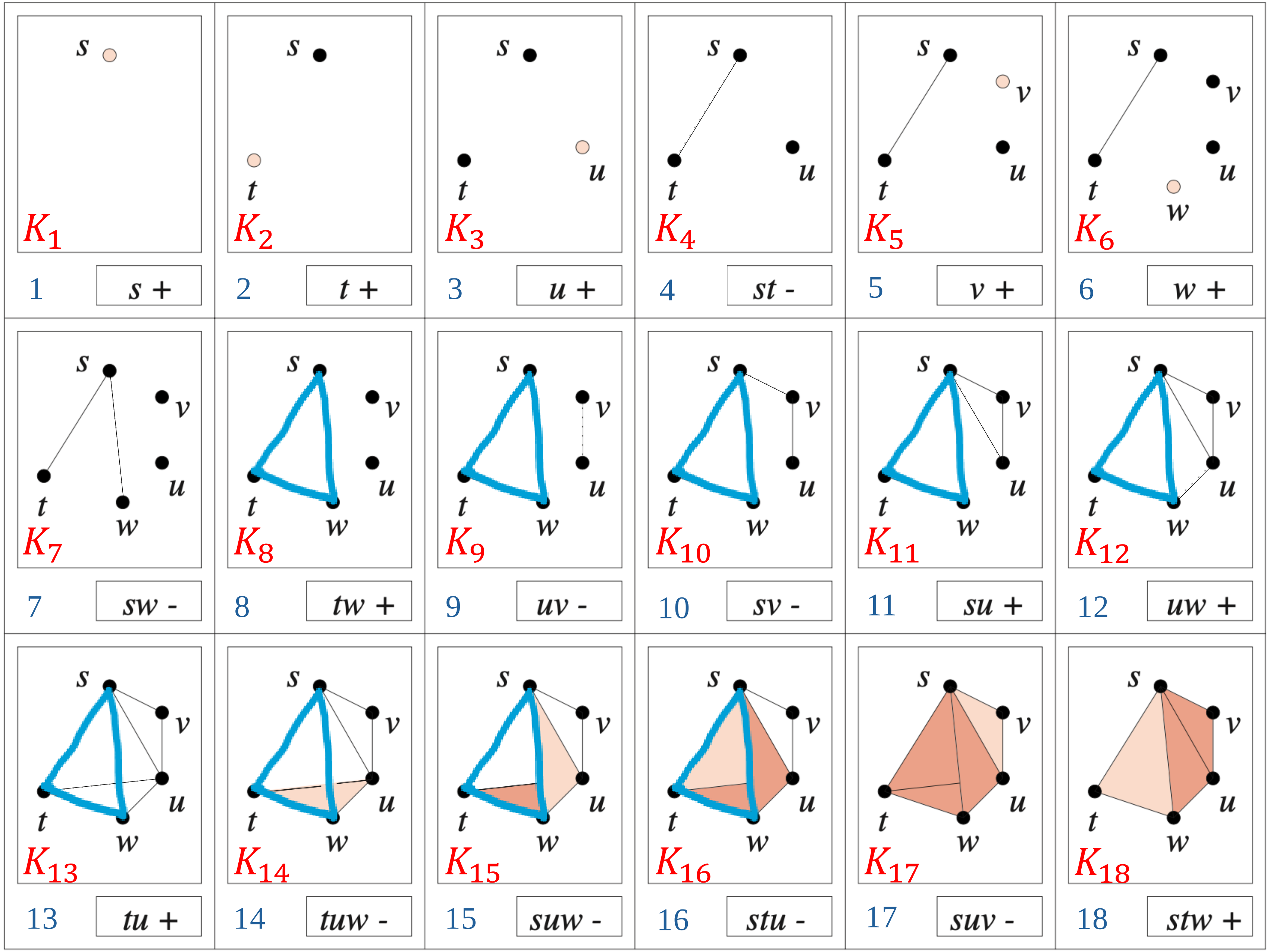
- E.g., inserting $\sigma_{16} = stu$ kills the blue 1d hole



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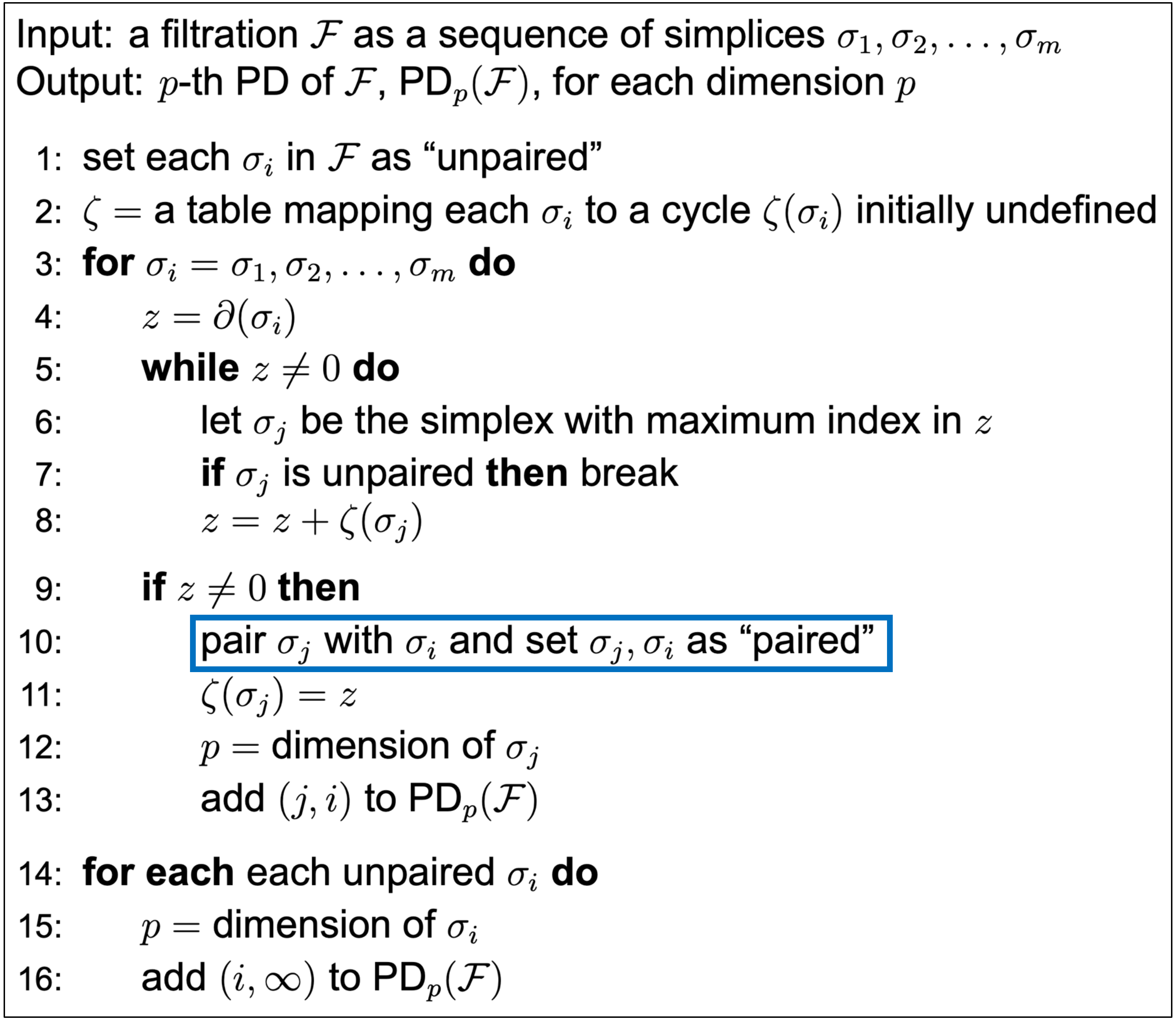
We have that line 10 in the algorithm is always pairing

- a positive simplex σ_j

with

- a negative simplex σ_i



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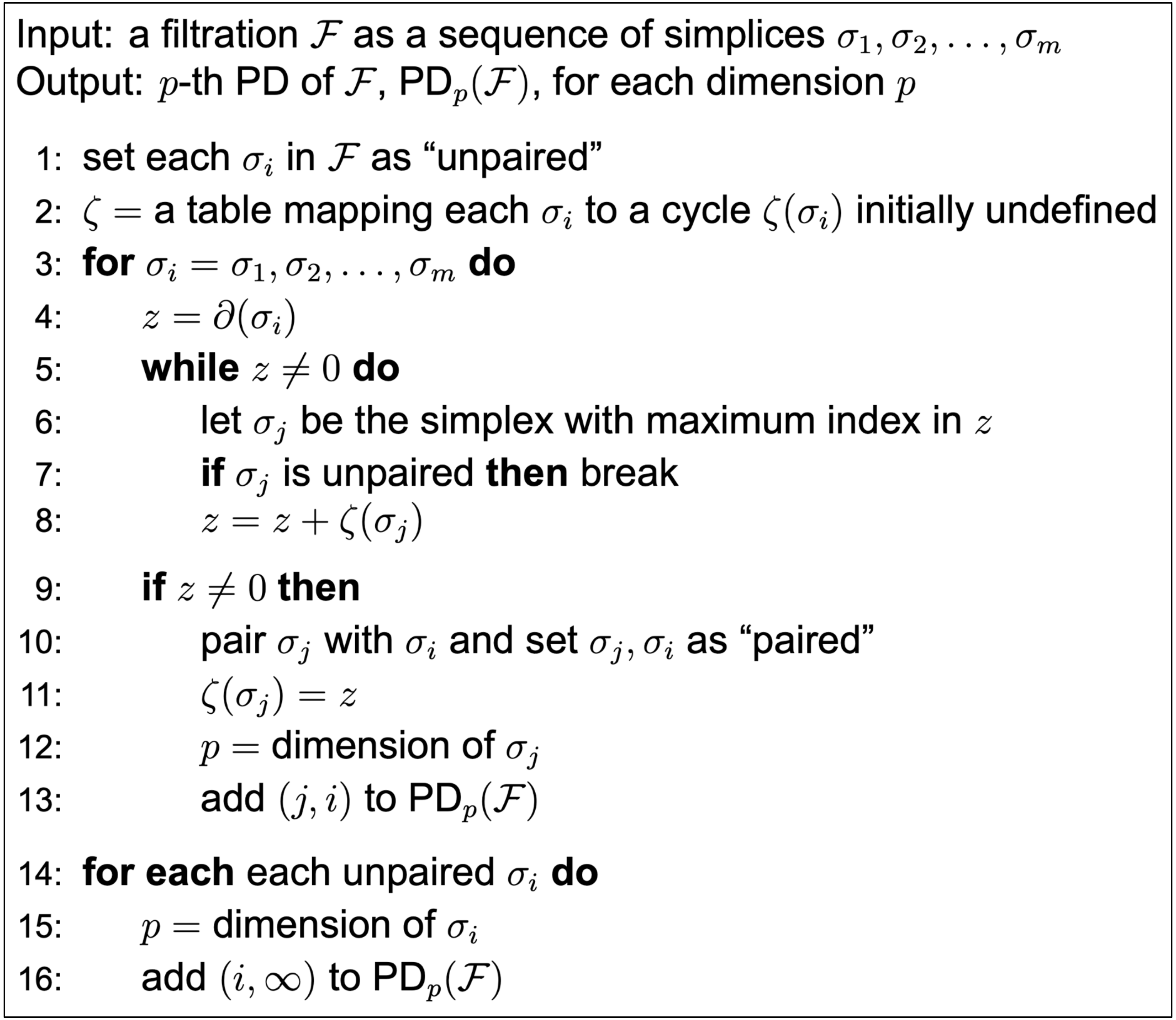
The algorithm takes $O(m^3)$ time:



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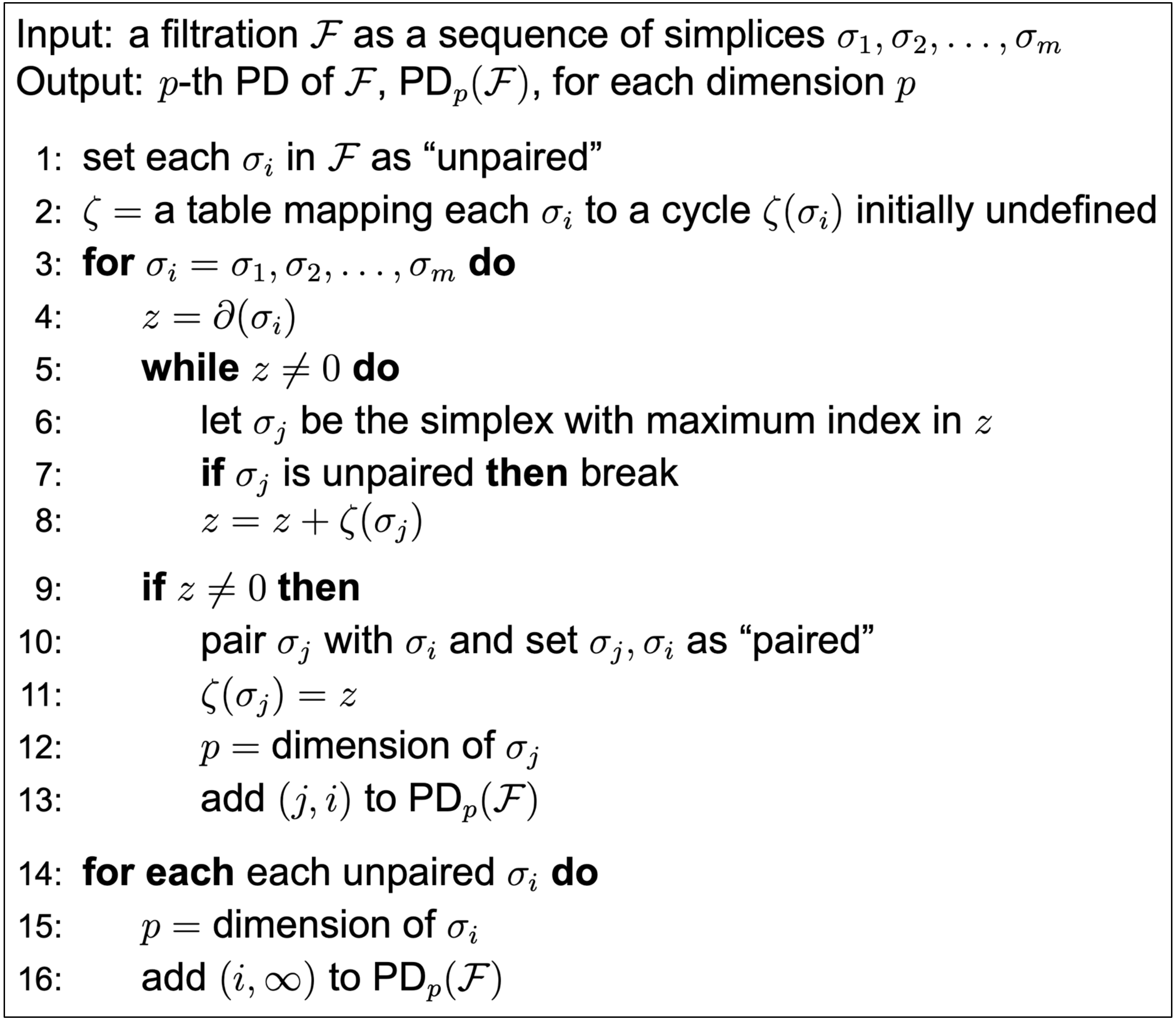

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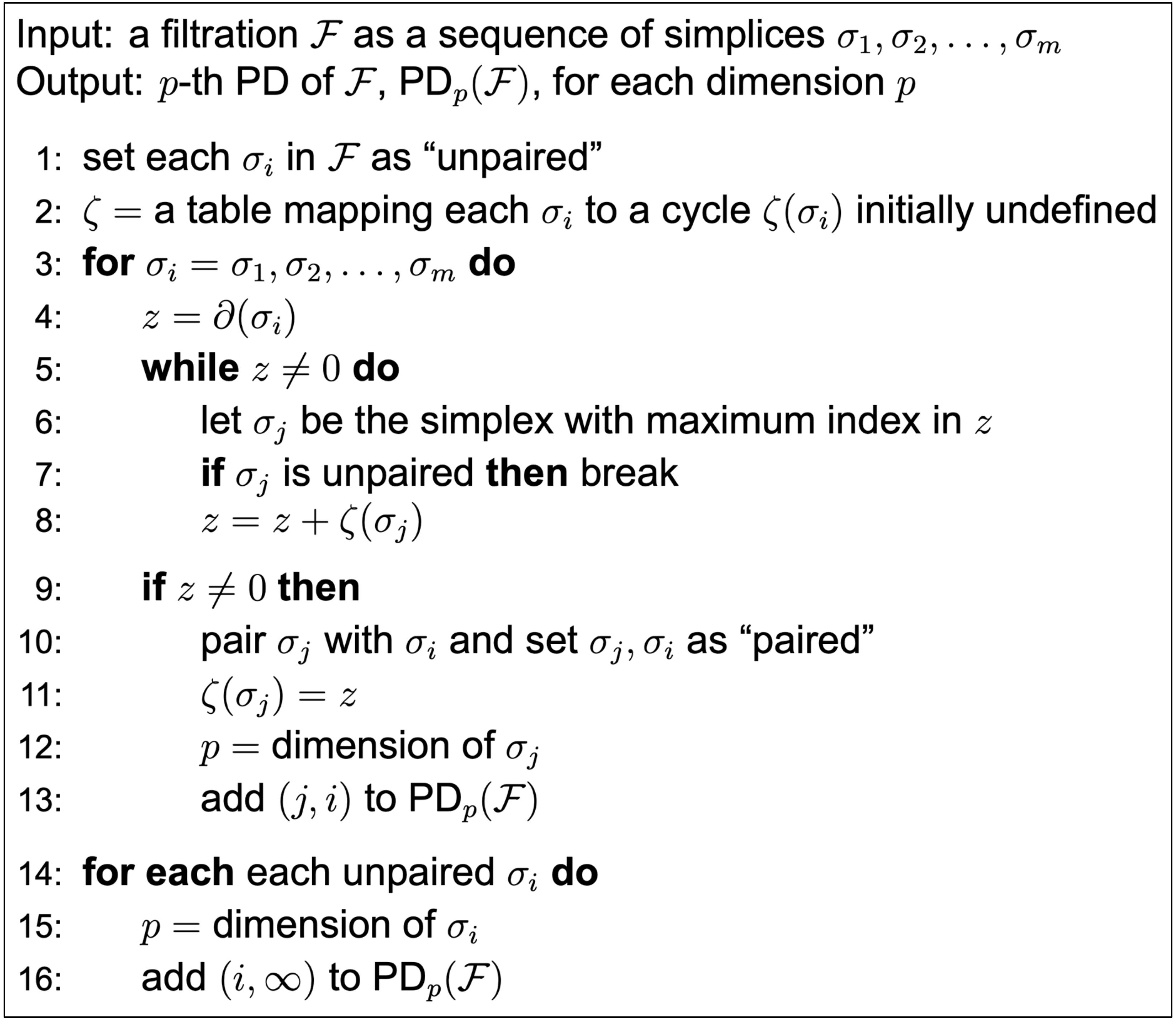

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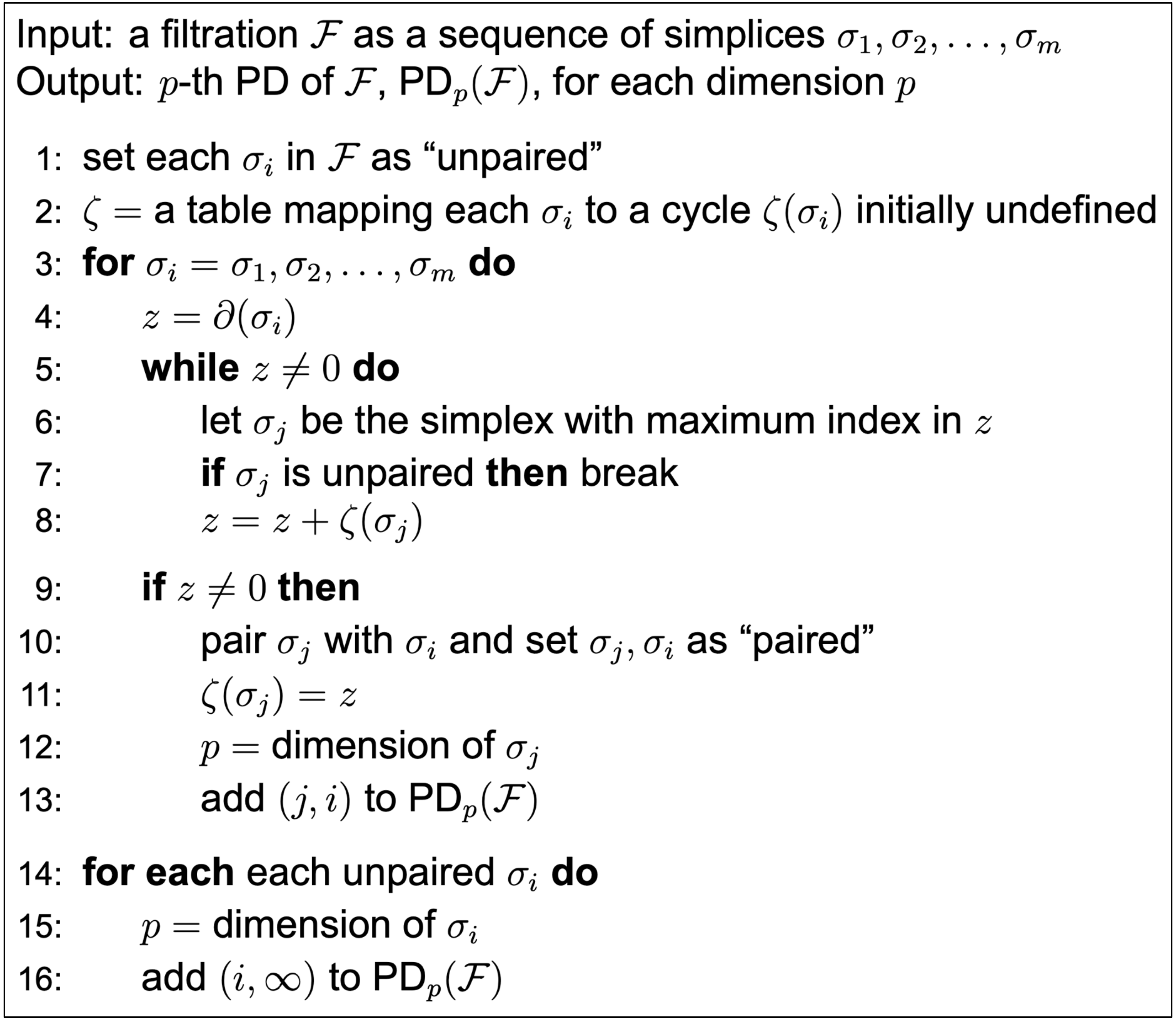
In the worst case, both inner and outer loop iterates $O(m)$ time, and hence $O(m^3)$ oveall



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  2. Compute $\mathrm{PD}(\mathcal{F}')$
  3. Convert $\mathrm{PD}(\mathcal{F}')$ into $\mathrm{PD}(\mathcal{F})$ by "**contracting**" each interval $\mathrm{PD}(\mathcal{F}')$ based on the correspondence between

PD for General Filtration

- Recall part of the reason we introduce the previous algorithm for computing PD is to formally define PD on a discrete filtration
- But the algorithm only takes a simplex-wise filtration as input, so technically we only defined PD on a simplex-wise filtration
- We shall now define PD on a general filtration not necessarily simplex-wise
- The process is as follows:
  1. "**Expand**" the general filtration $\mathcal{F}$ into a simplex-wise one $\mathcal{F}'$
     - Aka, for an inclusion in $\mathcal{F}$ which inserts k number of simplices, we convert it into k inclusions each inserting a single simplex
  2. Compute $\mathrm{PD}(\mathcal{F}')$
  3. Convert $\mathrm{PD}(\mathcal{F}')$ into $\mathrm{PD}(\mathcal{F})$ by "**contracting**" each interval $\mathrm{PD}(\mathcal{F}')$ based on the correspondence between
  4. During the contraction, some intervals in $\mathrm{PD}(\mathcal{F}')$ may disappear (birth and death coincide)

Expand general filtration to simplex wise

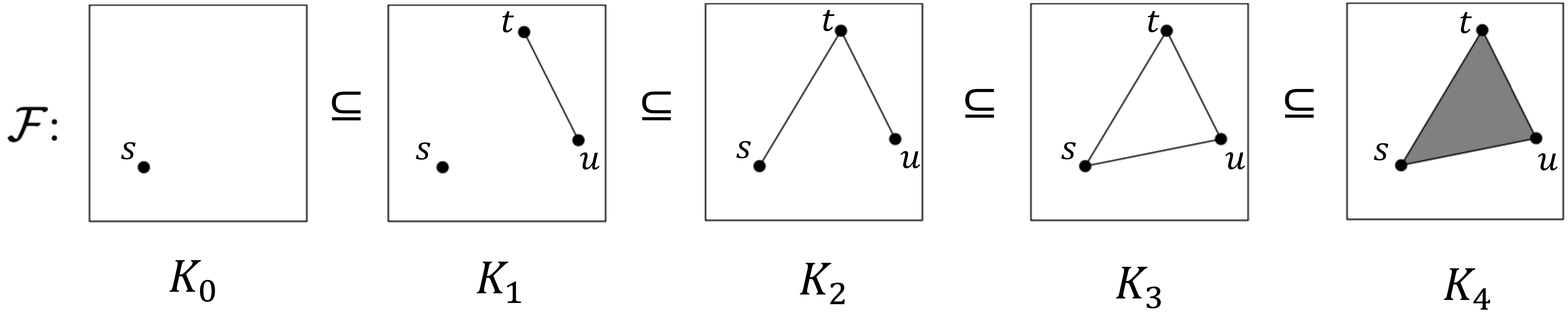
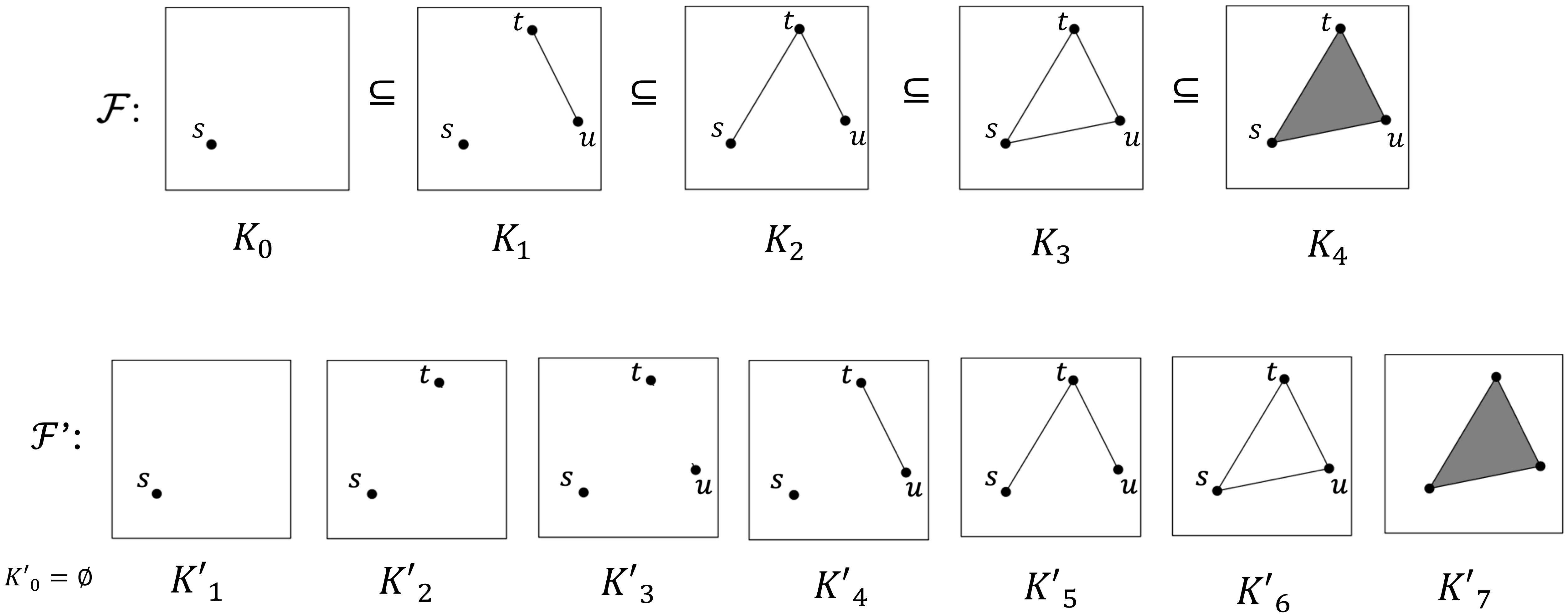


Image source: Patrick Schnider. Introduction to Topological Data Analysis Lecture Notes FS 2023

Expand general filtration to simplex wise



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Expand general filtration to simplex wise

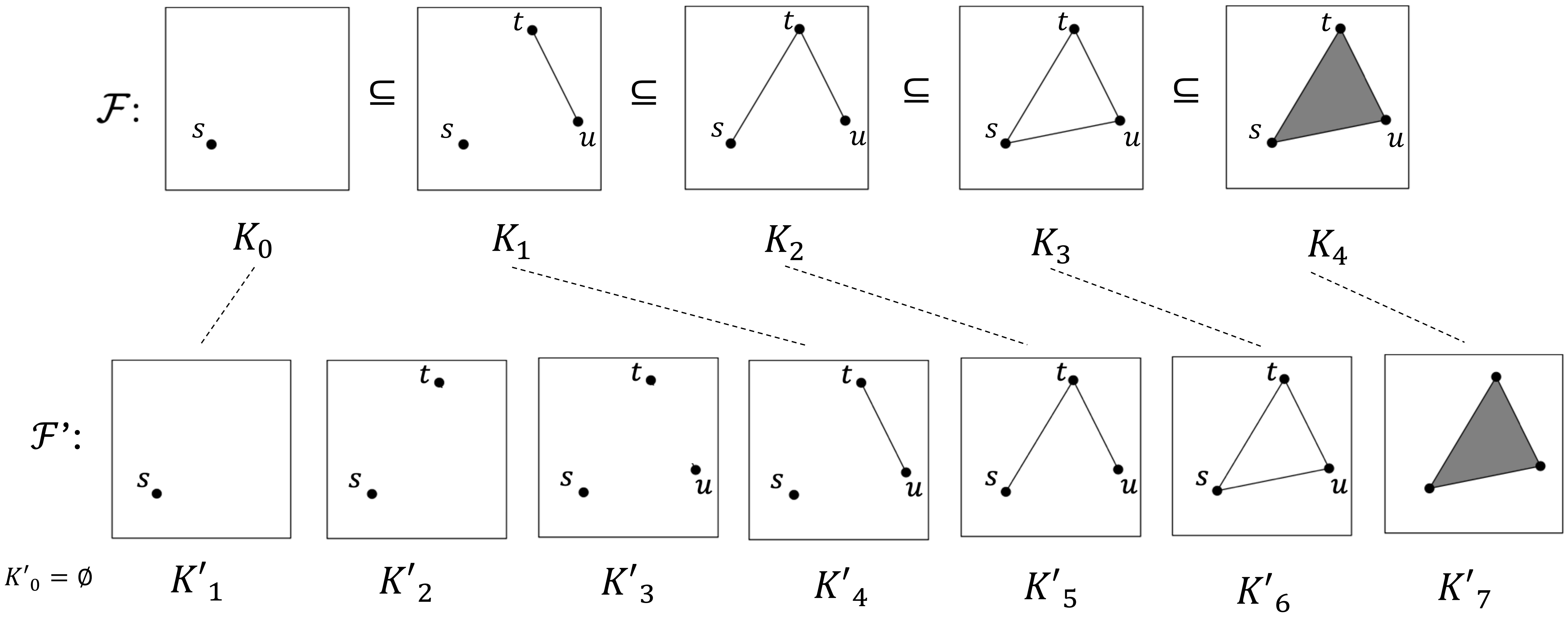


Image source: Patrick Schnider. Introduction to Topological Data Analysis Lecture Notes FS 2023

Expand general filtration to simplex wise

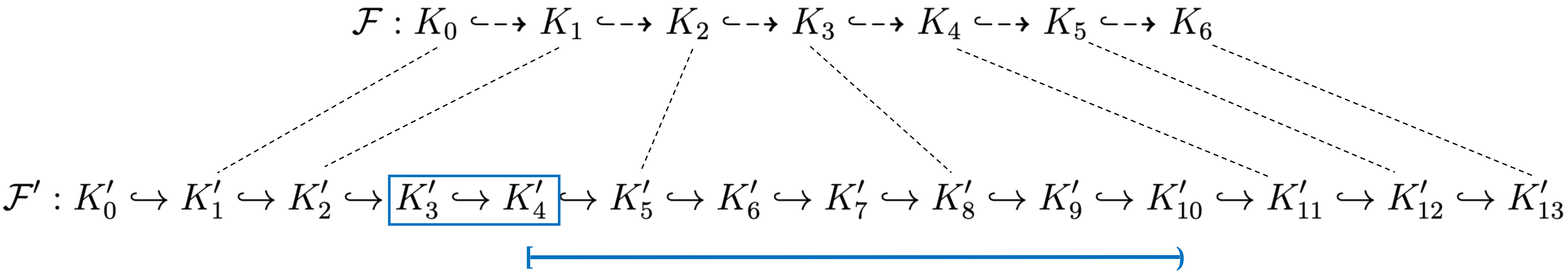
- Another interactive example for correspondence between a general filtration and its simplex-wise version: https://iuricichf.github.io/ICT/algorithm.html

PD for General Filtration

$$\begin{tikzcd}
 & & & \mathcal{F} : & K_0 \arrow[r, hook, dashed] \arrow[dll, dashed, no head] & K_1 \arrow[r, hook, dashed] \arrow[dll, dashed, no head] & K_2 \arrow[r, hook, dashed] \arrow[d, dashed, no head] & K_3 \arrow[r, hook, dashed] \arrow[drr, dashed, no head] & K_4 \arrow[r, hook, dashed] \arrow[drrrr, dashed, no head] & K_5 \arrow[r, hook, dashed] \arrow[drrrr, dashed, no head] & K_6 \arrow[drrrr, dashed, no head] & & & & \\
\mathcal{F}' : & K'_0 \arrow[r, hook] & K'_1 \arrow[r, hook] & K'_2 \arrow[r, hook] & K'_3 \arrow[r, hook] & K'_4 \arrow[r, hook] & K'_5 \arrow[r, hook] & K'_6 \arrow[r, hook] & K'_7 \arrow[r, hook] & K'_8 \arrow[r, hook] & K'_9 \arrow[r, hook] & K'_{10} \arrow[r, hook] & K'_{11} \arrow[r, hook] & K'_{12} \arrow[r, hook] & K'_{13}
\end{tikzcd}$$

“Contracting” $[4,10) \in PD(\mathcal{F}')$ into one for $PD(\mathcal{F})$:

PD for General Filtration

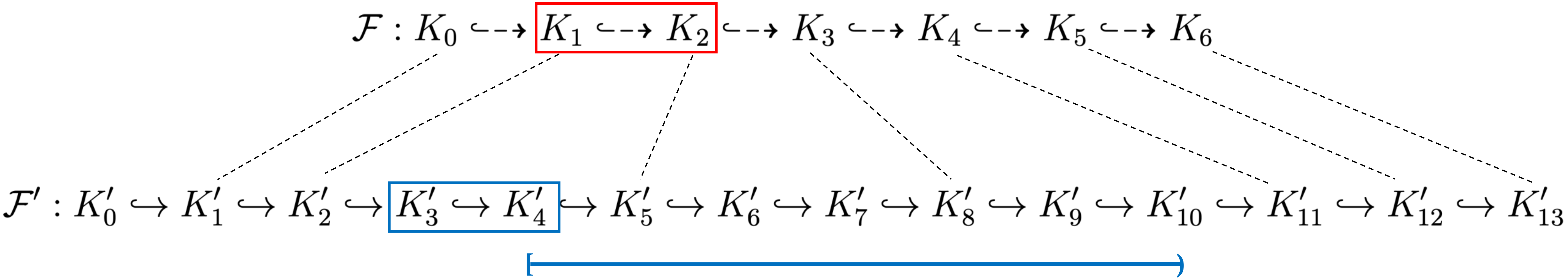


$$\begin{tikzcd}
 & & \mathcal{F} : & K_0 \arrow[r, hook, dashed] \arrow[dl, dash, dashed] & K_1 \arrow[r, hook, dashed] \arrow[dl, dash, dashed] & K_2 \arrow[r, hook, dashed] \arrow[dr, dash, dashed] & K_3 \arrow[r, hook, dashed] \arrow[drrr, dash, dashed] & K_4 \arrow[r, hook, dashed] \arrow[drrrrr, dash, dashed] & K_5 \arrow[r, hook, dashed] \arrow[drrrrr, dash, dashed] & K_6 \arrow[drrrrr, dash, dashed] & & & & & \\
\mathcal{F}' : & K'_0 \arrow[r, hook] & K'_1 \arrow[r, hook] & K'_2 \arrow[r, hook] & K'_3 \arrow[r, hook] & K'_4 \arrow[r, hook] & K'_5 \arrow[r, hook] & K'_6 \arrow[r, hook] & K'_7 \arrow[r, hook] & K'_8 \arrow[r, hook] & K'_9 \arrow[r, hook] & K'_{10} \arrow[r, hook] & K'_{11} \arrow[r, hook] & K'_{12} \arrow[r, hook] & K'_{13}
\end{tikzcd}$$

“Contracting” $[4,10) \in PD(\mathcal{F}')$ into one for $PD(\mathcal{F})$:

- $[4,10) \in PD(\mathcal{F}')$ is born in K'_4, which is when go from K'_3 to K'_4 in $\mathcal{F}'$

PD for General Filtration



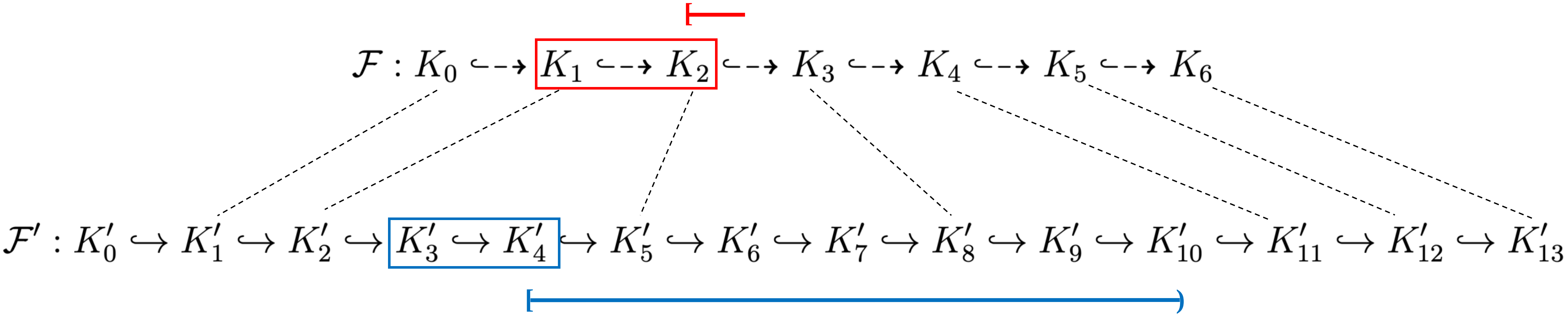
$$\mathcal{F} : K_0 \dashrightarrow \boxed{K_1 \dashrightarrow K_2} \dashrightarrow K_3 \dashrightarrow K_4 \dashrightarrow K_5 \dashrightarrow K_6$$

$$\mathcal{F}' : K'_0 \hookrightarrow K'_1 \hookrightarrow K'_2 \hookrightarrow \boxed{K'_3 \hookrightarrow K'_4} \hookrightarrow K'_5 \hookrightarrow K'_6 \hookrightarrow K'_7 \hookrightarrow K'_8 \hookrightarrow K'_9 \hookrightarrow K'_{10} \hookrightarrow K'_{11} \hookrightarrow K'_{12} \hookrightarrow K'_{13}$$

"Contracting" $[4,10) \in PD(\mathcal{F}')$ into one for $PD(\mathcal{F})$:

- $[4,10) \in PD(\mathcal{F}')$ is born in ${K'}_4$, which is when go from ${K'}_3$ to ${K'}_4$ in $\mathcal{F}'$
- In $\mathcal{F}$, the homology feature is born when we go from K_1 to K_2, aka in K_2

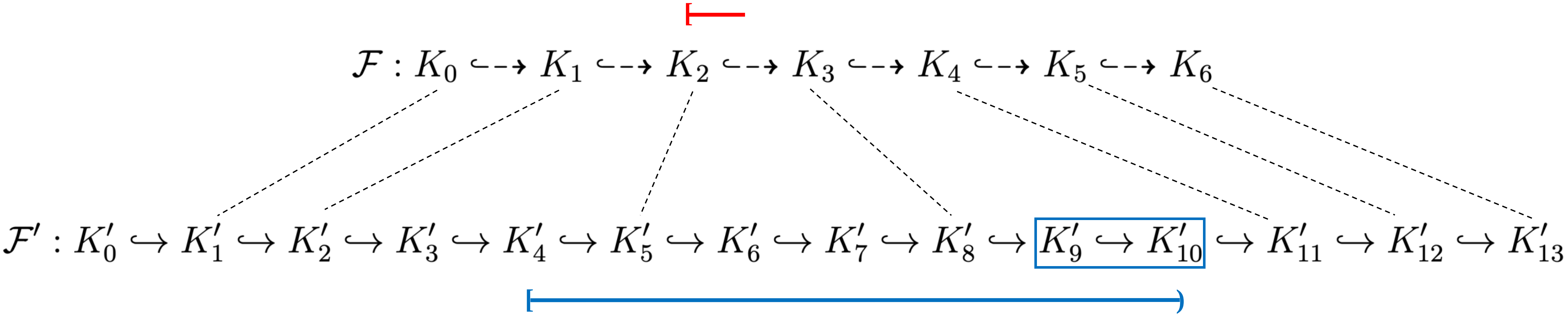
PD for General Filtration



“Contracting” $[4{,}10) \in PD(\mathcal{F}')$ into one for $PD(\mathcal{F})$:

- $[4{,}10) \in PD(\mathcal{F}')$ is born in K'_4, which is when go from K'_3 to K'_4 in $\mathcal{F}'$
- In $\mathcal{F}$, the homology feature is born when we go from K_1 to K_2, aka in K_2
- So the birth of the corresponding interval in $PD(\mathcal{F})$ is 2

PD for General Filtration



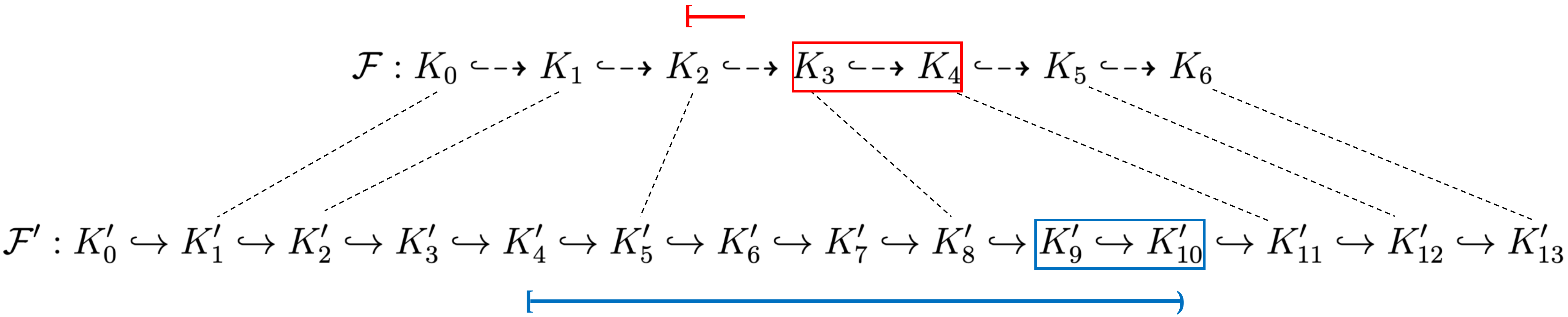
$$\mathcal{F} : K_0 \hookrightarrow K_1 \hookrightarrow K_2 \hookrightarrow K_3 \hookrightarrow K_4 \hookrightarrow K_5 \hookrightarrow K_6$$

$$\mathcal{F}' : K'_0 \hookrightarrow K'_1 \hookrightarrow K'_2 \hookrightarrow K'_3 \hookrightarrow K'_4 \hookrightarrow K'_5 \hookrightarrow K'_6 \hookrightarrow K'_7 \hookrightarrow K'_8 \hookrightarrow \boxed{K'_9 \hookrightarrow K'_{10}} \hookrightarrow K'_{11} \hookrightarrow K'_{12} \hookrightarrow K'_{13}$$

"Contracting" $[4,10) \in PD(\mathcal{F}')$ into one for $PD(\mathcal{F})$:

- $[4,10) \in PD(\mathcal{F}')$ dies in K'_{10}, which specifically is when go from K'_9 to K'_{10}

PD for General Filtration

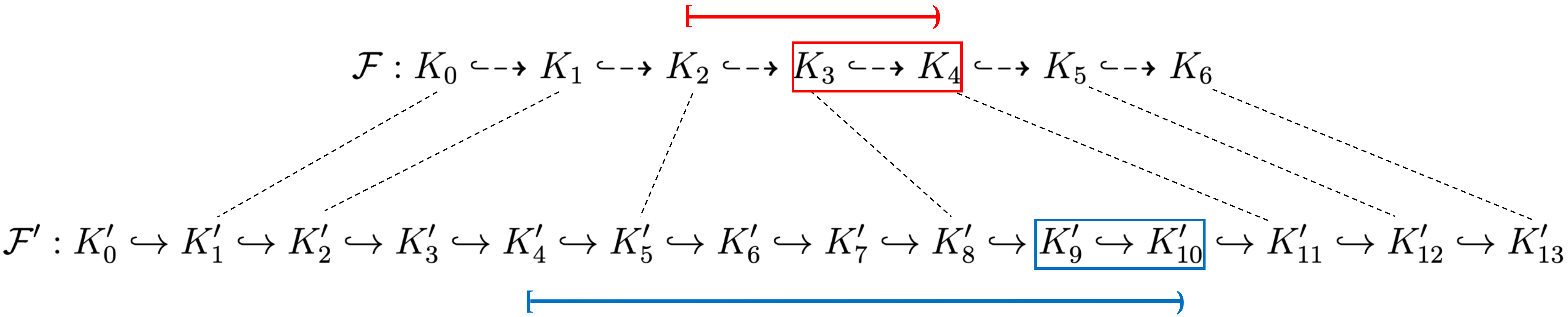


$$\begin{tikzcd}
 & & & \mathcal{F} : & K_0 \arrow[r, hook, dashed] \arrow[dll, dash, dashed] & K_1 \arrow[r, hook, dashed] \arrow[dll, dash, dashed] & K_2 \arrow[r, hook, dashed] \arrow[d, dash, dashed] & K_3 \arrow[r, hook, dashed] \arrow[drr, dash, dashed] & K_4 \arrow[r, hook, dashed] \arrow[drrrr, dash, dashed] & K_5 \arrow[r, hook, dashed] \arrow[drrrr, dash, dashed] & K_6 \arrow[drrrr, dash, dashed] \\
\mathcal{F}' : & K'_0 \arrow[r, hook] & K'_1 \arrow[r, hook] & K'_2 \arrow[r, hook] & K'_3 \arrow[r, hook] & K'_4 \arrow[r, hook] & K'_5 \arrow[r, hook] & K'_6 \arrow[r, hook] & K'_7 \arrow[r, hook] & K'_8 \arrow[r, hook] & K'_9 \arrow[r, hook] & K'_{10} \arrow[r, hook] & K'_{11} \arrow[r, hook] & K'_{12} \arrow[r, hook] & K'_{13}
\end{tikzcd}$$

"Contracting" $[4,10) \in PD(\mathcal{F}')$ into one for $PD(\mathcal{F})$:

- $[4,10) \in PD(\mathcal{F}')$ dies in K'_{10}, which specifically is when go from K'_9 to K'_{10}
- In $\mathcal{F}$, the homology feature dies when we go from K_3 to K_4, aka in K_4

PD for General Filtration



$$\mathcal{F} : K_0 \hookrightarrow K_1 \hookrightarrow K_2 \hookrightarrow \boxed{K_3 \hookrightarrow K_4} \hookrightarrow K_5 \hookrightarrow K_6$$

$$\mathcal{F}' : K'_0 \hookrightarrow K'_1 \hookrightarrow K'_2 \hookrightarrow K'_3 \hookrightarrow K'_4 \hookrightarrow K'_5 \hookrightarrow K'_6 \hookrightarrow K'_7 \hookrightarrow K'_8 \hookrightarrow \boxed{K'_9 \hookrightarrow K'_{10}} \hookrightarrow K'_{11} \hookrightarrow K'_{12} \hookrightarrow K'_{13}$$

“Contracting” $[4{,}10) \in PD(\mathcal{F}')$ into one for $PD(\mathcal{F})$:

- $[4{,}10) \in PD(\mathcal{F}')$ dies in K'_{10}, which specifically is when go from K'_9 to K'_{10}
- In $\mathcal{F}$, the homology feature dies when we go from K_3 to K_4, aka in K_4
- So the corresponding interval in $PD(\mathcal{F})$ is $[2{,}4)$

PD for General Filtration

$$\begin{tikzcd}
 & \mathcal{F} : K_0 \arrow[r, hook, dashed] \arrow[d, dash, dashed] & K_1 \arrow[rrr, hook, dashed] \arrow[d, dash, dashed] & & & K_2 \arrow[rrr, hook, dashed] \arrow[d, dash, dashed] & & & K_3 \arrow[rr, hook, dashed] \arrow[d, dash, dashed] & & K_4 \arrow[rr, hook, dashed] & & K_5 \arrow[r, hook, dashed] \arrow[d, dash, dashed] & K_6 \arrow[d, dash, dashed] \\
\mathcal{F}' : K'_0 \arrow[r, hook] & K'_1 \arrow[r, hook] & K'_2 \arrow[r, hook] & K'_3 \arrow[r, hook] & K'_4 \arrow[r, hook] & K'_5 \arrow[r, hook] & K'_6 \arrow[r, hook] & K'_7 \arrow[r, hook] & K'_8 \arrow[r, hook] & K'_9 \arrow[r, hook] & K'_{10} \arrow[r, hook] & K'_{11} \arrow[r, hook] & K'_{12} \arrow[r, hook] & K'_{13}
\end{tikzcd}$$

$[5,8) \in PD(\mathcal{F}')$ does not correspond to any interval in $PD(\mathcal{F})$:

- In $\mathcal{F}$, the homology feature is born in K_3 and dies also K_3 (so it's ephemeral)

- For the previous simplex-wise filtration, we can skip some complexes and renumber them

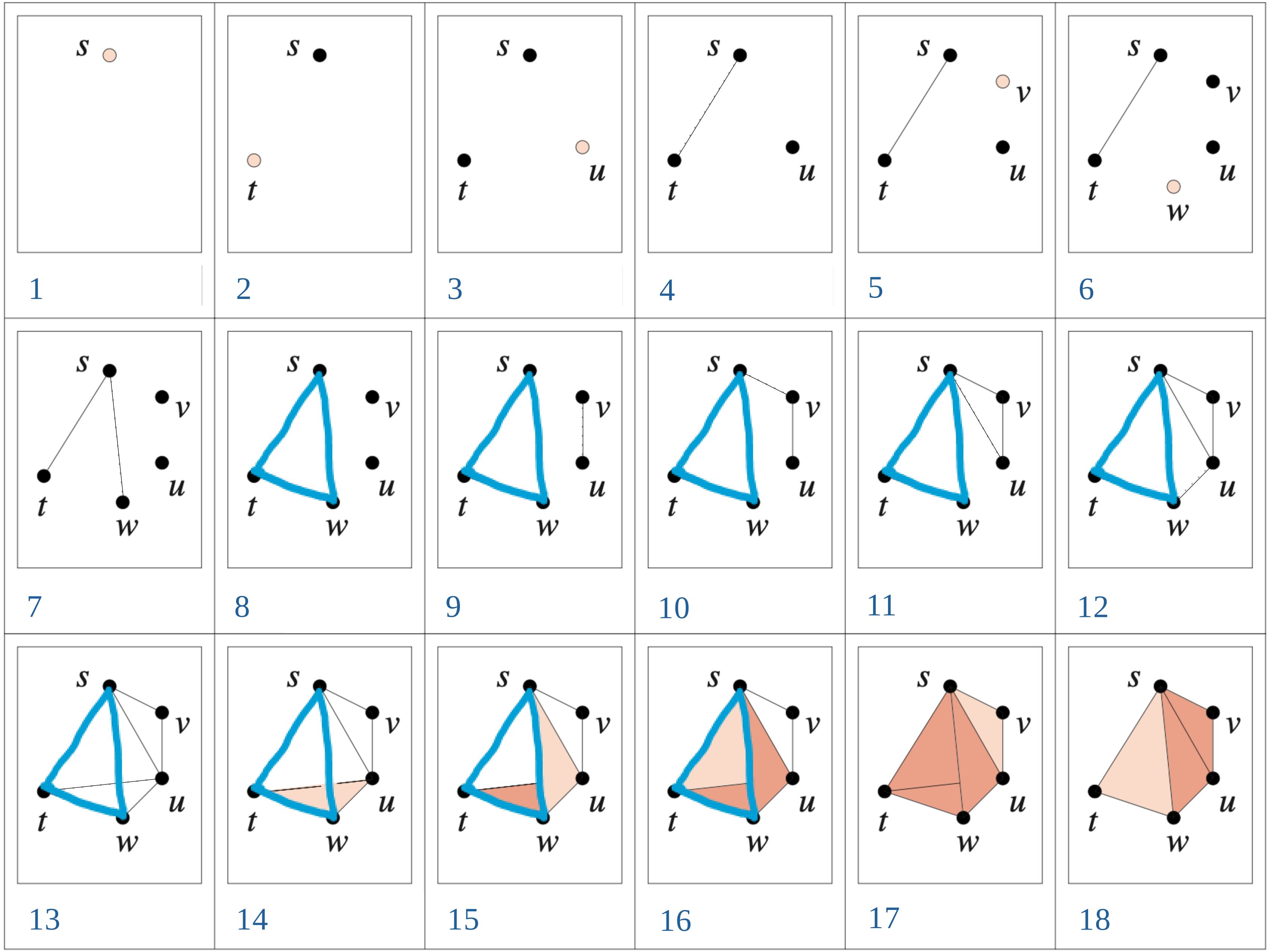


Image source: Edelsbrunner, Letscher, and Zomorodian. Topological persistence and simplification.

- For the previous simplex-wise filtration, we can skip some complexes and renumber them
- Then [8,16) in the simplex-wise filtration becomes [5,10) in the non-simplex-wise
- But they are essential "same" interval (representatives are the same)

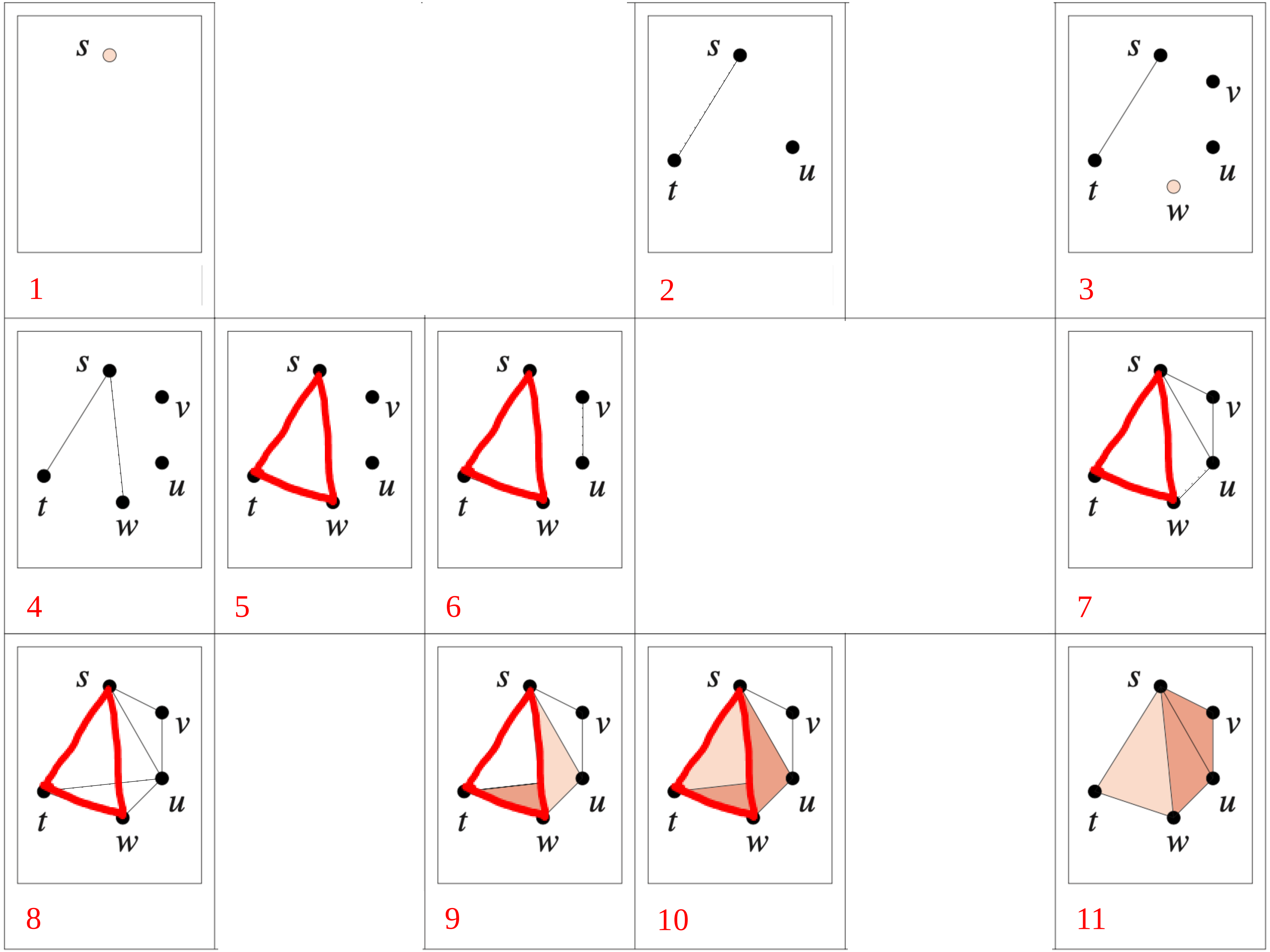


Image source: Edelsbrunner, Letscher, and Zomorodian. Topological persistence and simplification.