Persistent Homology: Filtration building techniques

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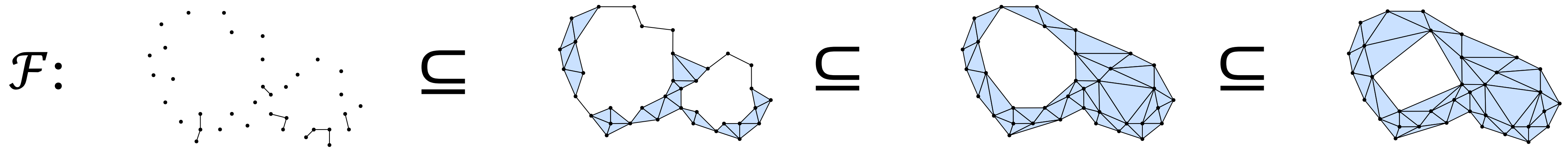
Outline for studying persistent homology

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

PD for continuous filtration

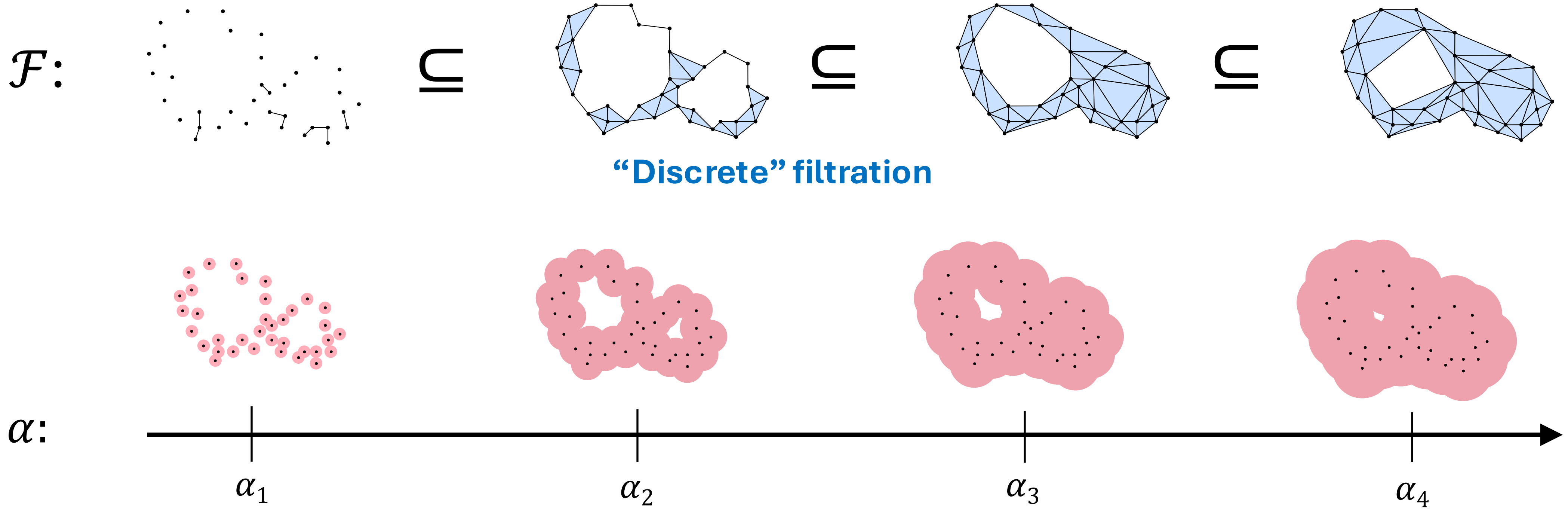
- So far, we have formally defined the PD for a (discrete) filtration, which is a finite sequence of simplicial complexes that are also nested



“Discrete” filtration

PD for continuous filtration

- So far, we have formally defined the PD for a (discrete) filtration, which is a finite sequence of simplicial complexes that are also nested
- But we haven't formally defined PD for a continuous filtration, where we have a space varying over $\alpha \in [0, \infty)$ (technically, there're infinitely many of them)



"Discrete" filtration

"Continuous" filtration

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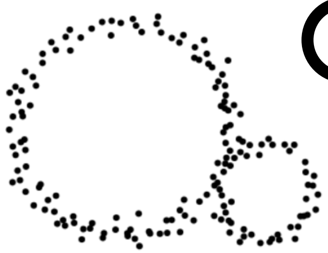
- So to harness the power of persistence, you have to do this
- So we shall not only formally define PD on input data (which are typically continuous at least theoretically), but also learn ways to preprocess the data into filtrations to feed into the persistent homology pipeline

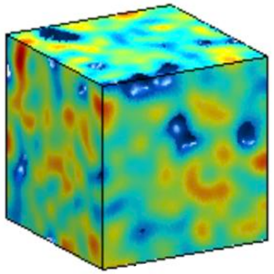
Persistent homology pipeline

1



Point cloud

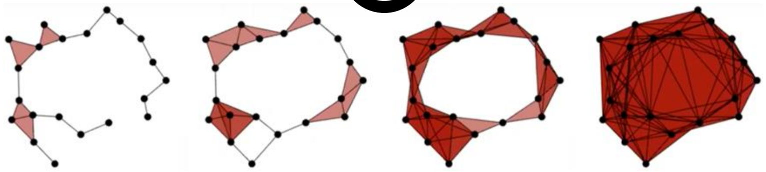
Image



3D volume data

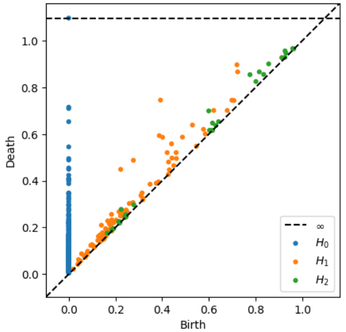
Build Filtration

2



Filtration

Persistent Homology

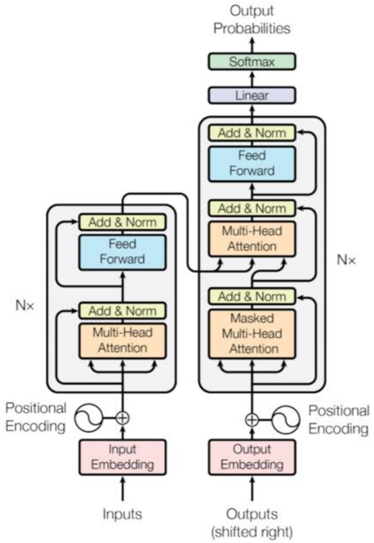


3

PD / barcode

Infer the shape / machine learning / visualization

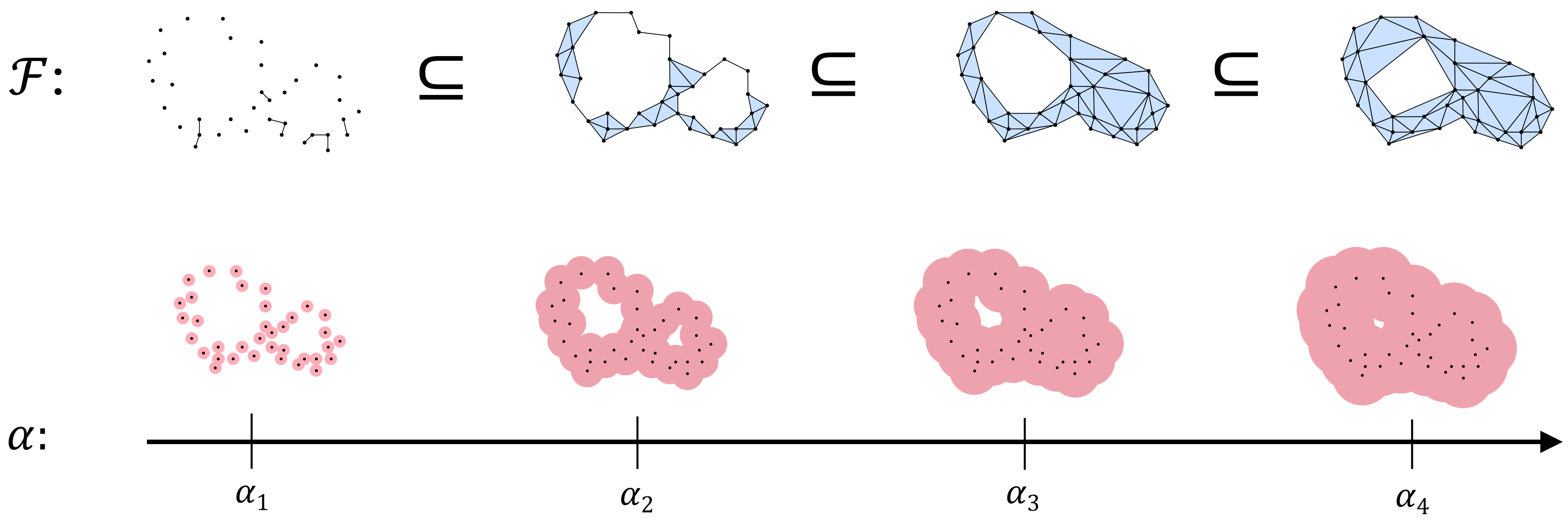
4



Some img from: AATRN; https://quantdare.com/understanding-the-shape-of-data-ii/; https://pixabay.com/photos/new-year-background-tree-sunset-736885/; Adler et al. Persistent homology for random fields and complexes.; https://builtin.com/artificial-intelligence/transformer-neural-network

PD for continuous filtration

- To formally define the PD for a continuous filtration, the idea is to "emulate" the continuous filtration using the discrete one, with no or minimal data loss



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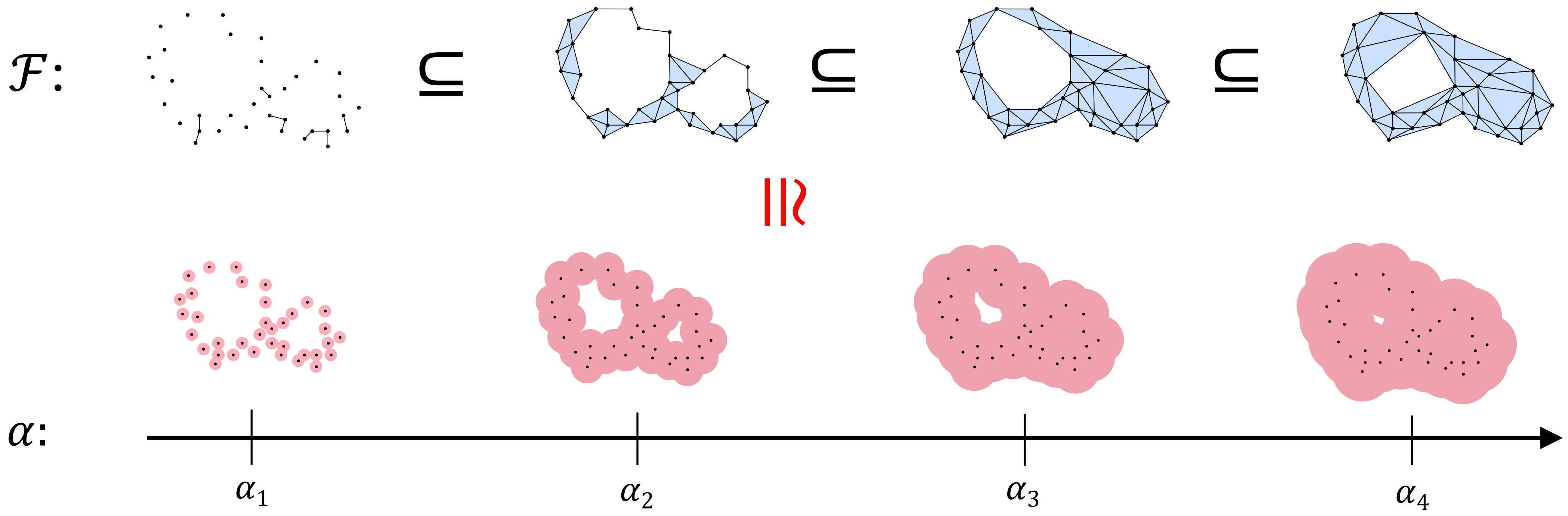
- We shall eventually show that continuous filtration is in some sense "equivalent" to the discrete one



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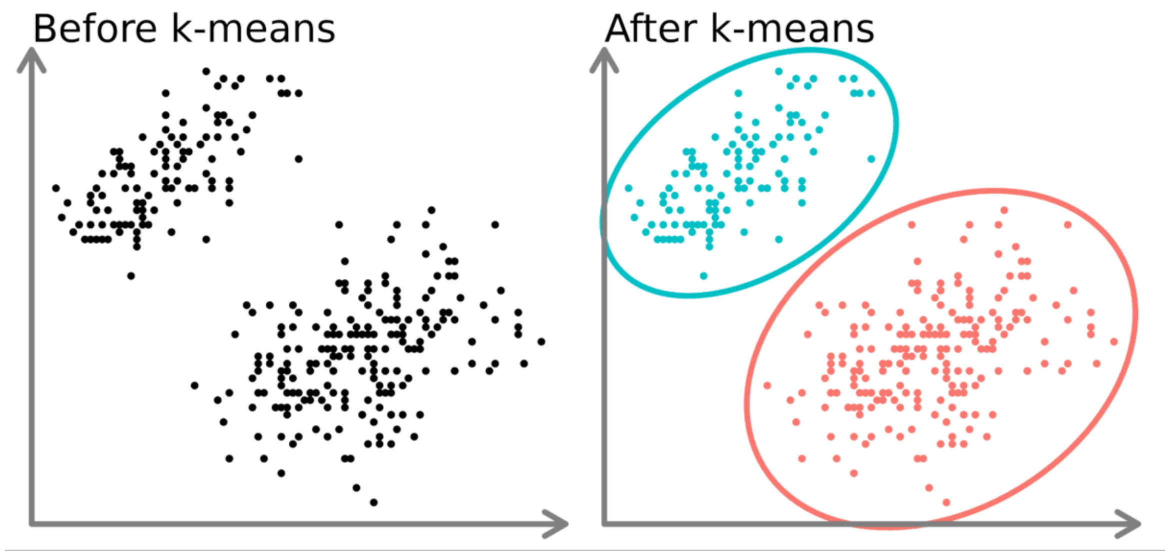

Image source: https://www.datacamp.com/tutorial/k-means-clustering-python

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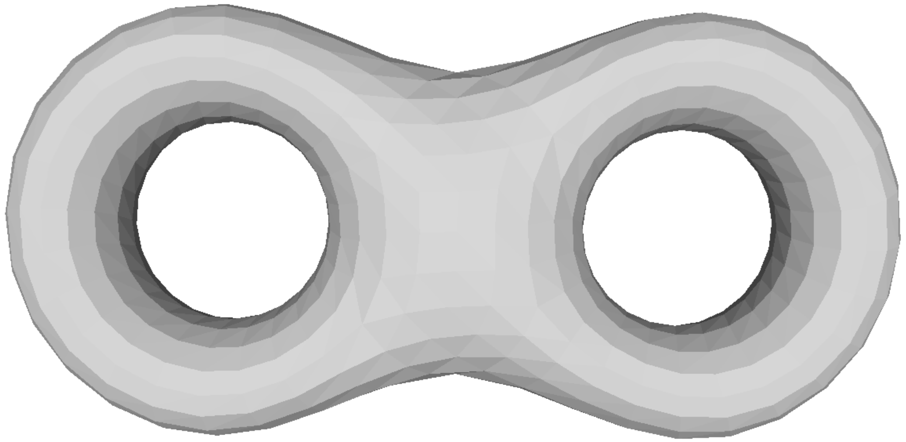
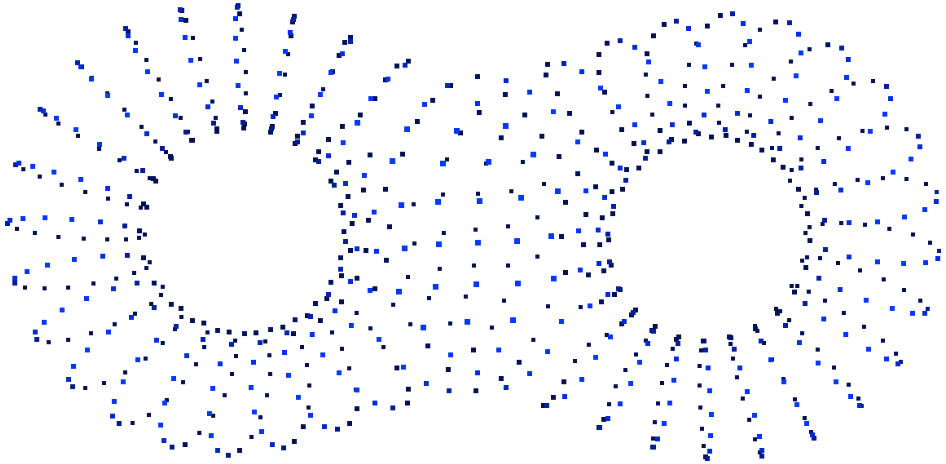
  - Even for supervised learning (another type of more popular? machine learning), if you ignore the “labels” for the data, then the data become point clouds
  - After all, each element in your data is in some sense a “point”

Growing balls for point clouds

- Furthermore, for geometric models (which topological methods are good with), e.g., triangular meshes, if you ignore the triangles and edges in the data and only focus on the vertices, then this is a point cloud





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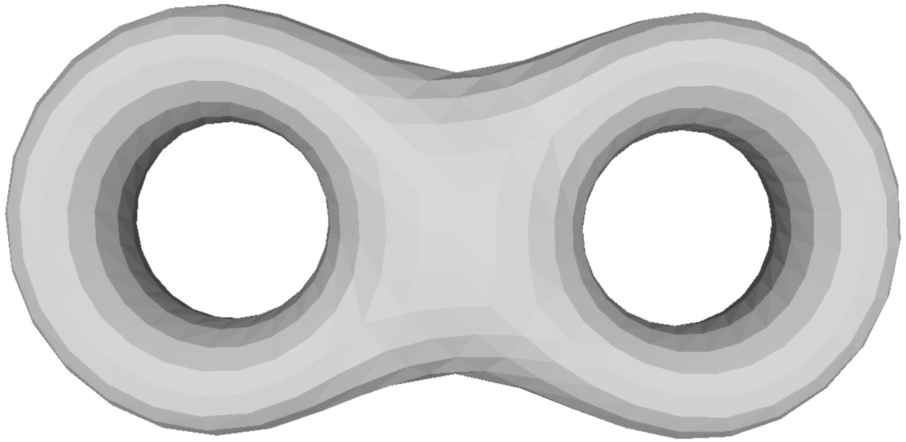
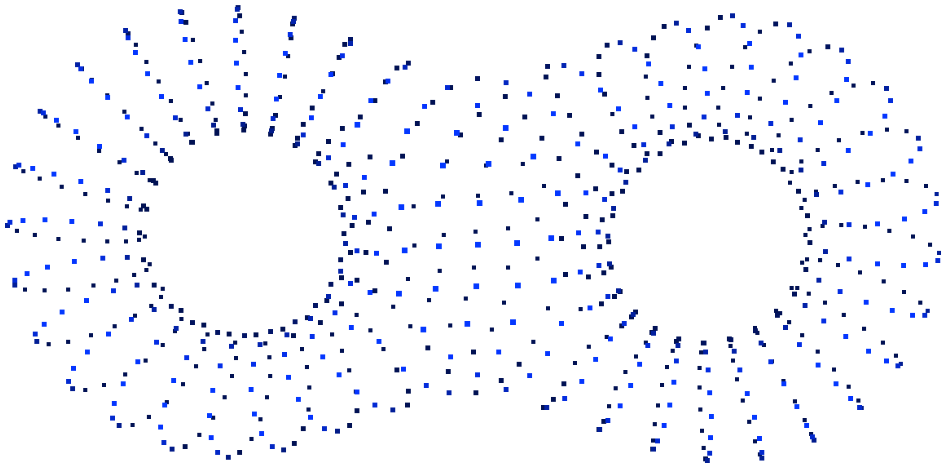
- Trying to infer the shape of point cloud is indeed a major motivation for topological data analysis





Build discrete filtration for “growing balls”

- Recall that each space in the “growing of balls” filtration is to take a ball of the same radius α centering in each point, and then take the union of the α-radius balls of all points
- To get the (continuous) filtration, we then let the radius α increase from 0 to ∞, and let the union of balls grow with it (see: https://gjkoplik.github.io/pers-hom-examples/0d_pers_2d_data_widget.html)

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- To construct a simplicial complex for the union of balls, we first let the point in the point cloud be all the vertices in the simplicial complex
- The remaining task is to build high-dimensional simplices out of the points (vertices)

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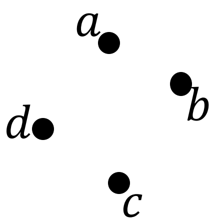
Simplices:

- a
- b
- c
- d



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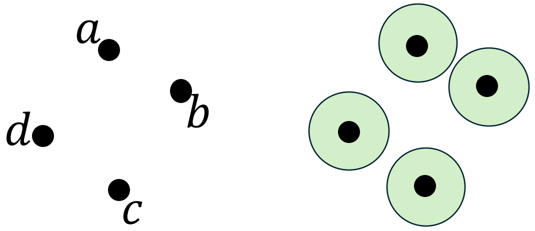

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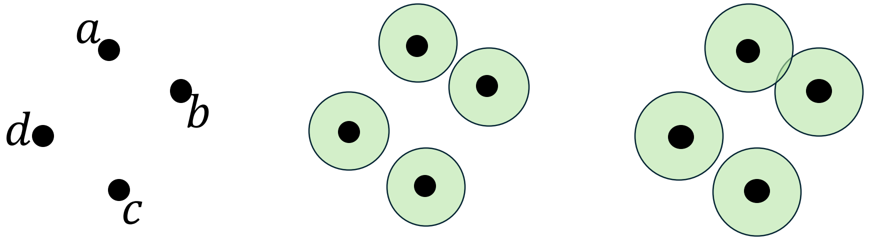

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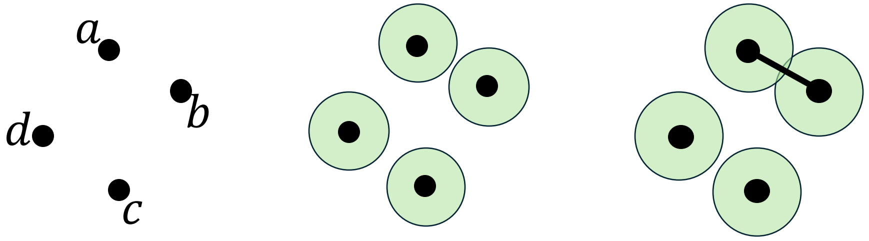

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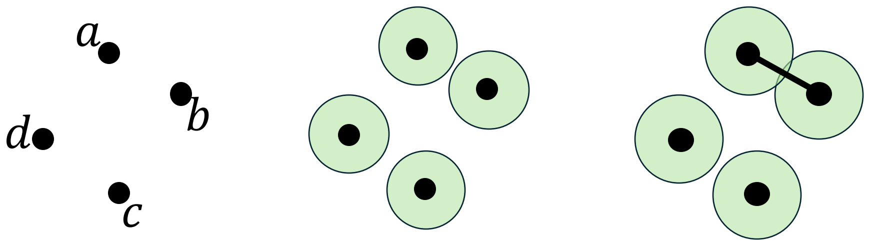

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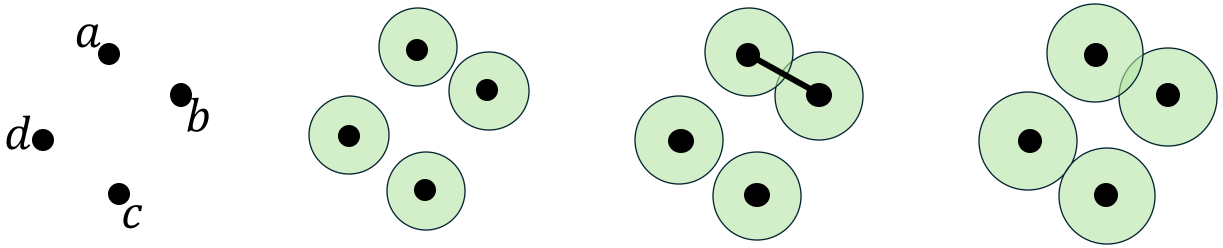

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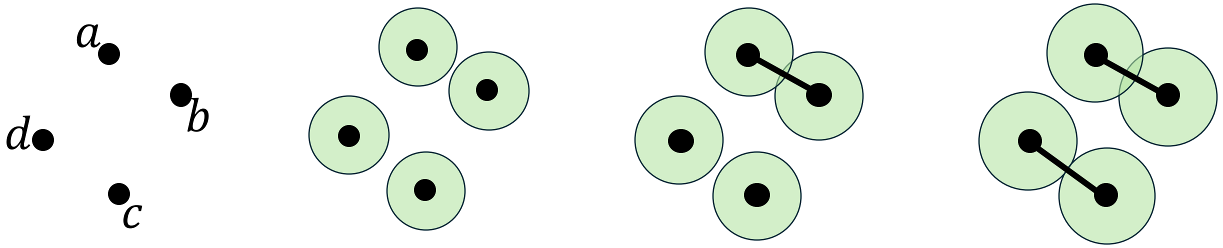

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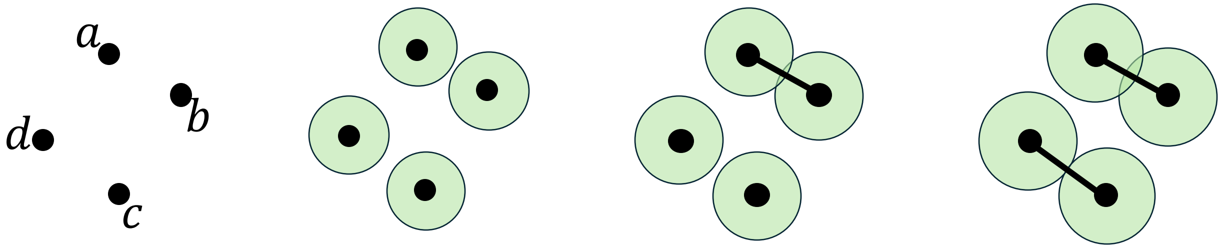

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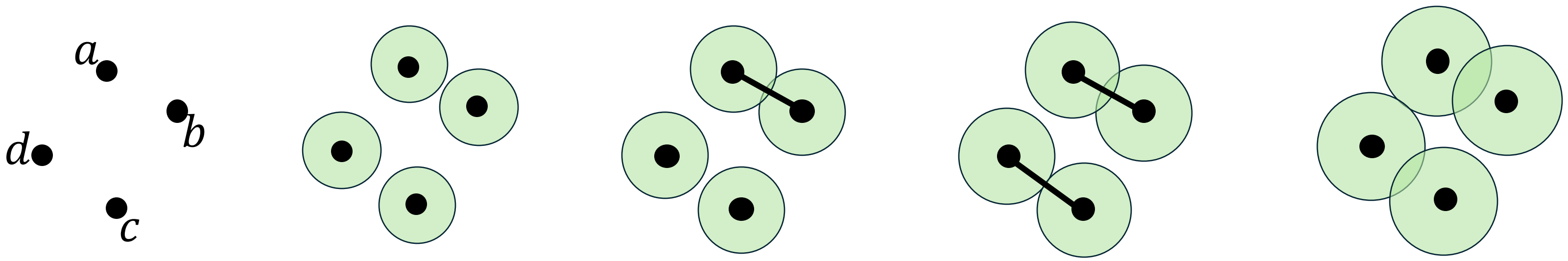

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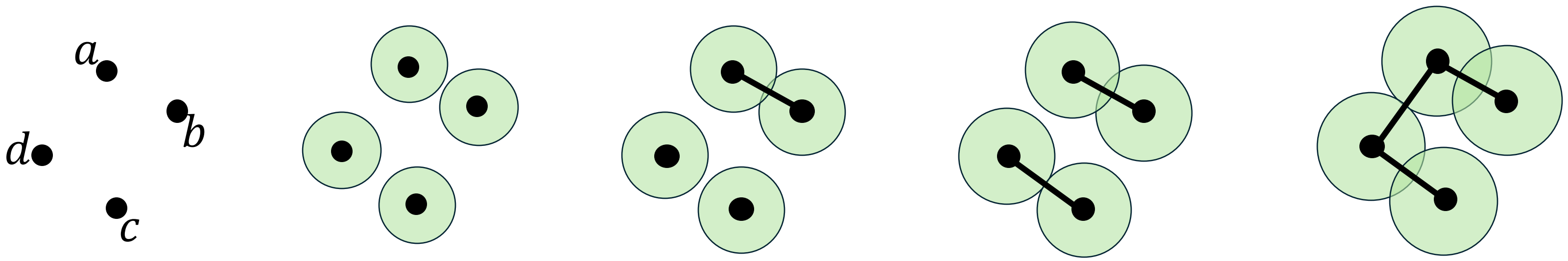

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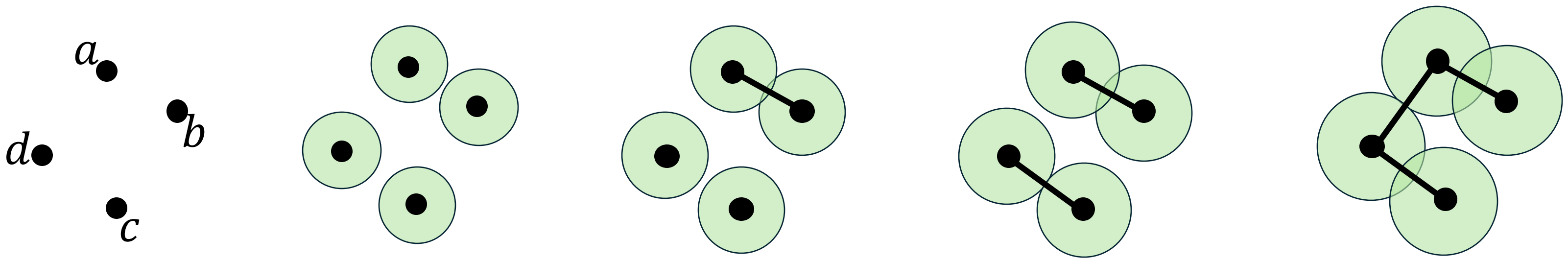

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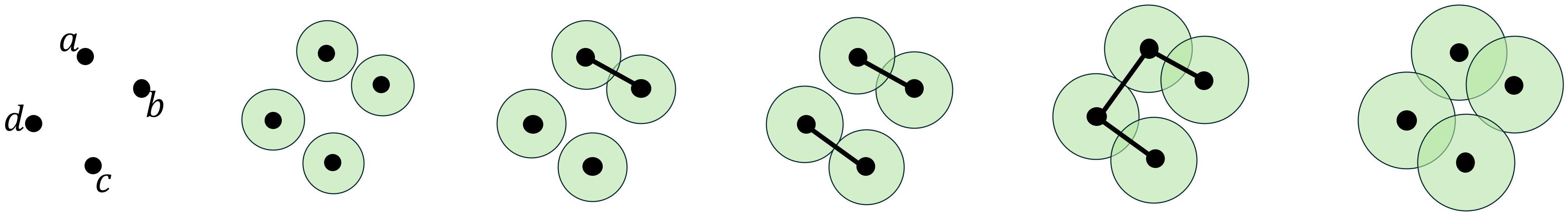

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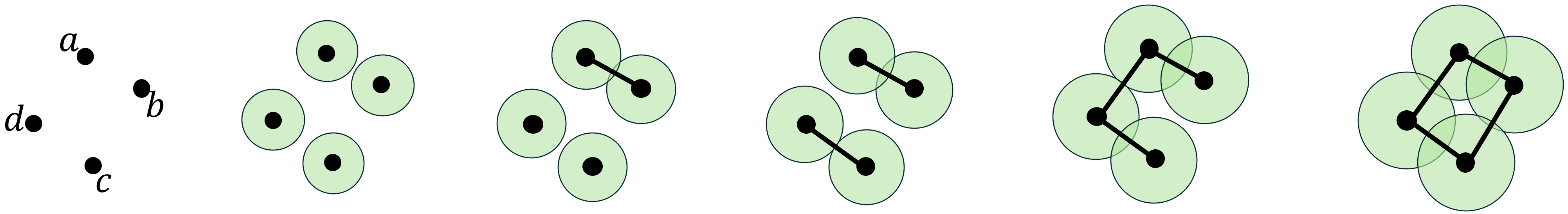

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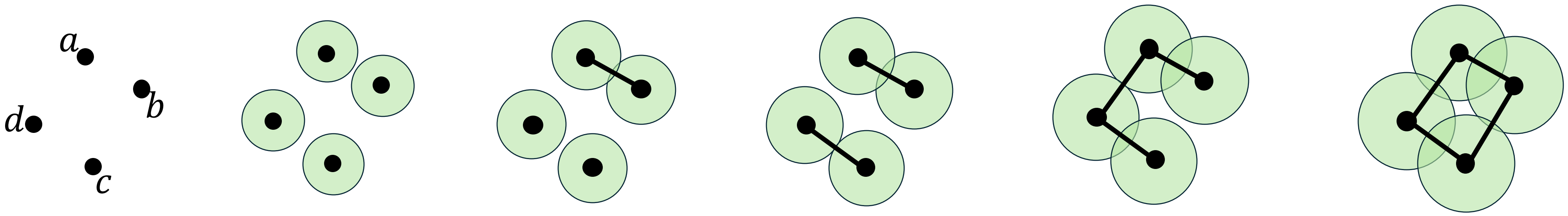

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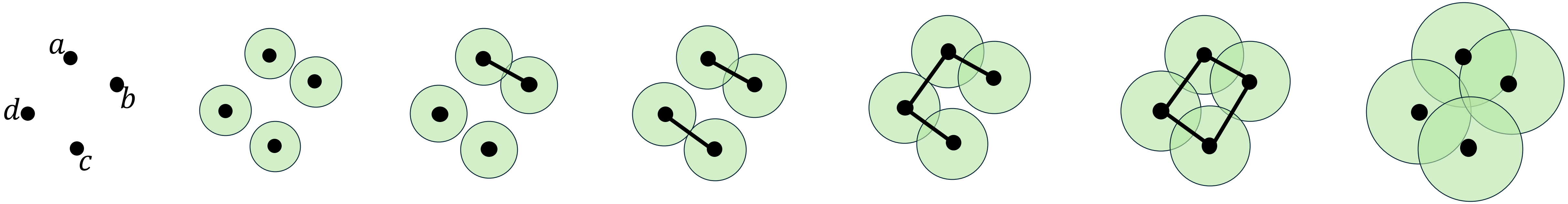

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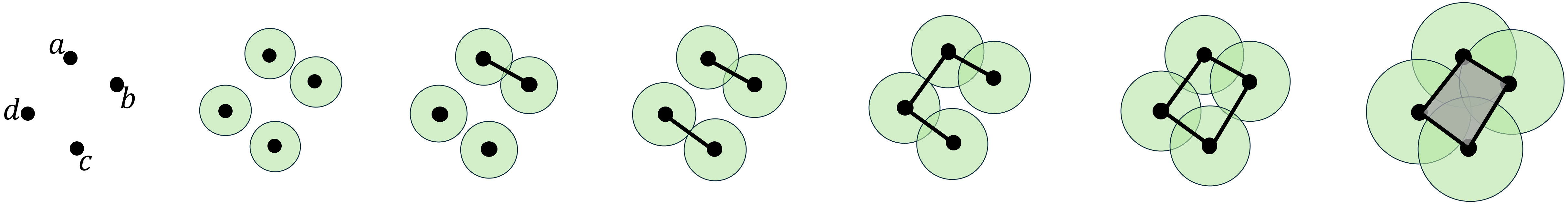

Čech Complex

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- Of course, in practice, the algorithms that people use to compute Čech Complexes are much more efficient ones

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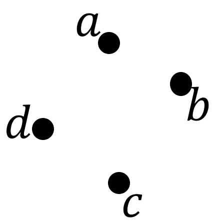

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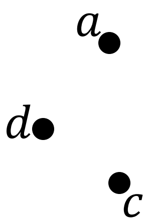

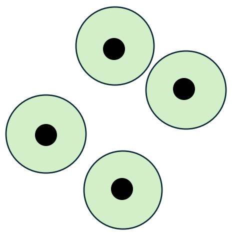

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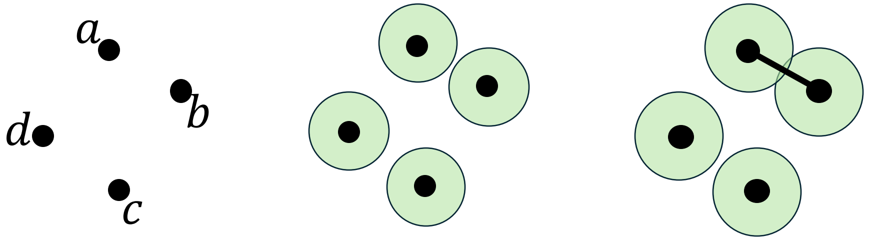

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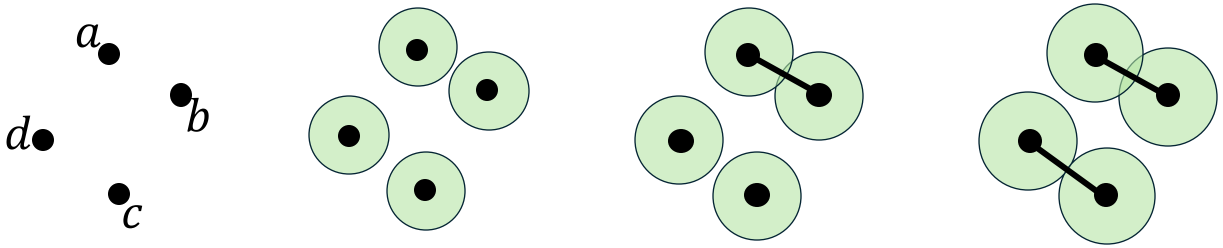

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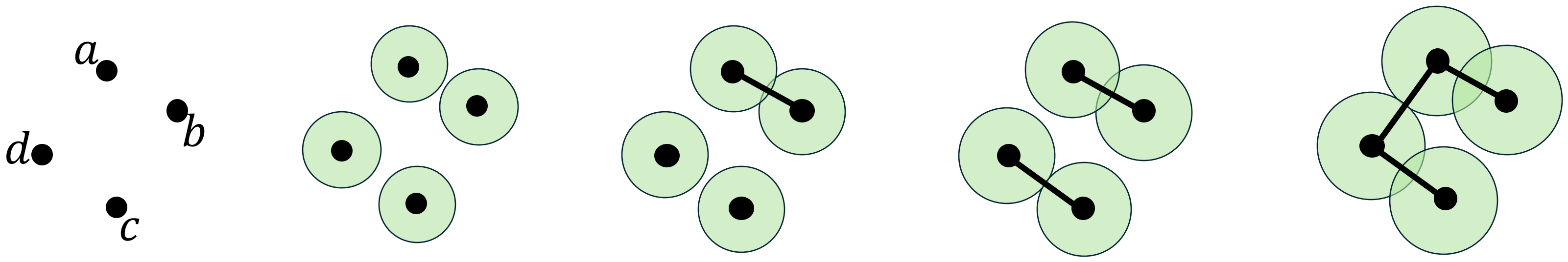

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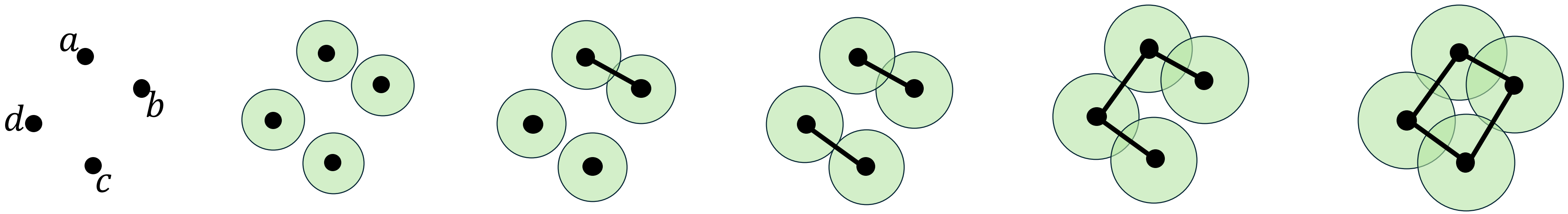

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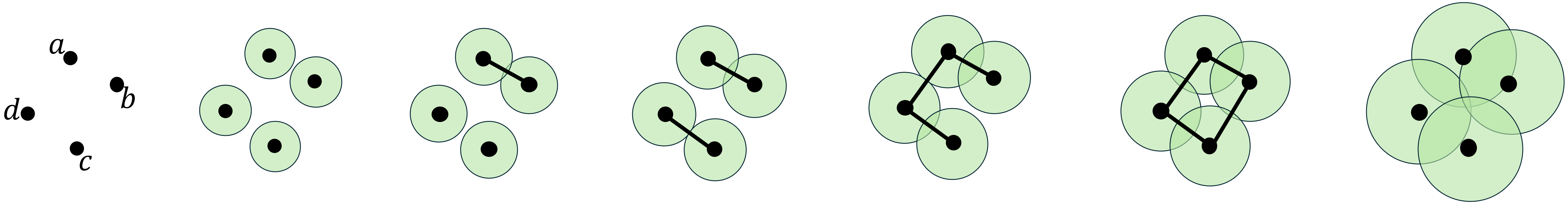

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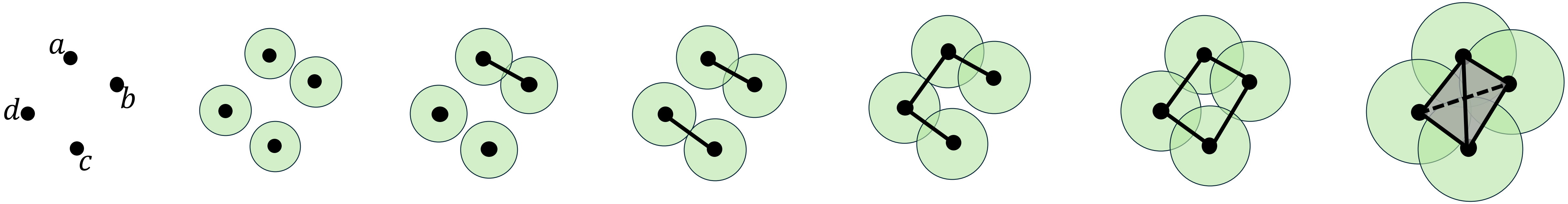
- $abcd$ with all its faces (abc, abd, acd, and bcd).



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- E.g., if three balls intersect, then any two balls also intersect. So the edges of the corresponding triangle are also in the Cech complex.

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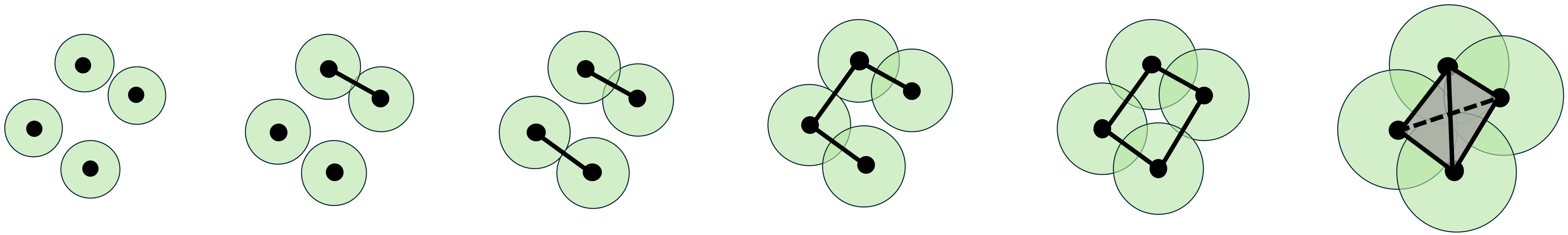

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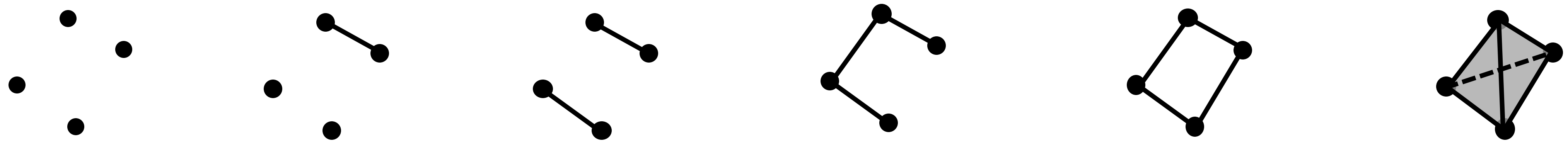

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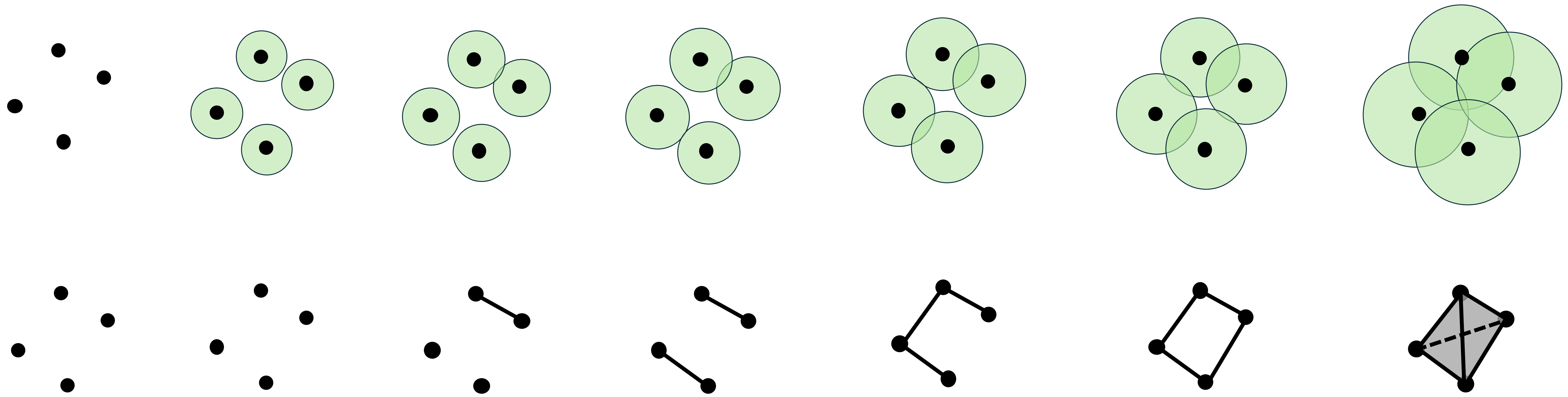

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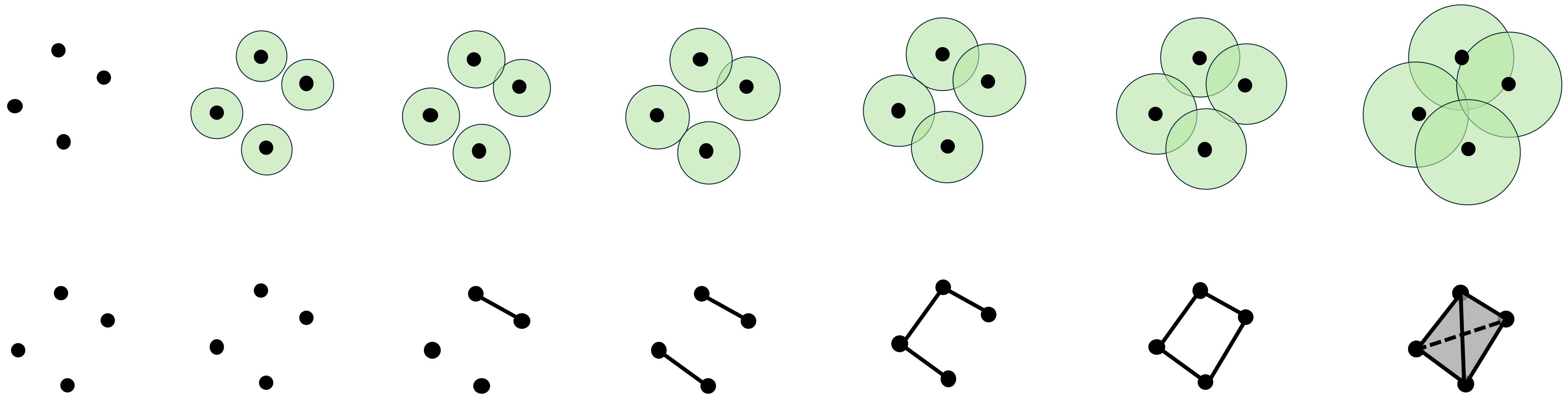
- The above "equivalence" is called the "homotopy equivalence" in algebraic topology, whose definition is beyond the scope



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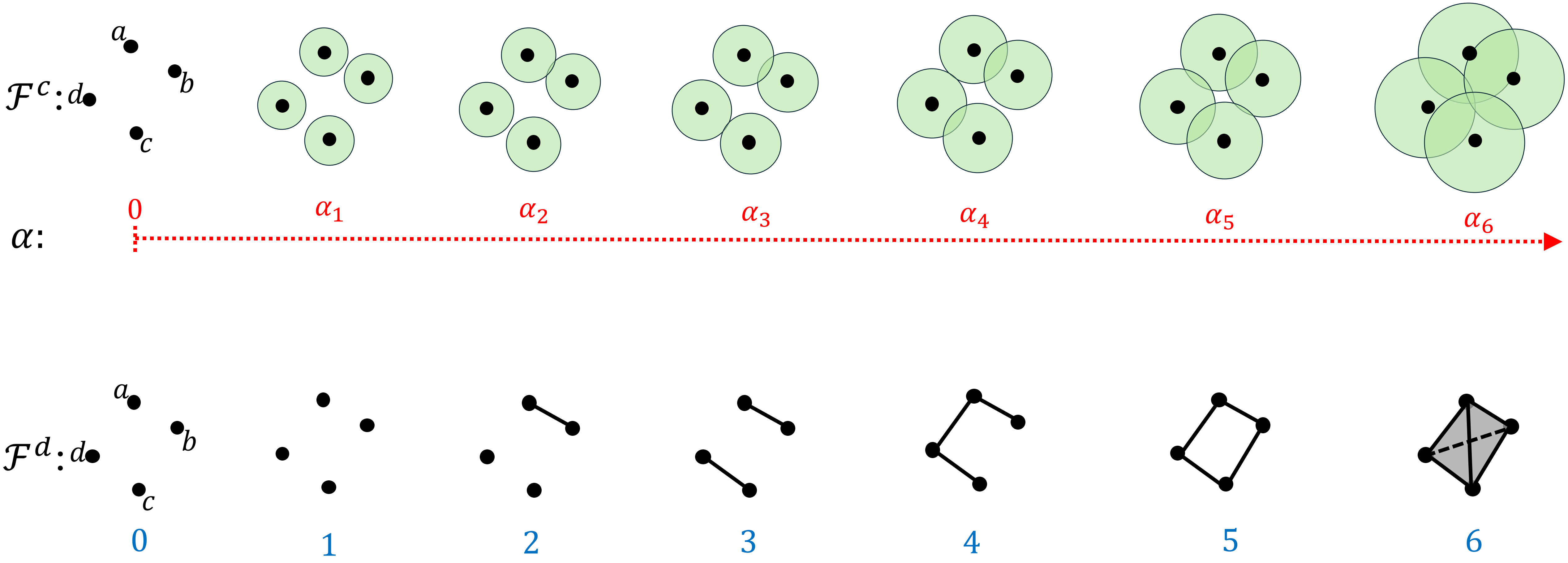

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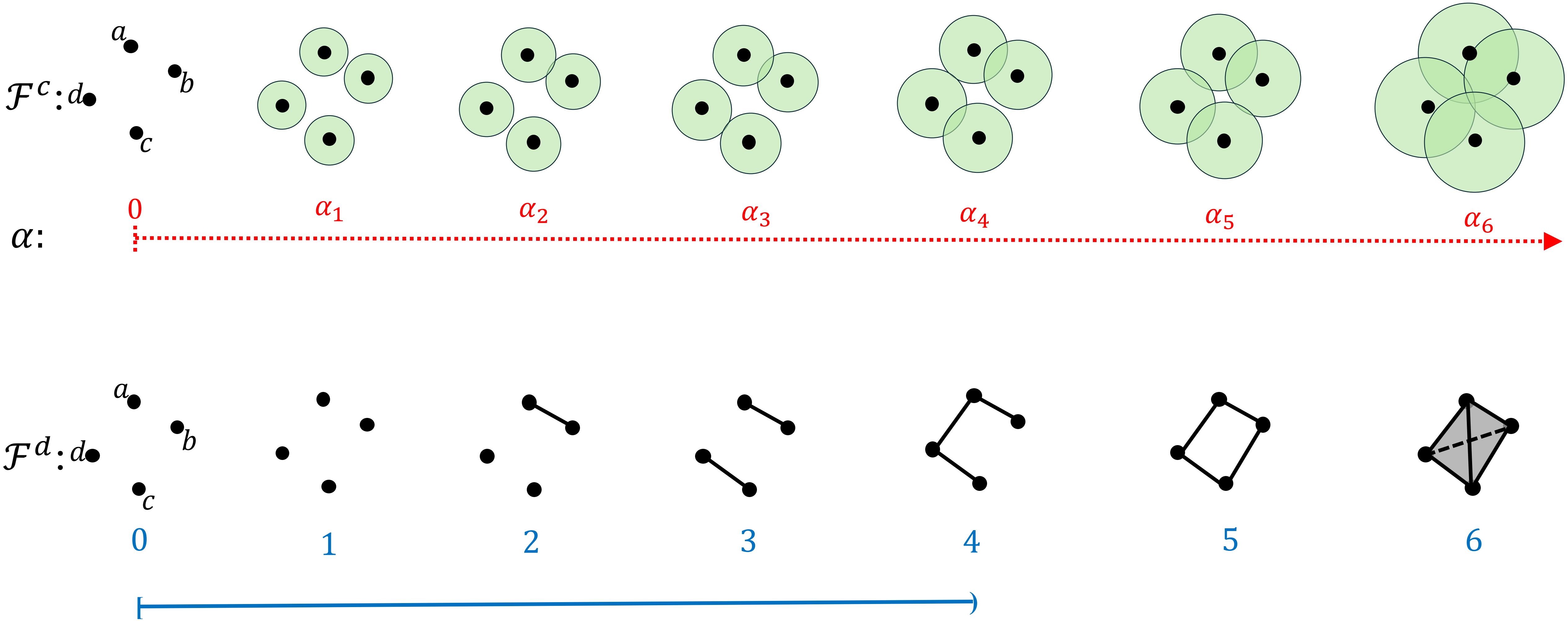

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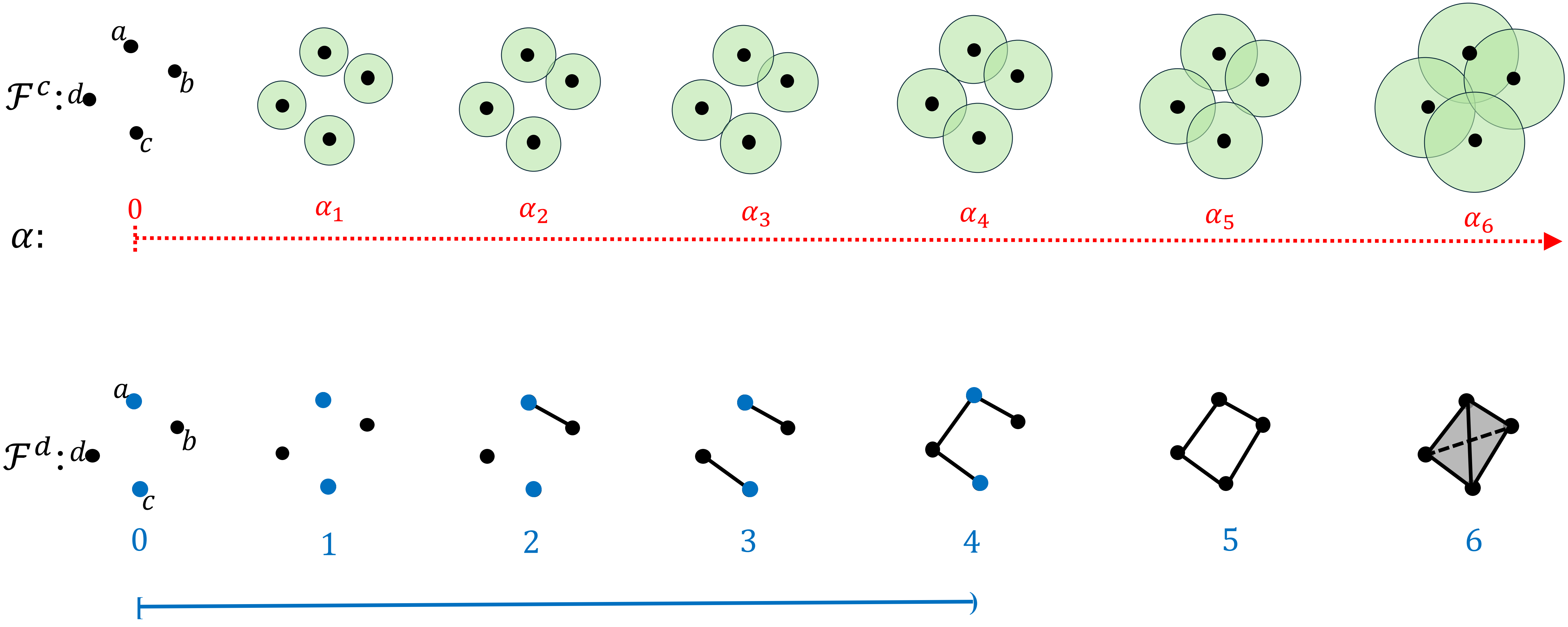

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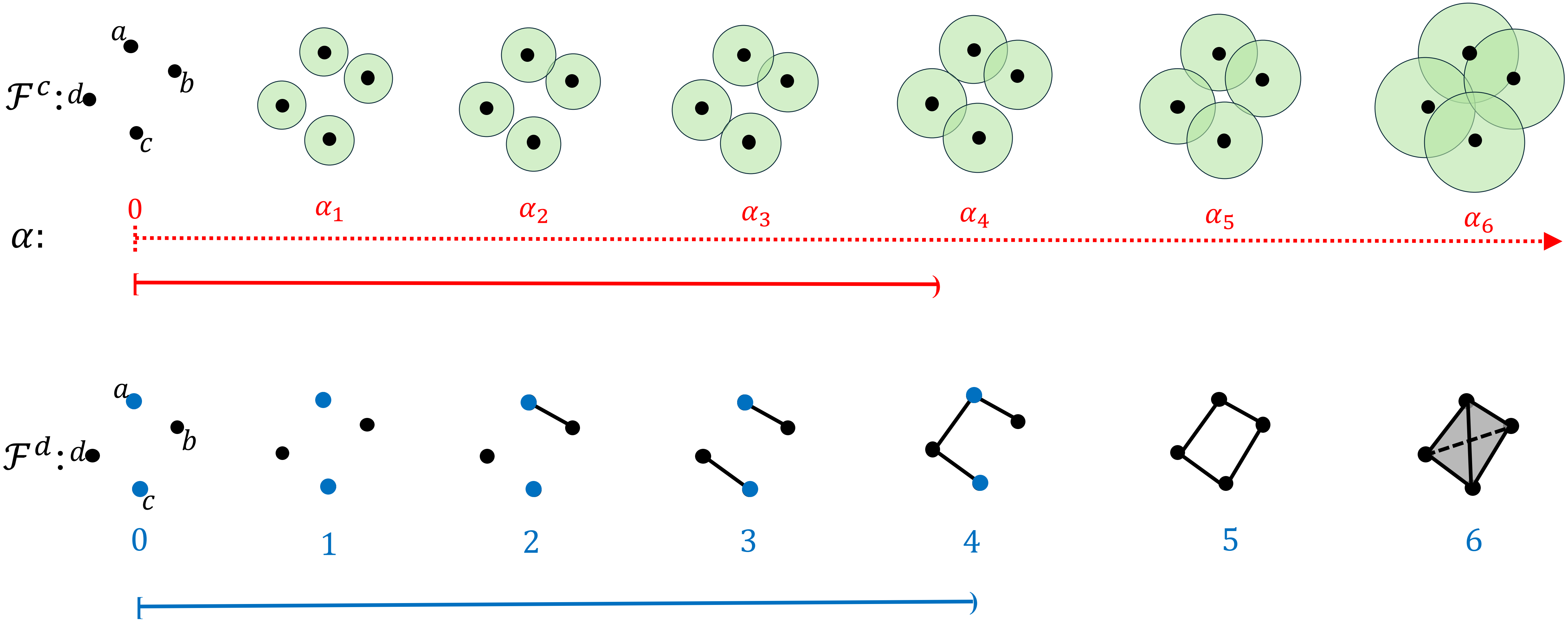

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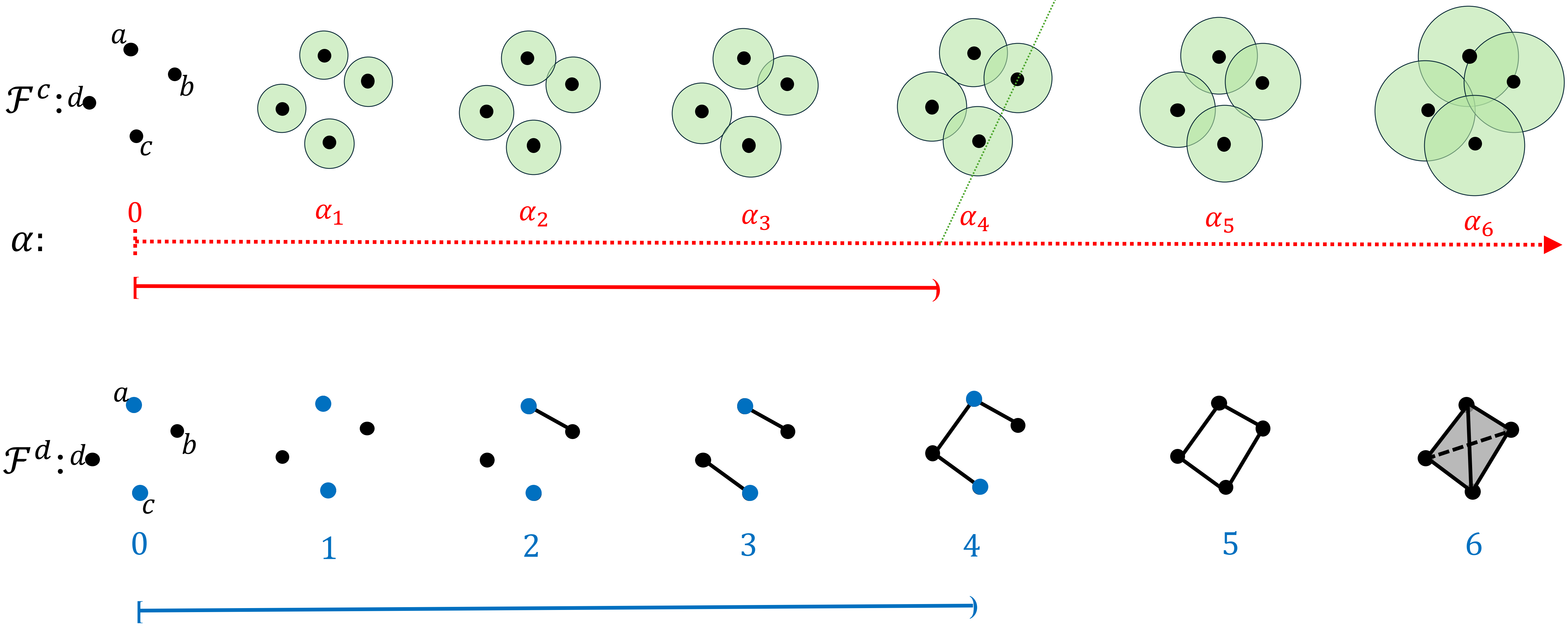
Between α_3 and α_4, balls of a and d touch so the gap between a and d filled



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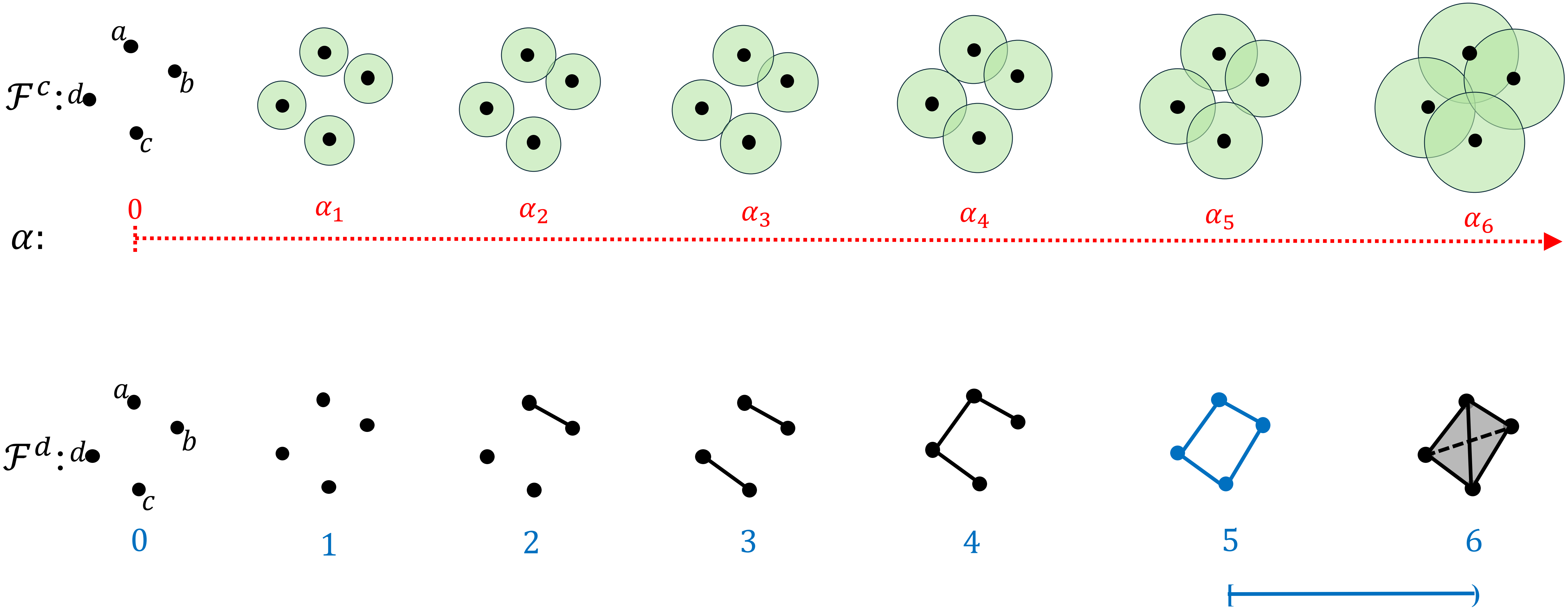

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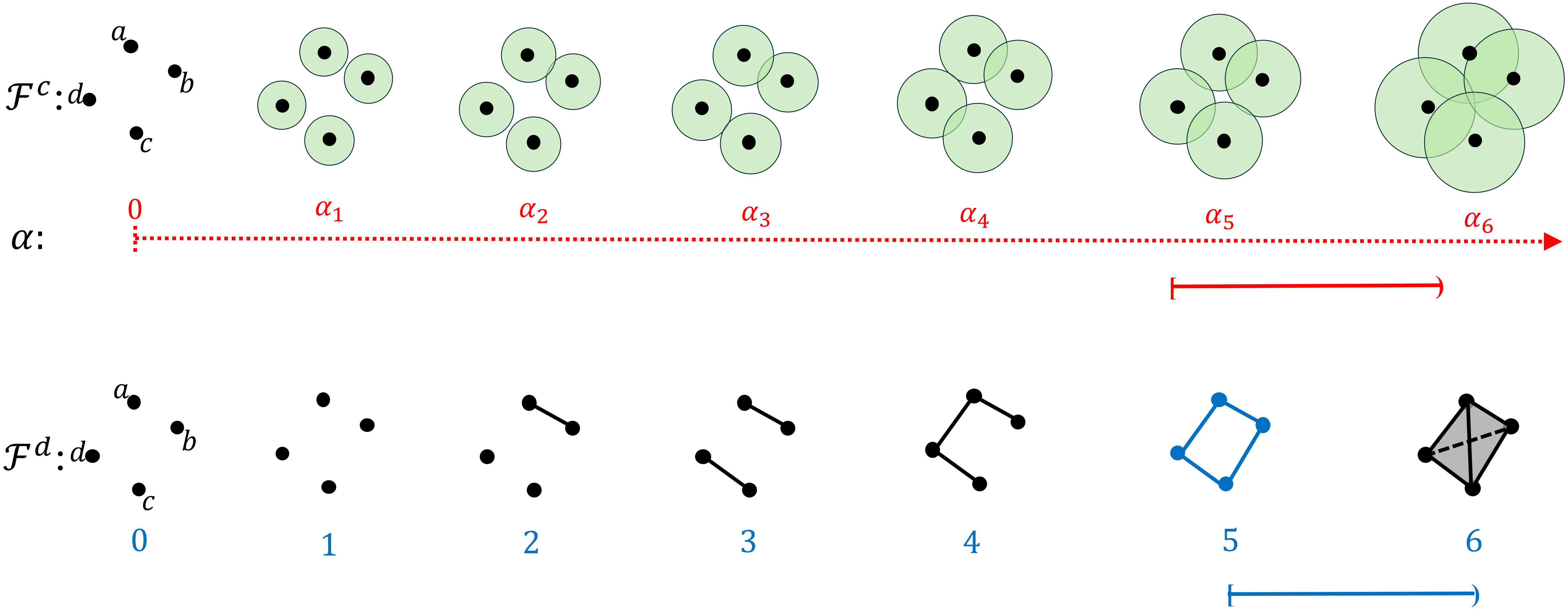

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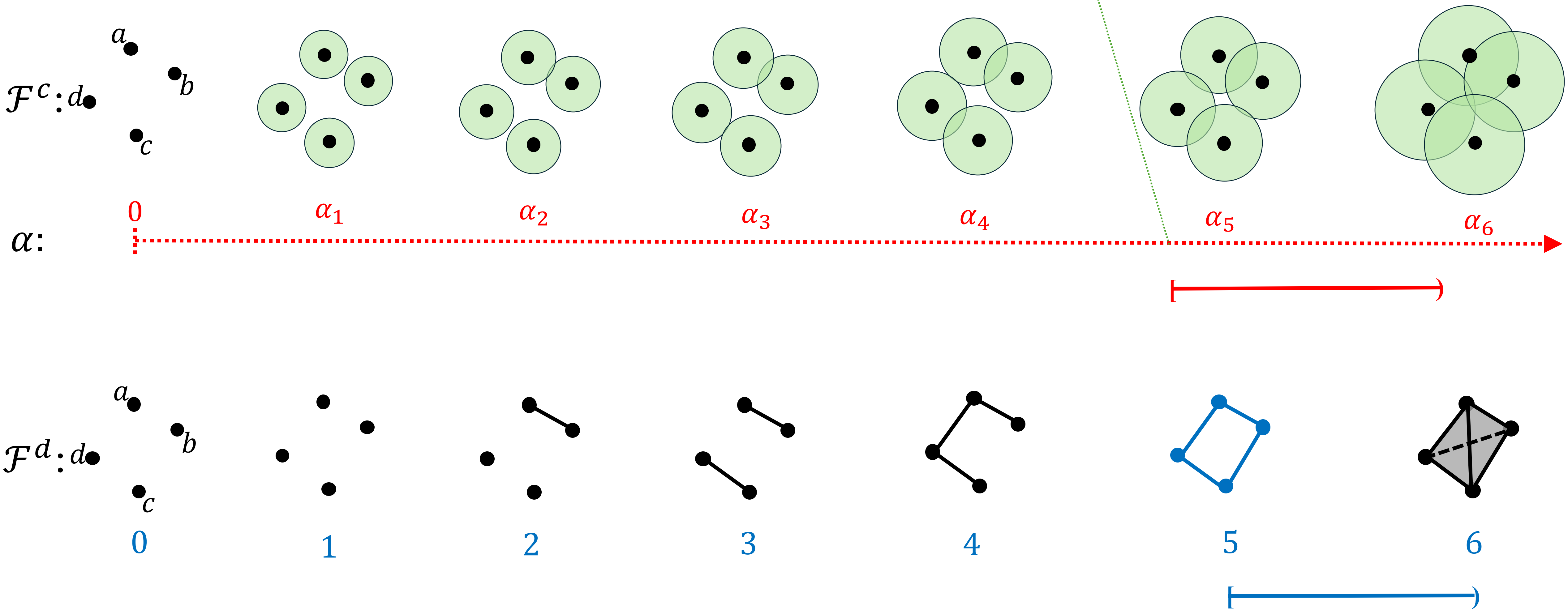
Between α_4 and α_5, balls of b and c touch so the blue 1-cycle forms



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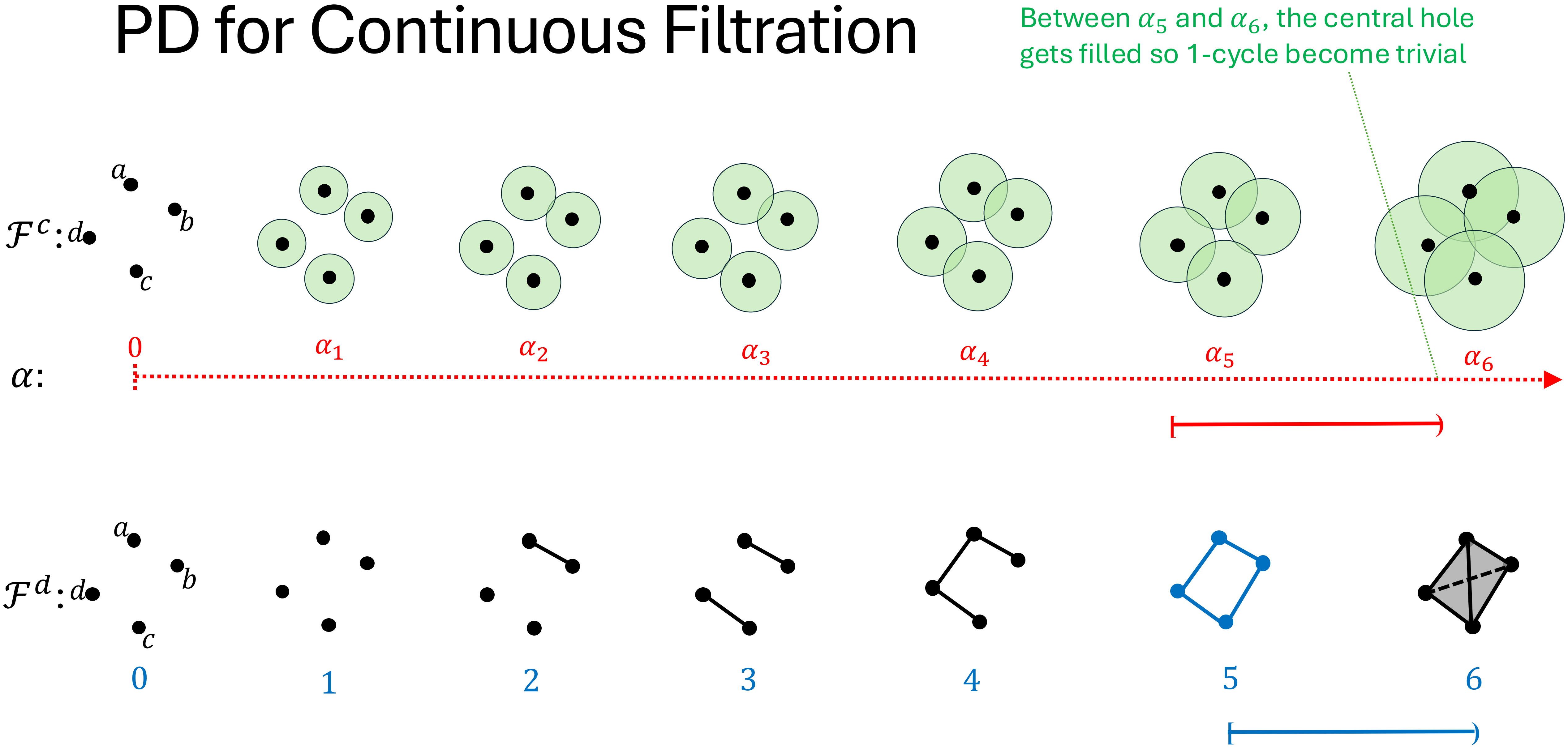

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- After all, trade-offs were made everywhere in computer science between efficiency and quality

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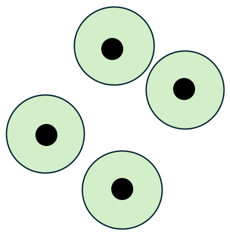

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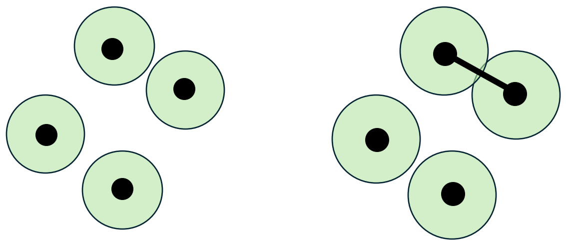

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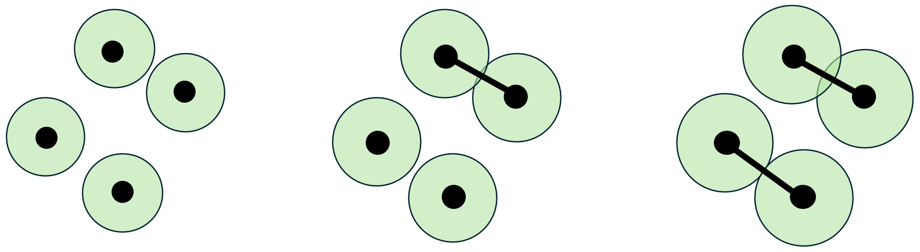

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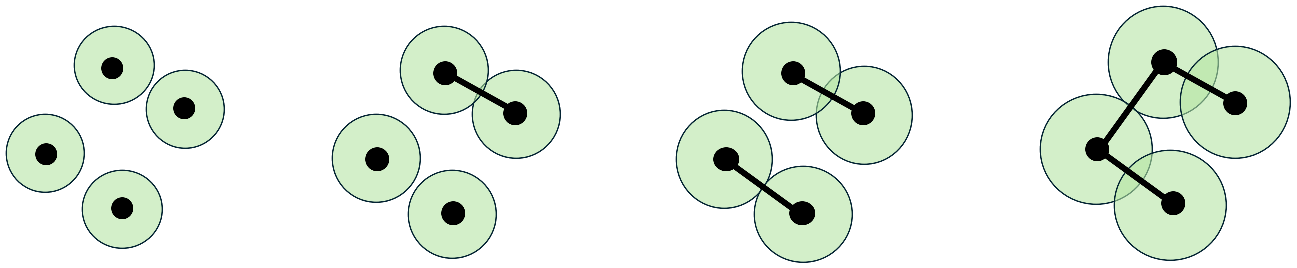

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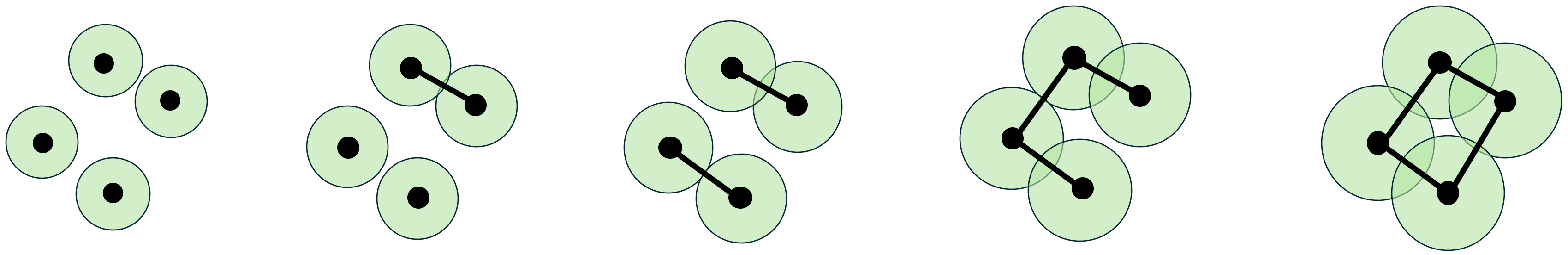

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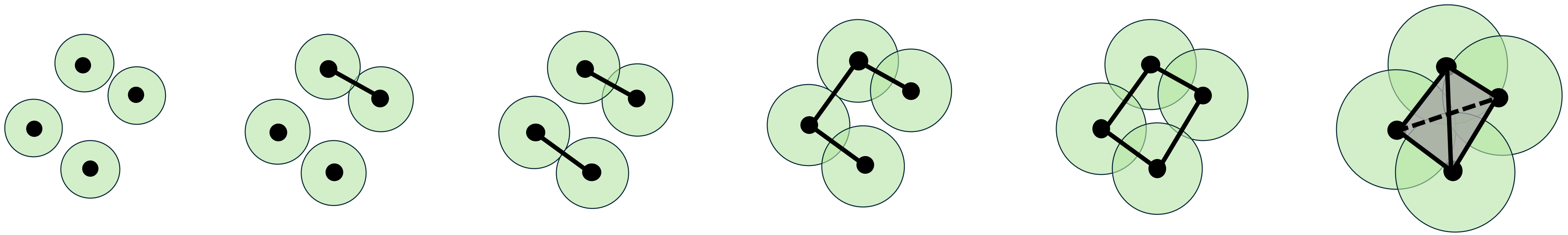

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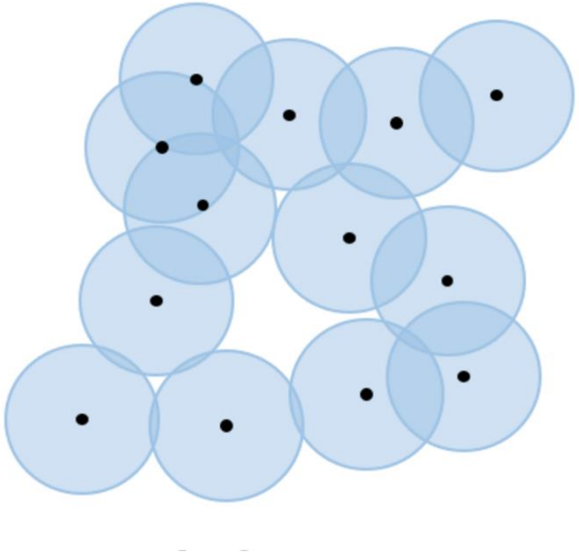

Image source: Reani, Bobrowski. Cycle Registration in Persistent Homology with Applications in Topological Bootstrap

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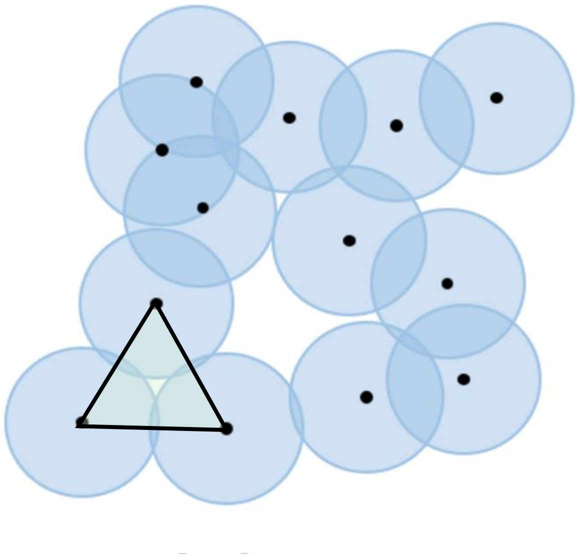

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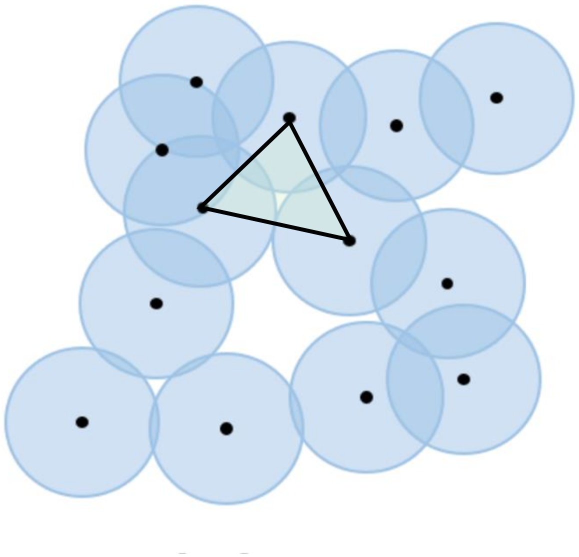

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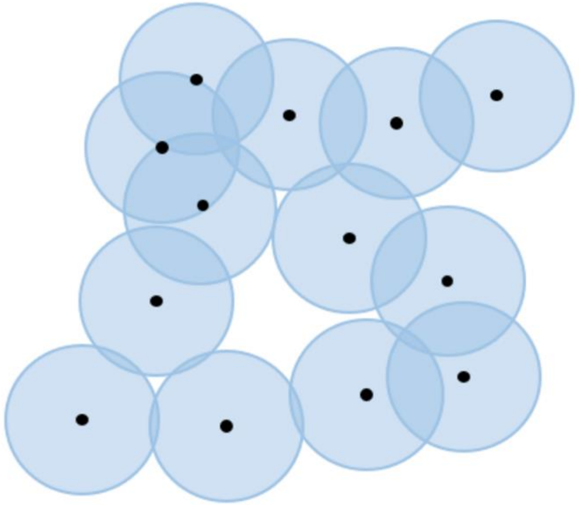

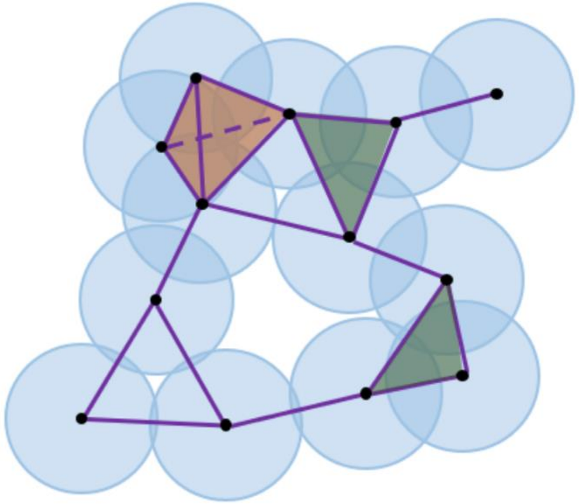

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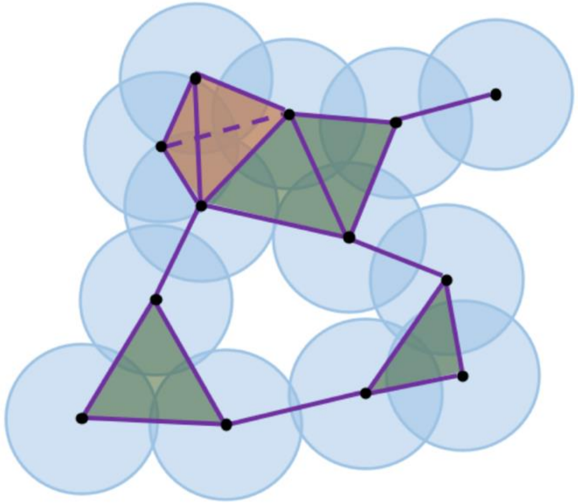

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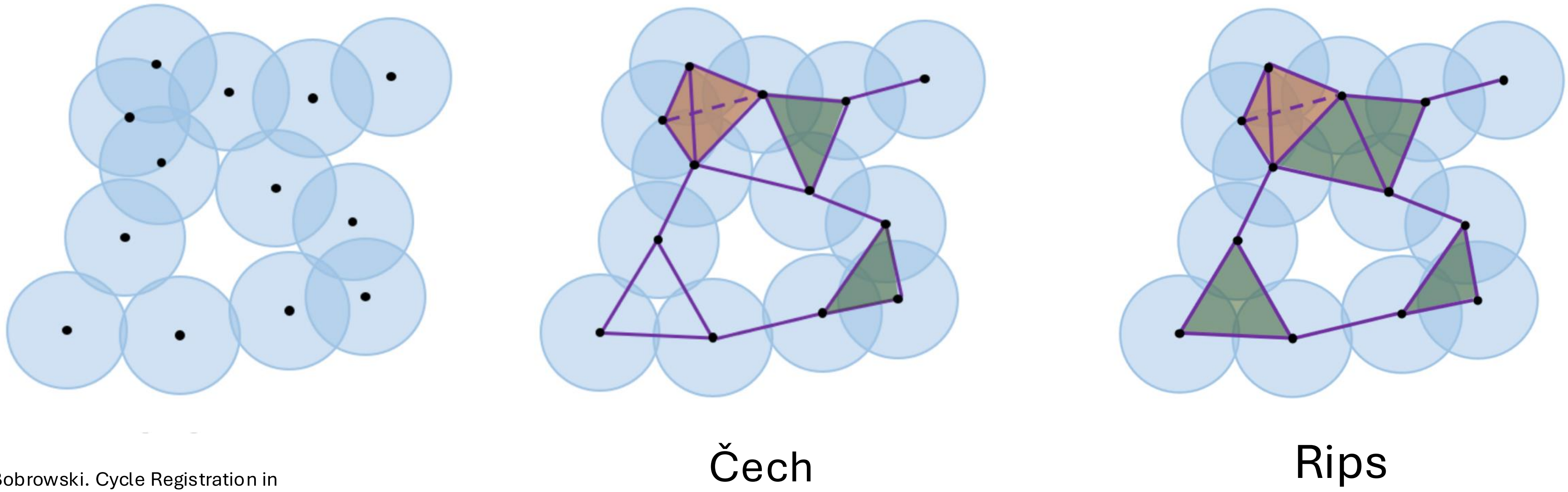

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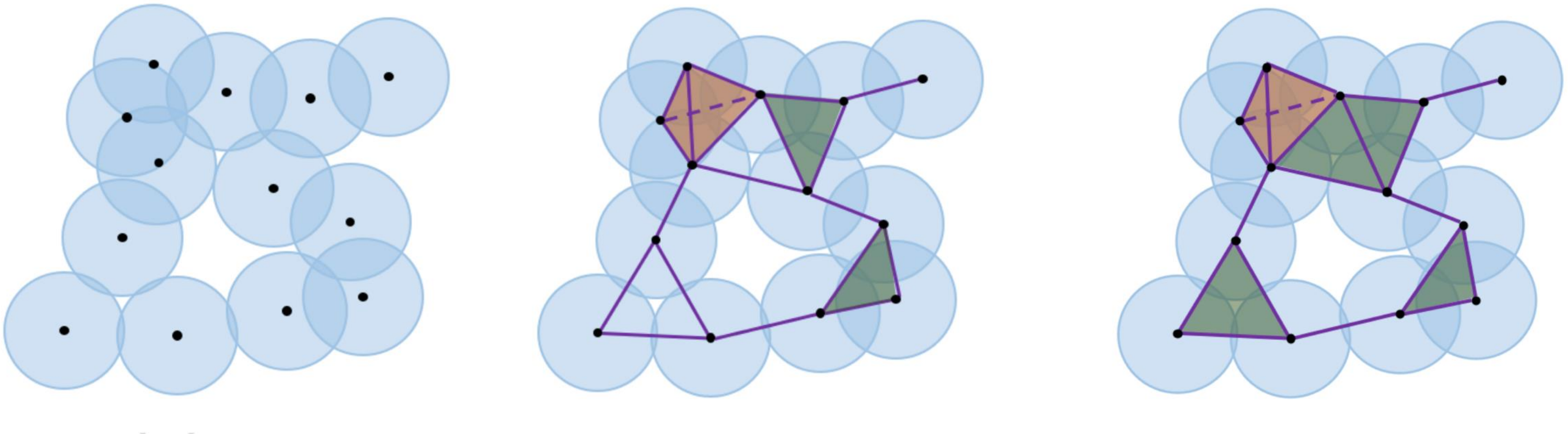
- Furthermore, if we increase the radius for Čech complex, the two missing two triangles will come into picture ---- in some sense, the sequences of Čech and Rips complexes are "interleaved with each other"



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- As for $\mathbb{C}^{\alpha}(P)$, we also need to show that $\mathbb{VR}^{\alpha}(P)$ is not only a set of simplices but also a simplicial complex, which is checking that the faces of each simplex in the set $\mathbb{VR}^{\alpha}(P)$ are also in $\mathbb{VR}^{\alpha}(P)$.
- **Verification**: Take any $\sigma \in \mathbb{VR}^{\alpha}(P)$ and a face τ of σ (a subset of σ, i.e.,$\tau \subseteq \sigma$).
- We have any pairs of the α-balls for the points in σ intersect. So any pairs of the α-balls for the points in τ intersect (because τ is a subset). So $\tau \in \mathbb{C}^{\alpha}(P)$

Remark

- For both the Čech and Vietoris-Rips filtration, all the vertices are always assumed to be present at *any* radius α starting from 0
- So at a certain radius α, you only need to figure out what are the edges and higher-dimensional simplices in the corresponding complex

PD for Vietoris-Rips Filtration

- We now also define PD for a continuous filtration using the discrete Rips filtration
- Again, define the PD for the continuous filtration $\mathcal{F}^c$ by "inducing" from the PD of the discrete Rips filtration $\mathcal{VR}(P)$:
  - Each complex in the discrete $\mathcal{VR}(P)$ corresponds to a range of α-values (and a range of spaces) in the continuous filtration
  - For each interval $[b, d) \in PD(\mathcal{VR}(P))$, consider the corresponding complexes in $\mathcal{VR}(P)$, which are $K_b, K_{b+1}, \dots, K_{d-1}$.
  - Then, the corresponding interval of $PD(\mathcal{F}^c)$ is the union of all the α-values corresponding to $K_b, K_{b+1}, \dots, K_{d-1}$.

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  - Then, the corresponding interval of $PD(\mathcal{F}^c)$ is the union of all the α-values corresponding to $K_b, K_{b+1}, \dots, K_{d-1}$.
- Notice now there is **data loss** introduced because $\mathcal{VR}(P)$ is not exactly the same as $\mathcal{C}(P)$

“Similarity” of Čech and Vietoris-Rips

- **Interleaving Theorem of Čech and Rips Filtration** : For any point set P and any radius α,

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- Remark: This “approximation well” thing will be made more formal later.

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- **Another observation**: The edges of the two Čech and Vietoris-Rips complexes for the same point set P over the same radius α are the same.
- Reason: Edges are formed by two points. If you check the definition of Čech and Vietoris-Rips (“all balls for a set of points intersect” and “each pair of balls for a set of points intersect”), when we only have two point, the two criteria become the same.

Vietoris-Rips Filtration: Alternative Definition

- **Definition**: Given a point set P and a distance r, the Vietoris-Rips complex of P corresponding to the distance r, denoted $\mathbb{VR}^r(P)$, is a simplicial complex whose vertices are points in P such that
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- The benefit of the above alternative definition is that we can completely eliminate balls and define Rips complexes / filtration **by only considering the pair-wise distances between points**

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- E.g., there could be data where we have objects which are not naturally coming from a Euclidean space $\mathbb{R}^n$, i.e., without positions (like points from a triangular mesh).

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- They are abstract objects but we have some pair-wise “distances” between these objects.

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- In this example, the data points are "regions of the brain", and we can calculate their "similarity" by measuring the correlation of their blood oxygen fluctuation over time (a time series data).

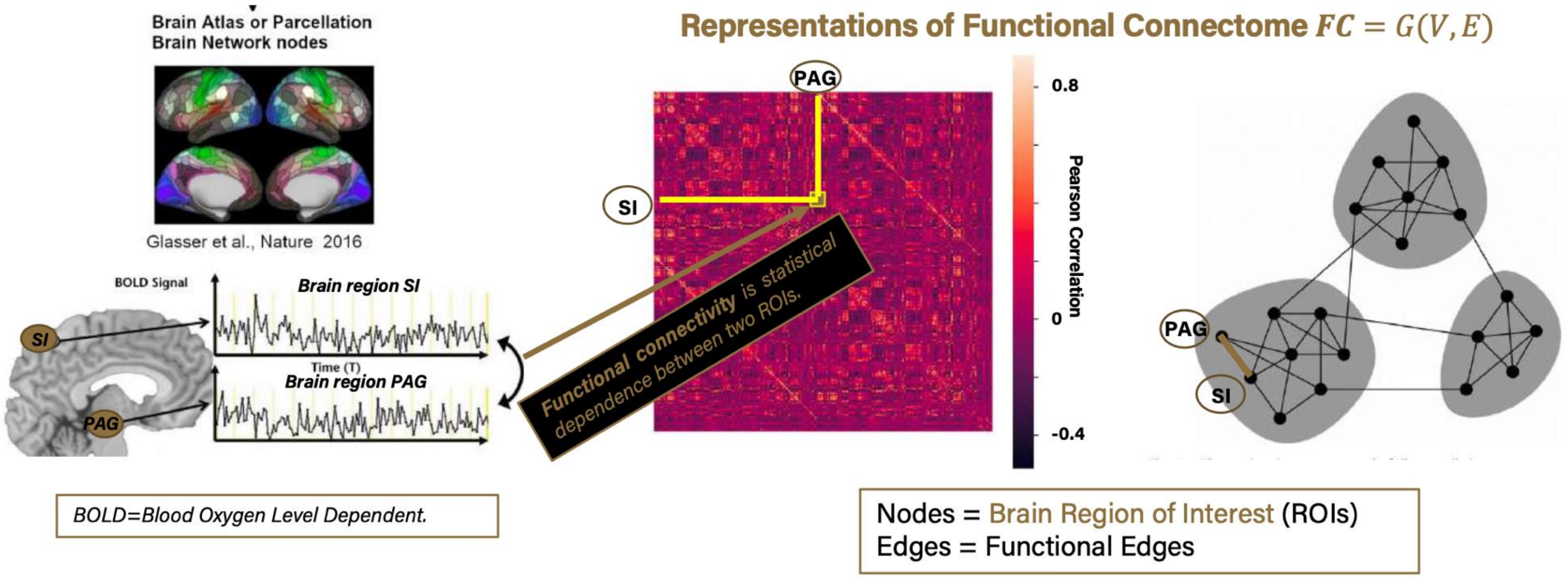

Figure courtesy of: Duy Duong-Tran

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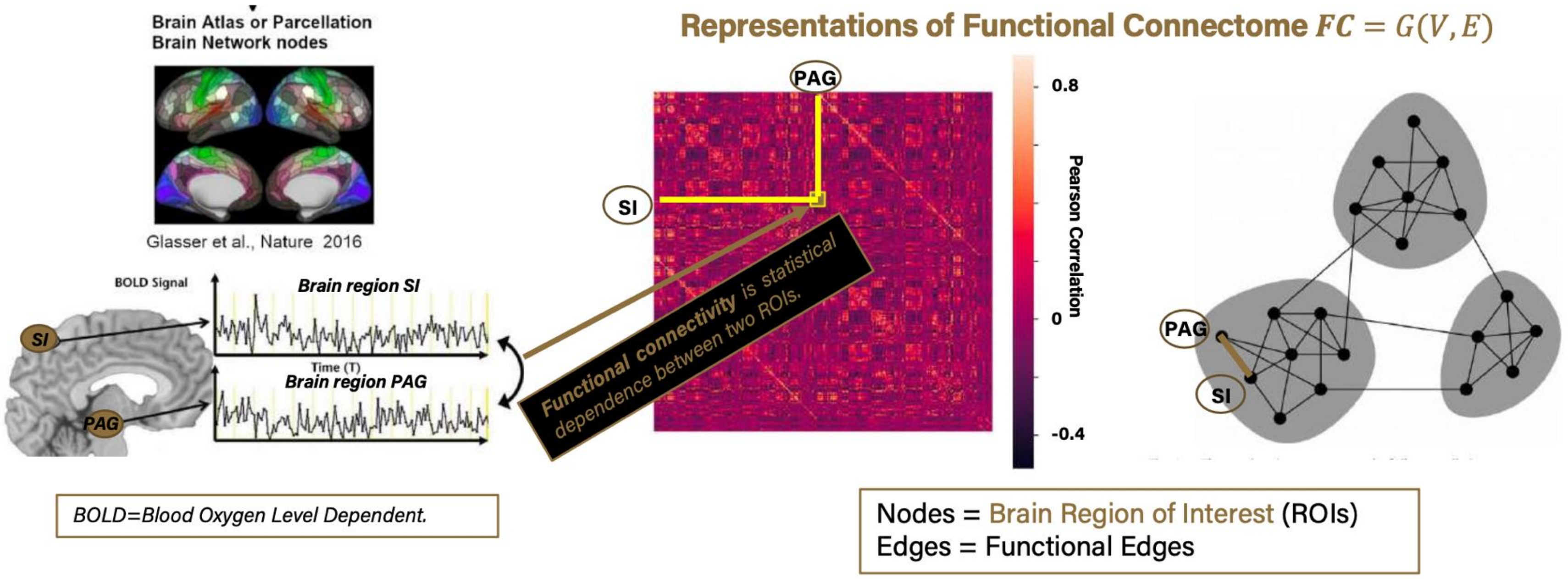

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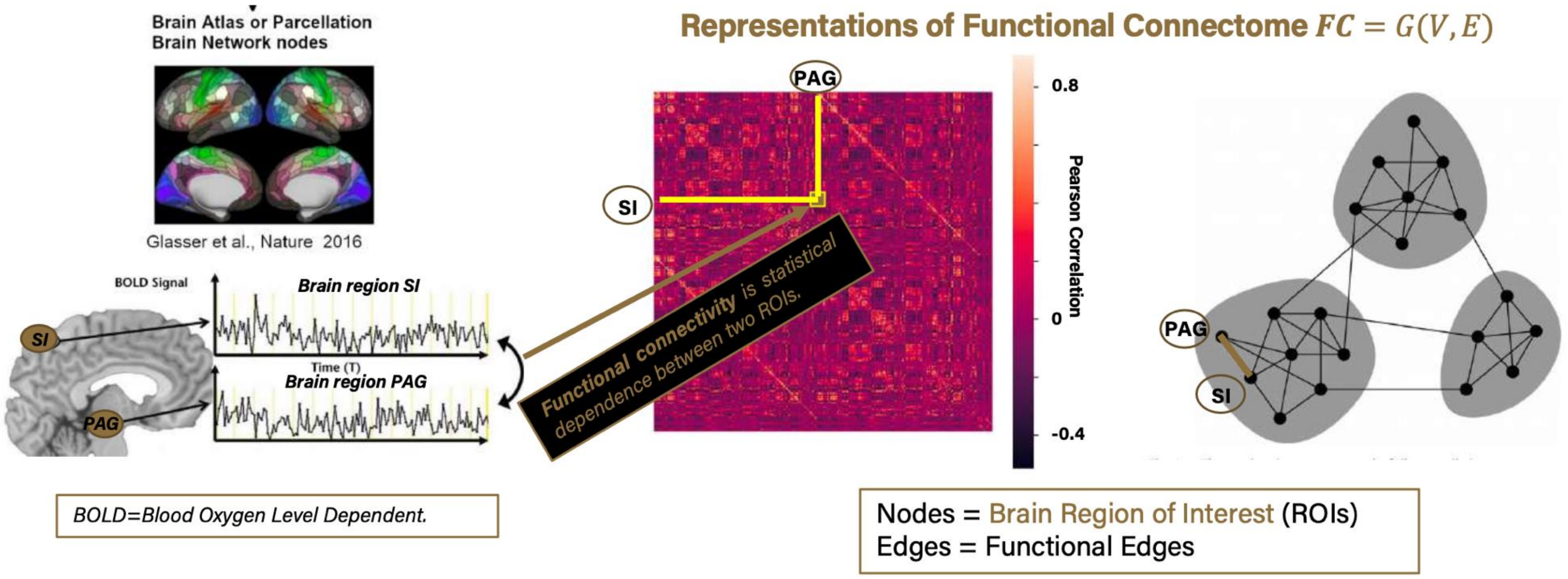
- These regions are not really technically having a position (each region is represented by a blood oxygen level function over time), but we have distances between the regions



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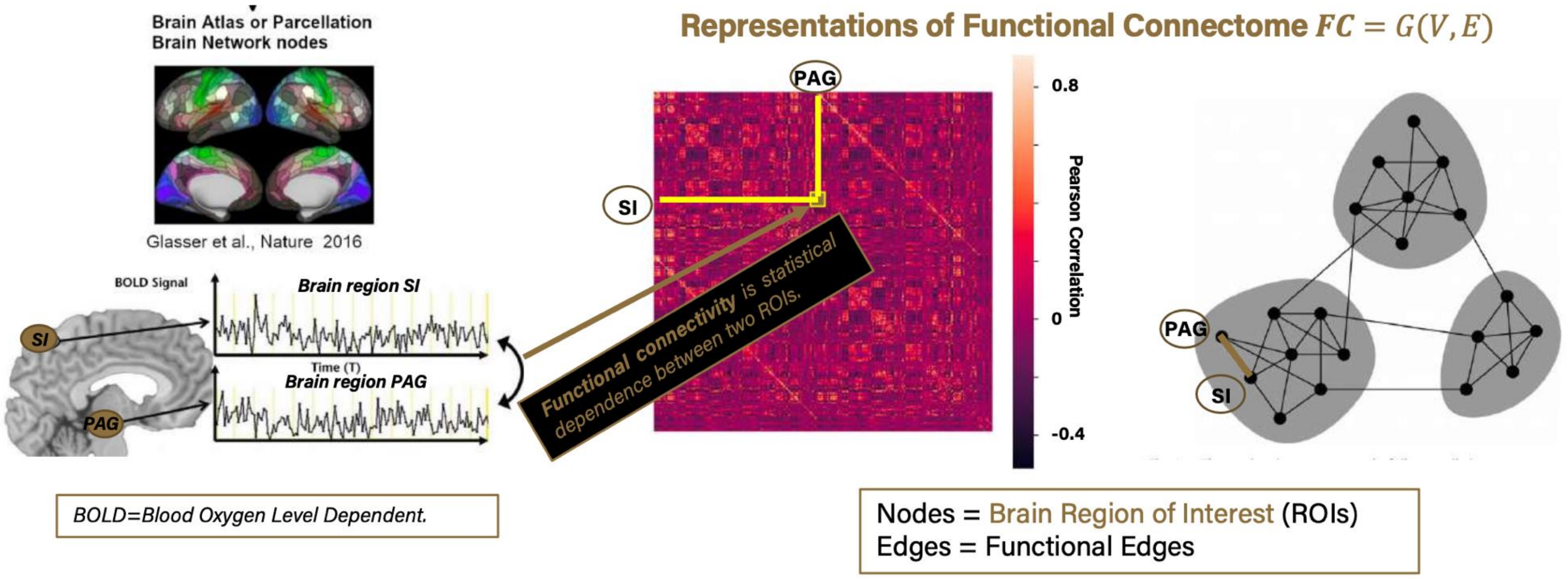
Vietoris-Rips Filtration: Alternative Definition

- For this data, we still can build Rips filtration on these brain regions



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Vietoris-Rips Filtration: Computation

- We shall briefly look at some facts concerning computing Rips Filtration.
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- This means that a Rips complex over a certain distance (radius) r is completely determined by the distances of each pair of points in P
- Since a pair of points form an edge, this also means that a $\mathbb{VR}^r(P)$ can be completely determined once we have figured out the edges (1-simplices) for $\mathbb{VR}^r(P)$

Vietoris-Rips Filtration: Computation

- So, for a certain r, to compute $\mathbb{VR}^r(P)$, our first thing to do: Enumerate each pair of points in P and check whether their distance is no more than r.
  - If this is true, we let the pair form an edge in $\mathbb{VR}^r(P)$
- By doing this, we have all the edges in $\mathbb{VR}^r(P)$.
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- $\mathbb{VR}^r(P)$ is then the **Clique complex** of the graph $\mathbb{G}^r(P)$.

Clique

- **Definition**: A **clique** of a graph $G = (V(G), E(G))$ is a subset S of $V(G)$ such that each pair of vertices of S form an edge in G.
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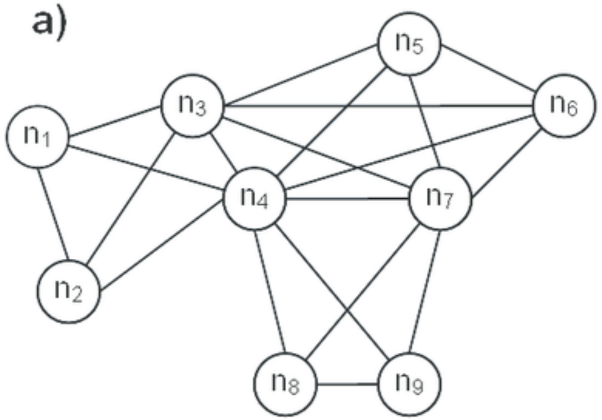

Image source: Santamaría, Therón. Overlapping Clustered Graphs: Co-authorship Networks Visualization

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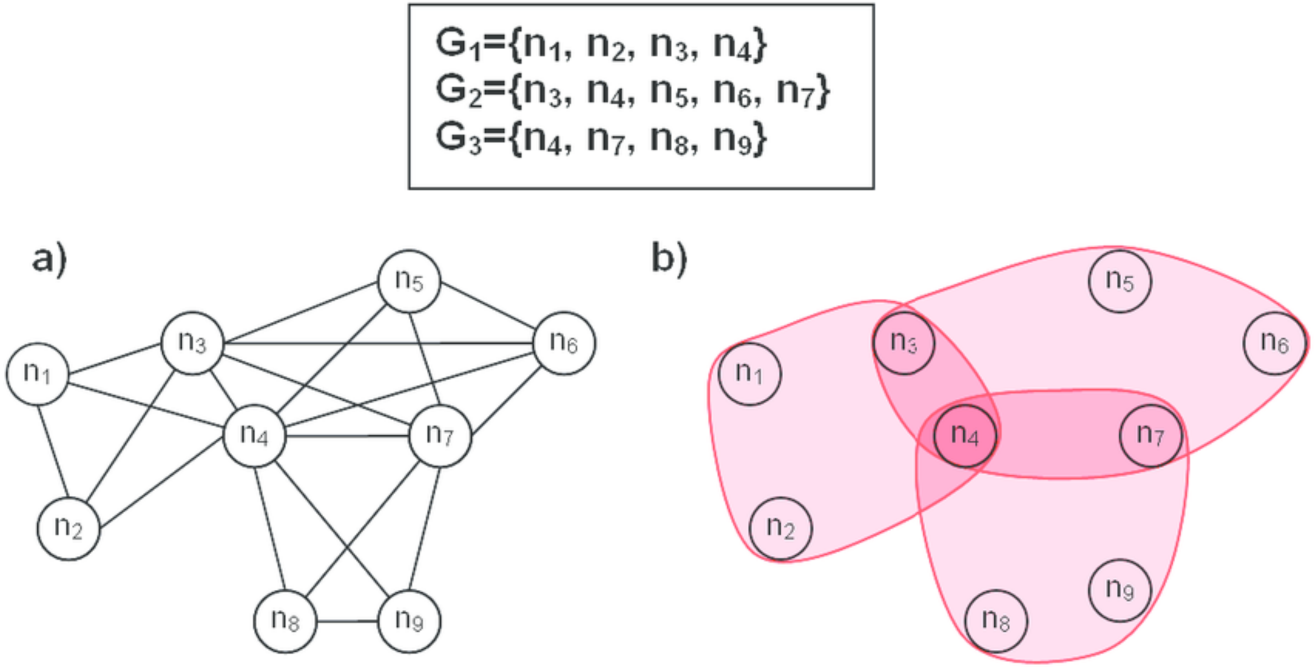
- E.g, the following graph has three maximal cliques (a clique not contained in another clique)



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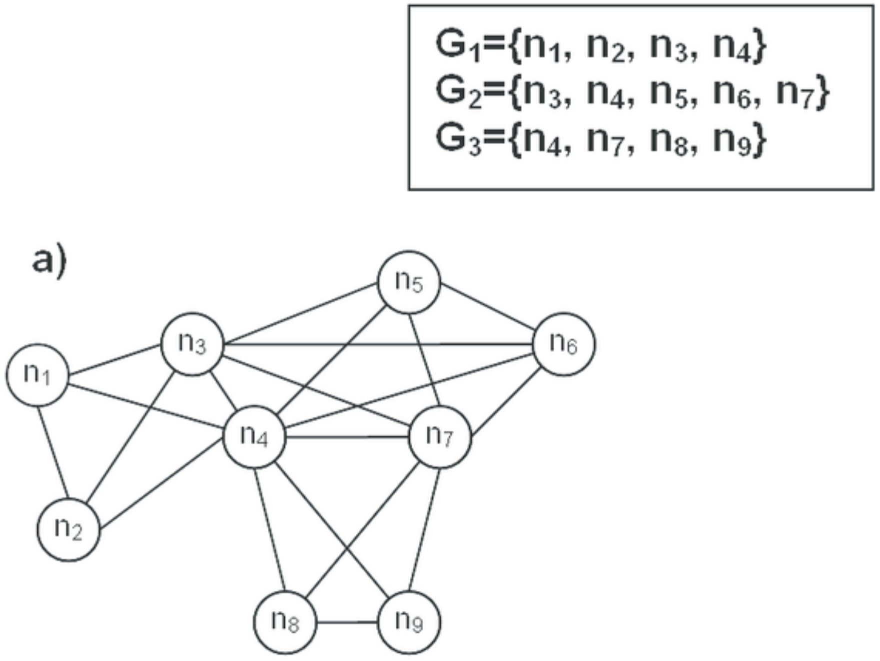

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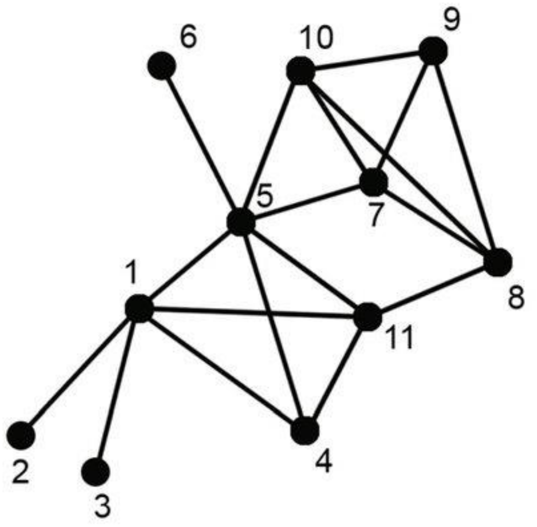

{1 4, 1 5, 1 11, 4 5, 4 11, 5 11} → [1, 4, 5, 11]
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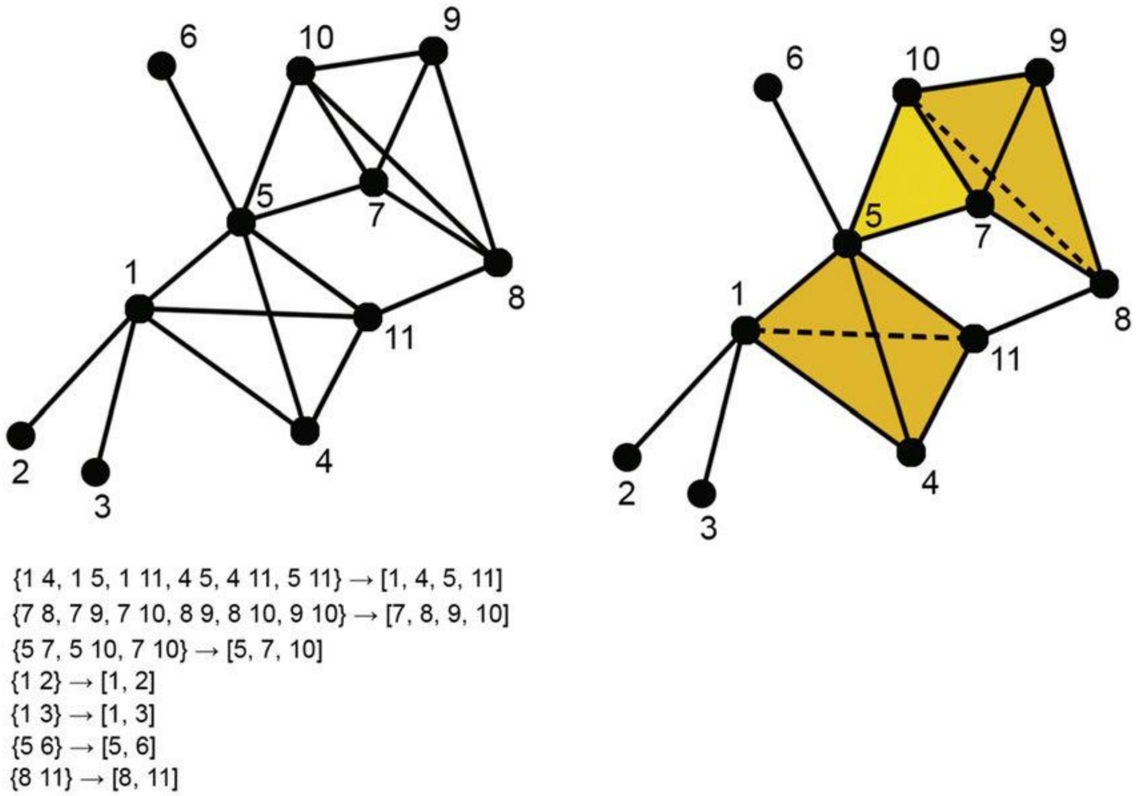

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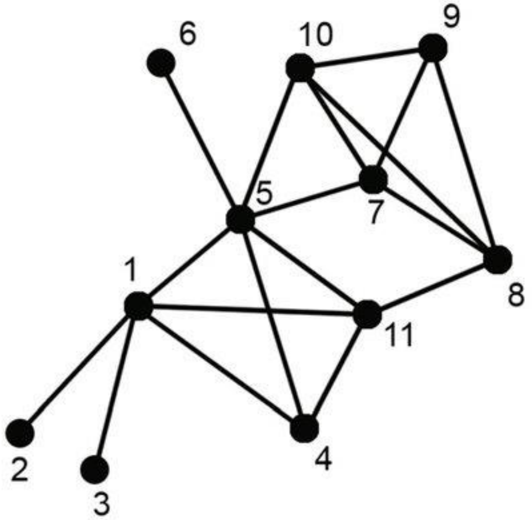

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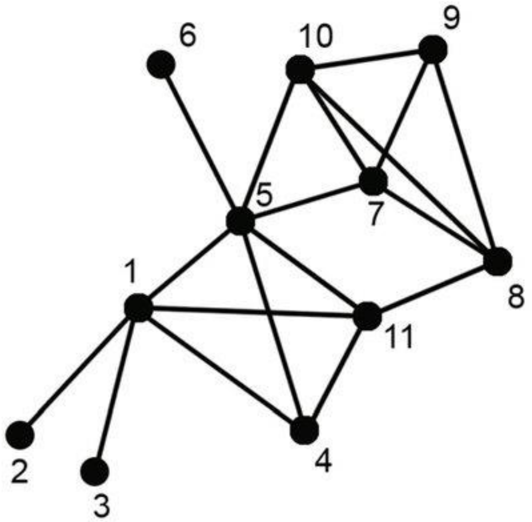

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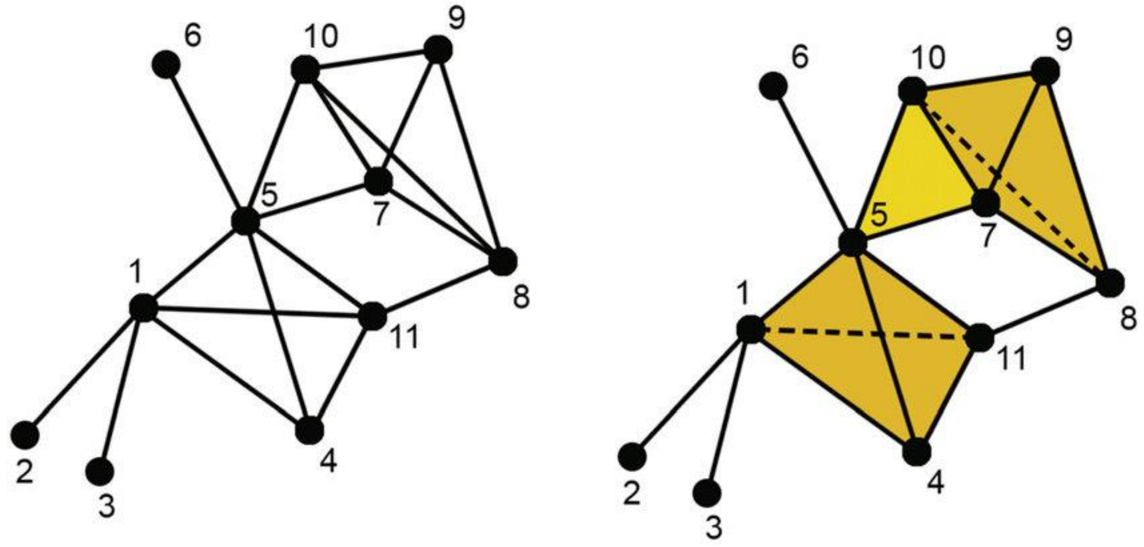

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    - Find the values r where $\mathbb{VR}^r(P)$ changes
    - This is equivalent to finding the values r where $\mathbb{G}^r(P)$ changes

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  - Finding these values takes $O(n^2 \log n)$ time dominated by the sorting, where n is the number of points in P

Another type of filtration

- **Delauney** complexes / filtrations: growing the balls around points, construct a simplex whenever their set of balls intersect (the same as Cech complexes)
- **Difference**: the part of a ball stops growing when touching another ball.

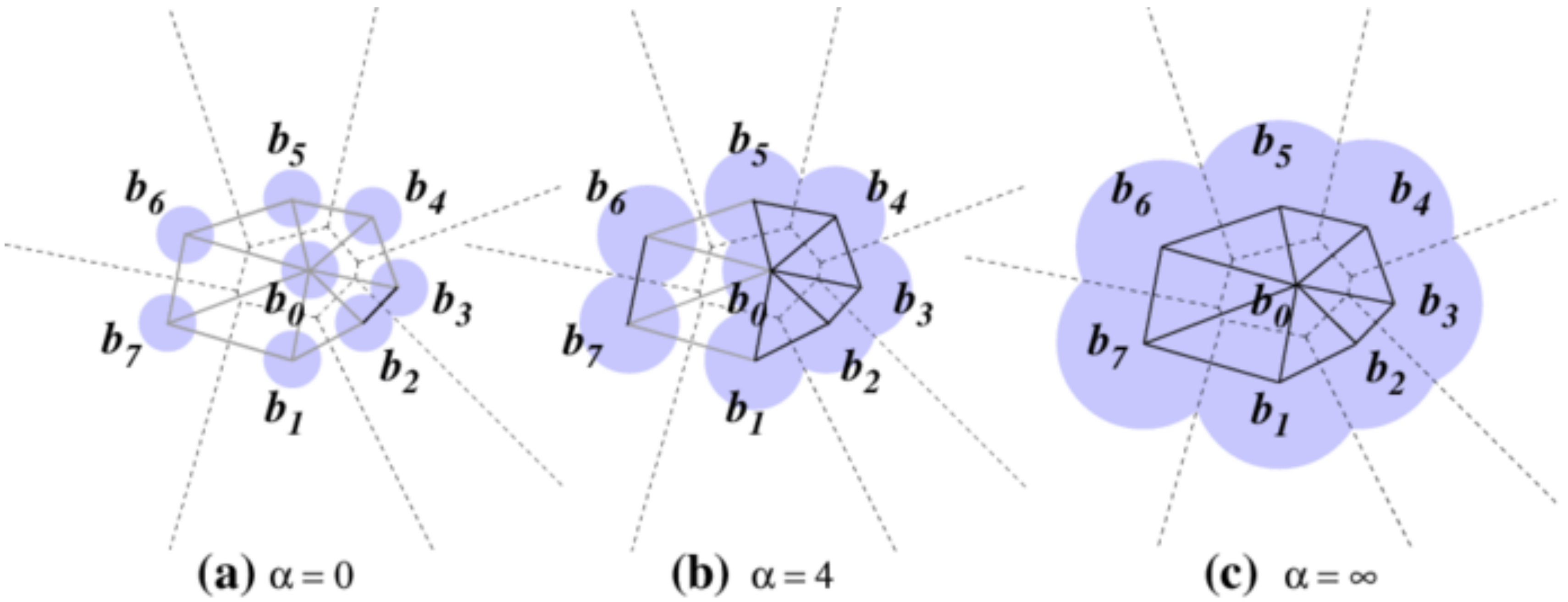

Image source: Li & Liang. Knowledge-Based Energy Functions for Computational Studies of Proteins

Delauney complexes / filtrations

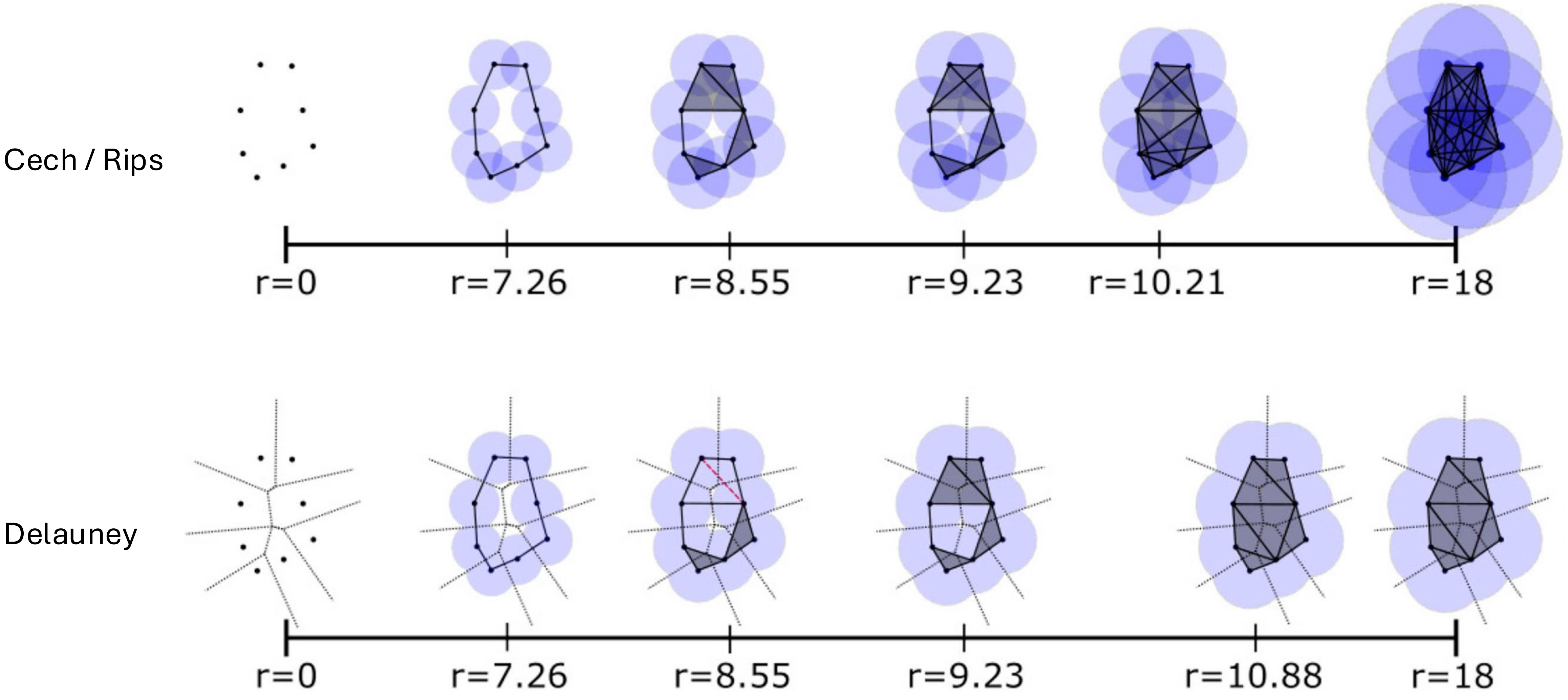

Image source: Mishra, Motta. Stability and machine learning applications of persistent homology using the Delaunay-Rips complex

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- Disadvantage of Delauney complexes: costly to compute, especially when the dimension of the points in the point cloud is high
- The go-to filtration for point cloud is **Rips filtration** because of (1) its computational efficiency and (2) the fact that it still faithfully recover the shape of the data (despite data loss)

Other types of complexes

- There are other types of complexes:
    - Witness complex
    - Graph-induced complex
    - Tangential complex
    - …
- Will not cover them at least for the time being

Data as a function

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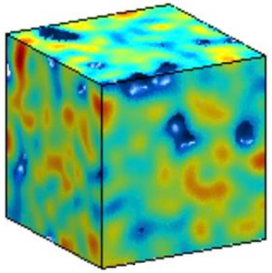
Image



3D volume data

Img source: https://pixabay.com/photos/new-year-background-tree-sunset-736885/; Adler et al. Persistent homology for random fields and complexes

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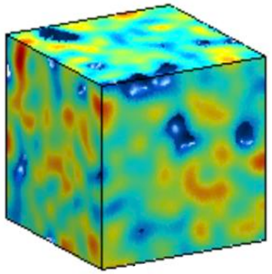

3D volume data

- E.g., all pixels in an image form the domain of a function and the color value on each pixel is basically the function value on a point of the domain

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  - Even if the range of the function is more than a single real value, say again, a colored image, we can take each channel (RGB), this will give you three individual real-valued functions. We can analyze each individually using persistence

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Image

➡ $f: X \to \mathbb{R}$ ➡ Filtration ➡ PD

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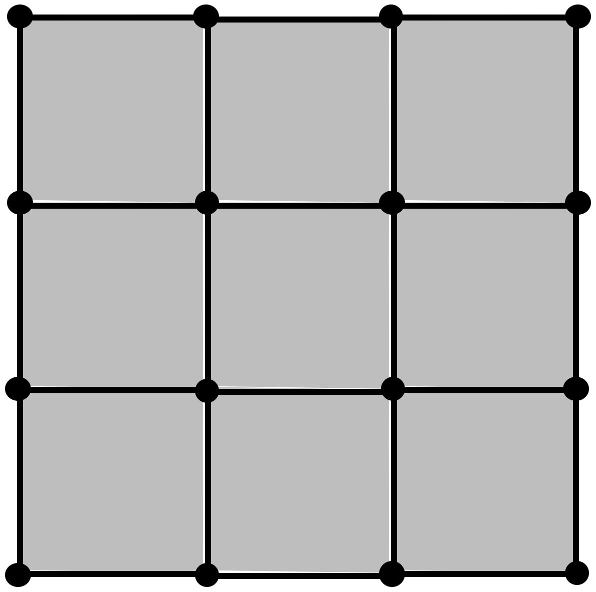

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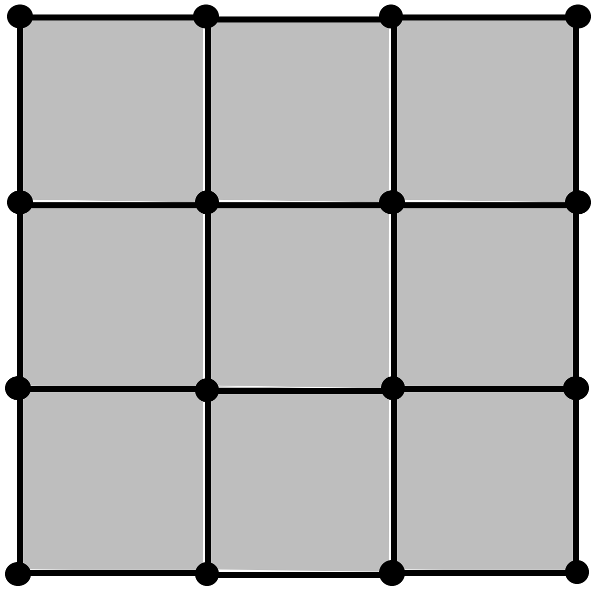

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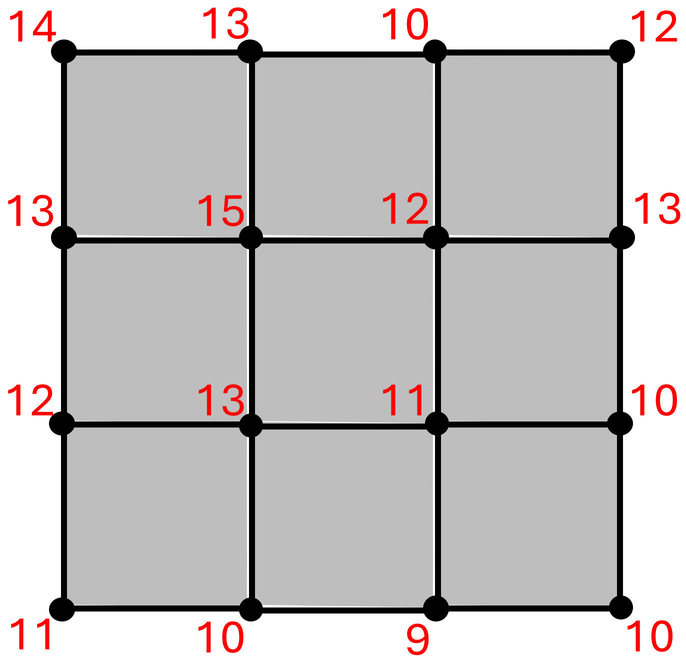


Image function

- Notice: the below regular grid does not form a simplicial complex (because of the square)

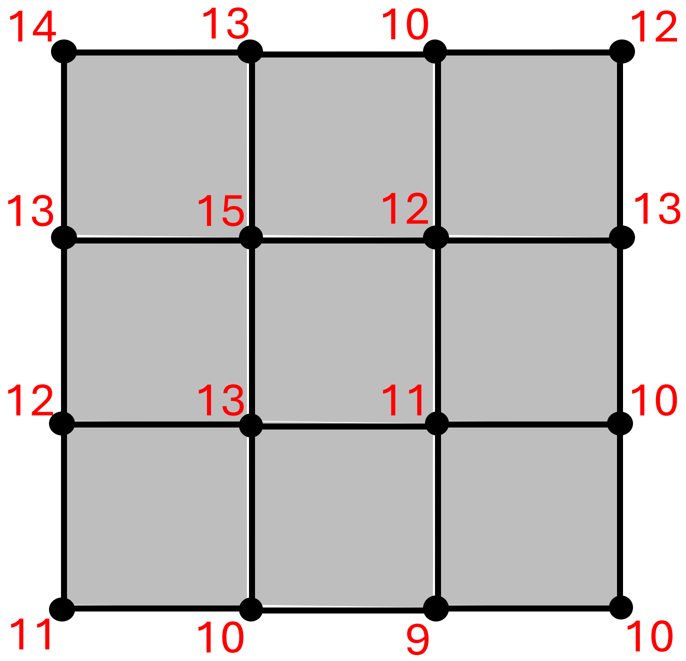


Image function

- Notice: the below regular grid does not form a simplicial complex (because of the square)
- So we subdivide the grid to be consisting of triangles, so X becomes a simplicial complex

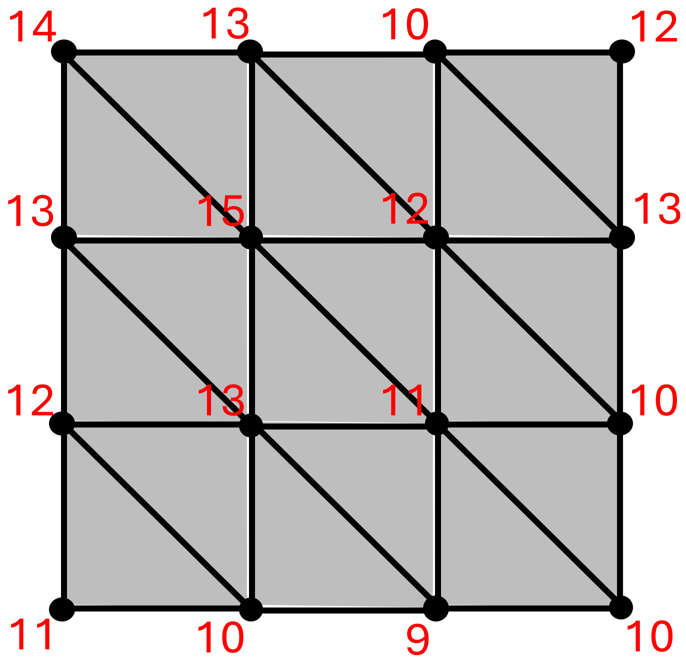
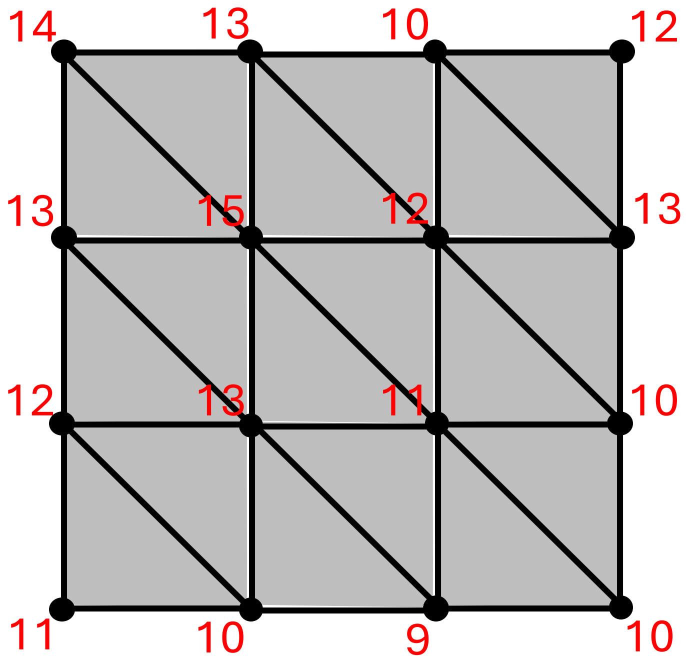


Image function

- Another problem: the function values are only given on the vertices (which are gray-scale values on the pixels from the given image)
- We need function values on the edges and triangles: for this we take the "maximum" value of the vertices that an edge or triangle contains



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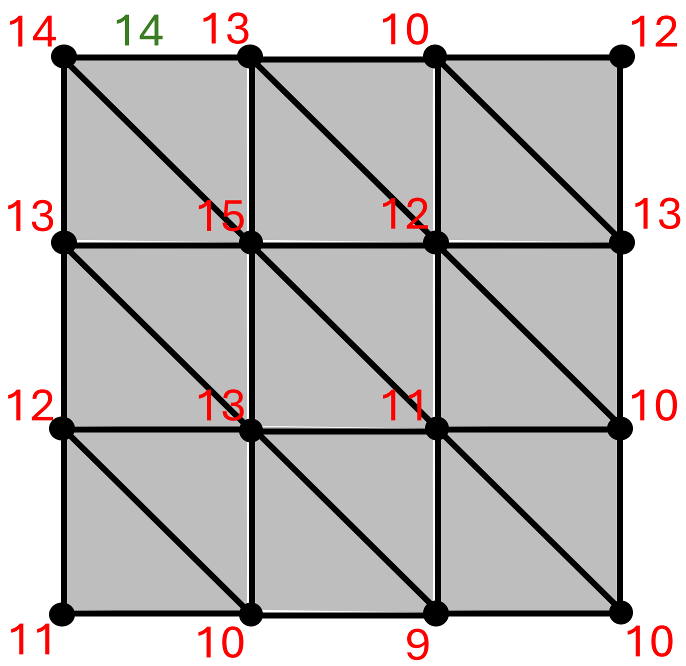

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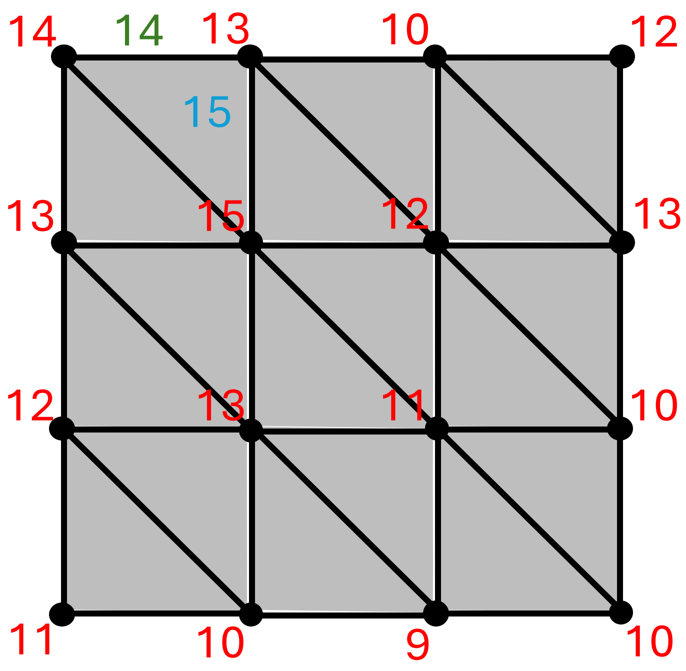

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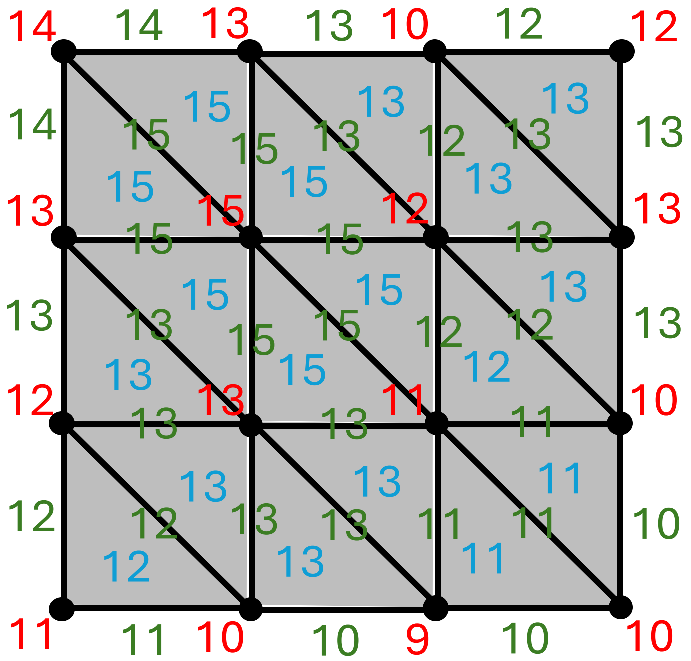

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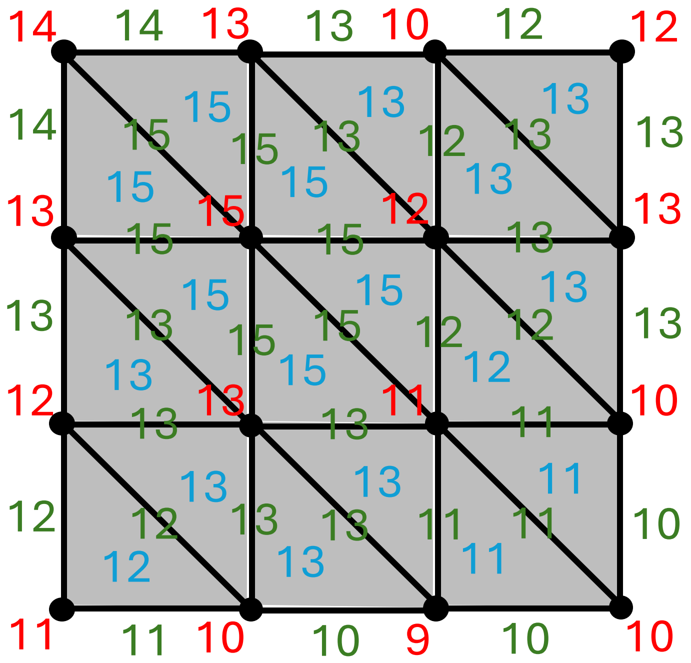
- It should be esay to verify that $f^{-1}(-\infty, \alpha_i] \subseteq f^{-1}(-\infty, \alpha_{i+1}]$ for any i

Sublevelset filtration

- $f^{-1}(9] \subseteq f^{-1}(10] \subseteq f^{-1}(11] \subseteq f^{-1}(12] \subseteq f^{-1}(13] \subseteq f^{-1}(14] \subseteq f^{-1}(15]$



Sublevelset filtration

- $f^{-1}(9]$

Sublevelset filtration

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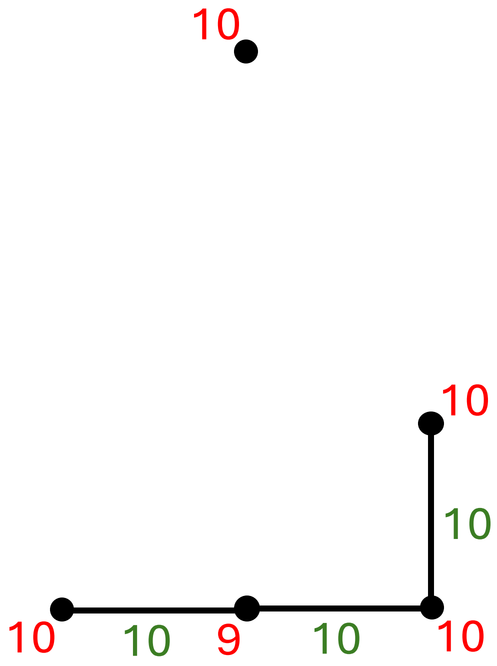

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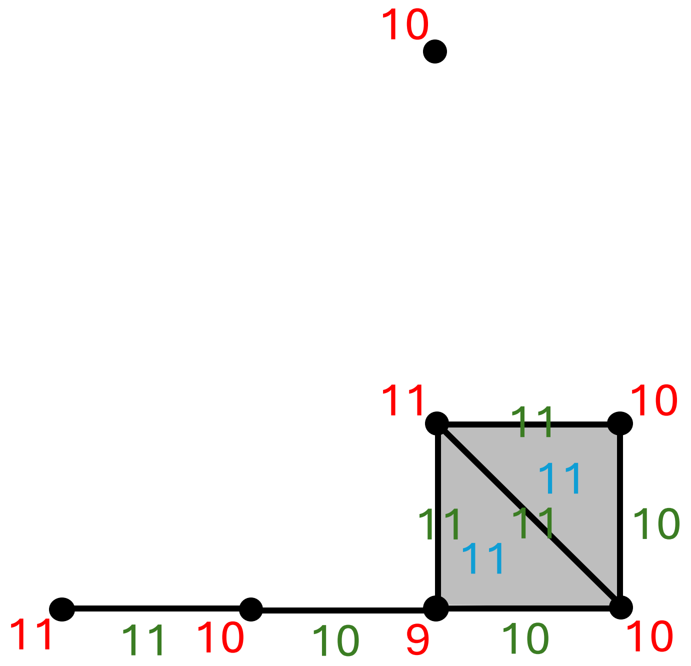

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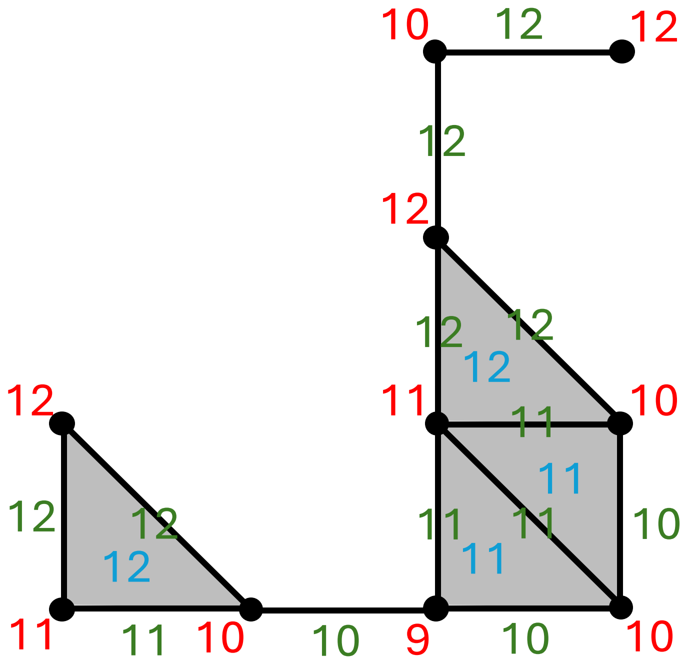

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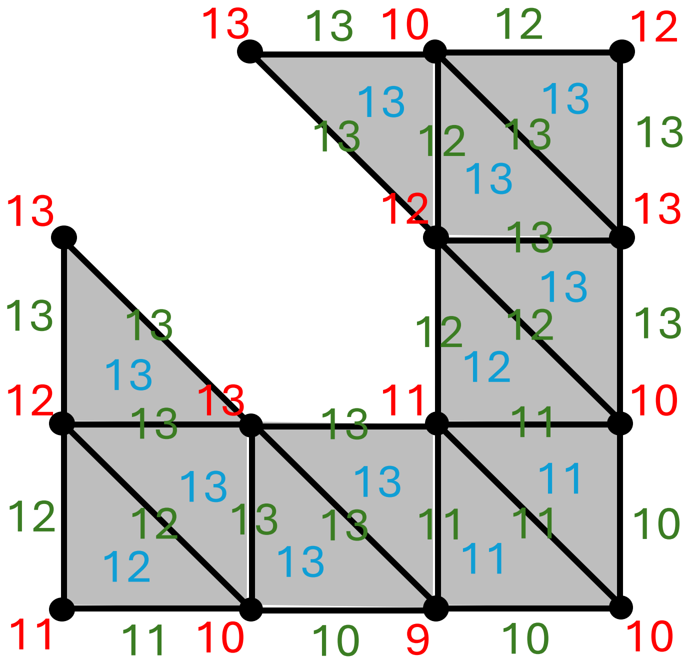

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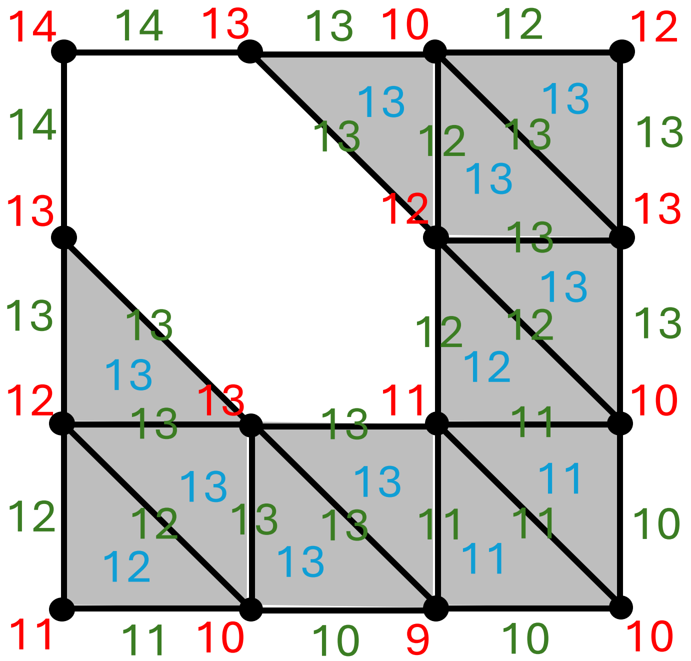

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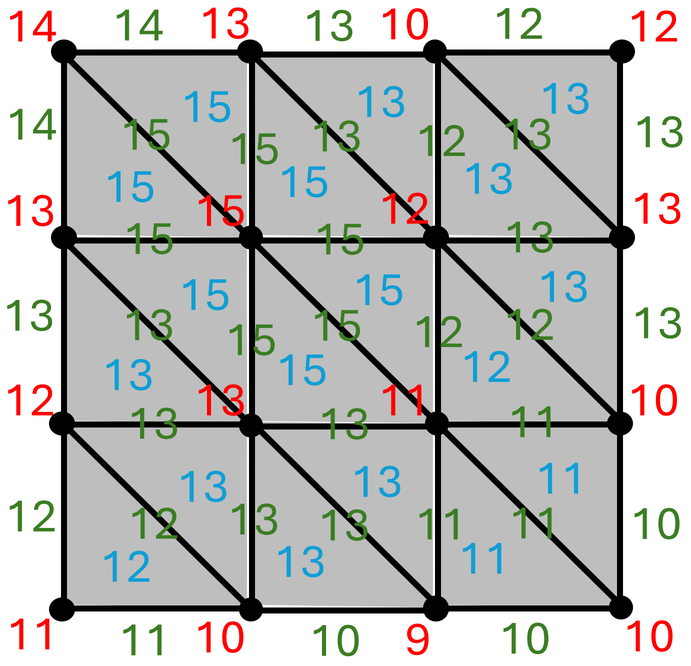

PD for the sublevelset filtration

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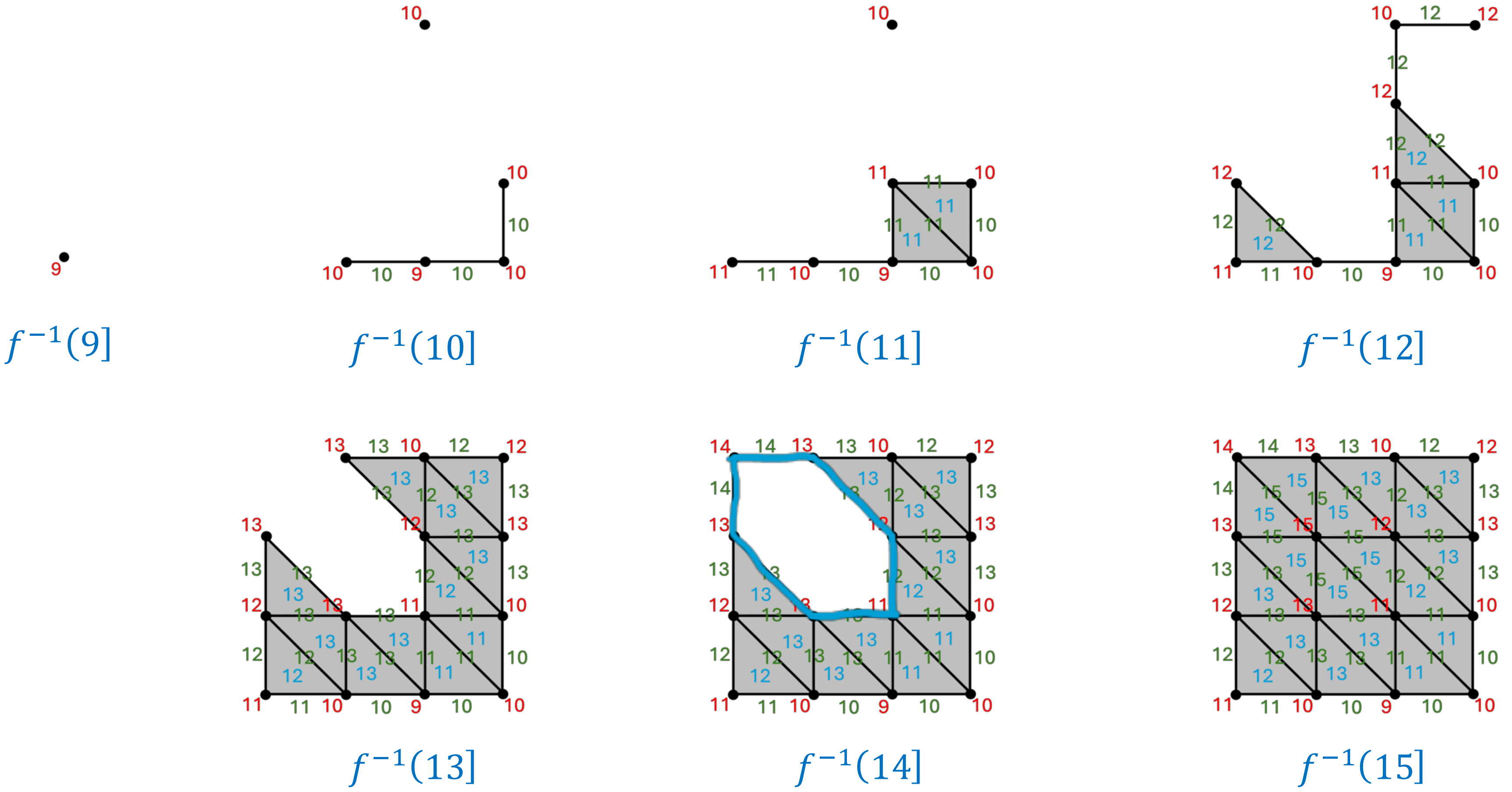
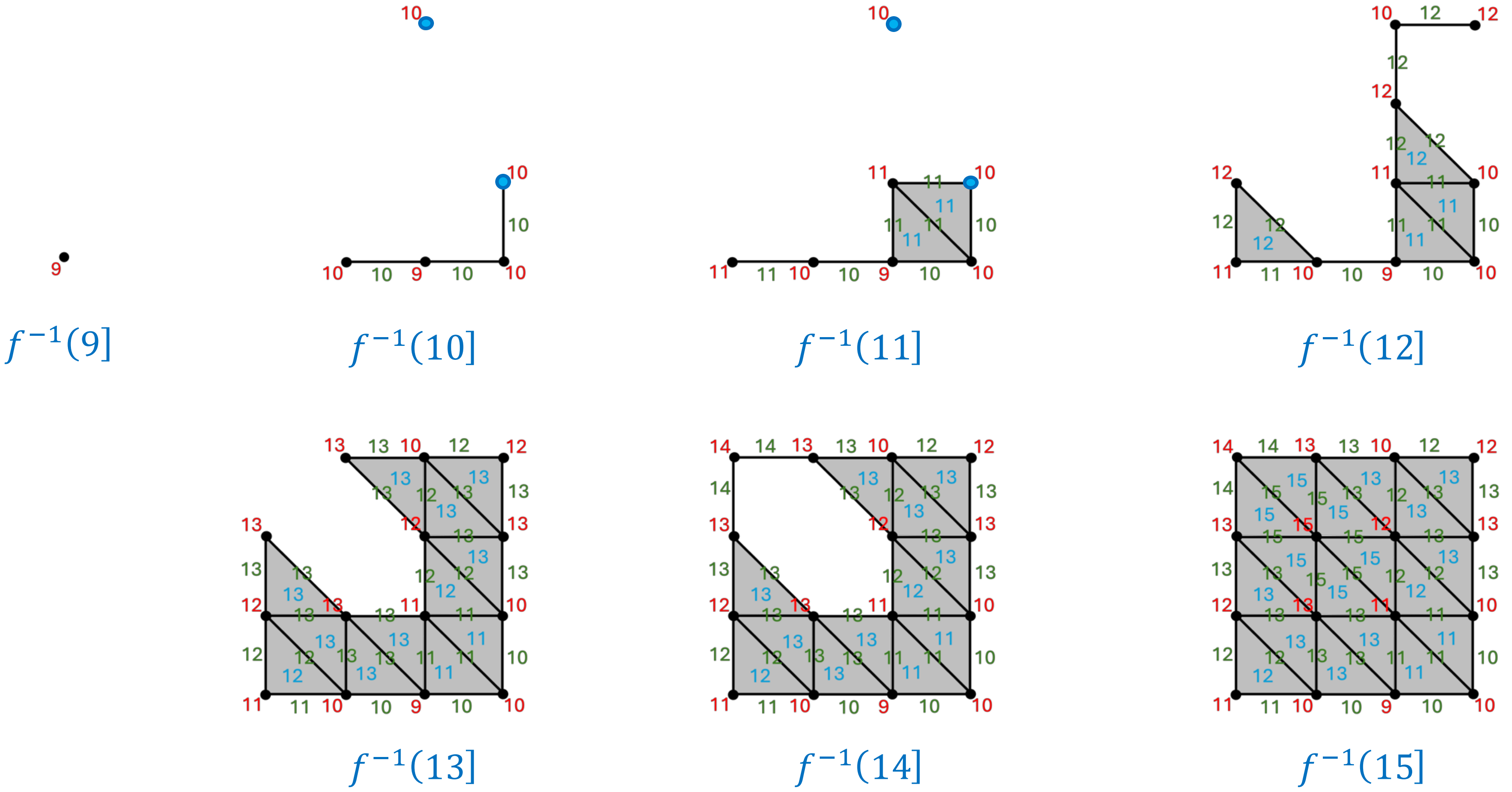
- There is a 1-dimensional bar $[14,15)$ in the PD



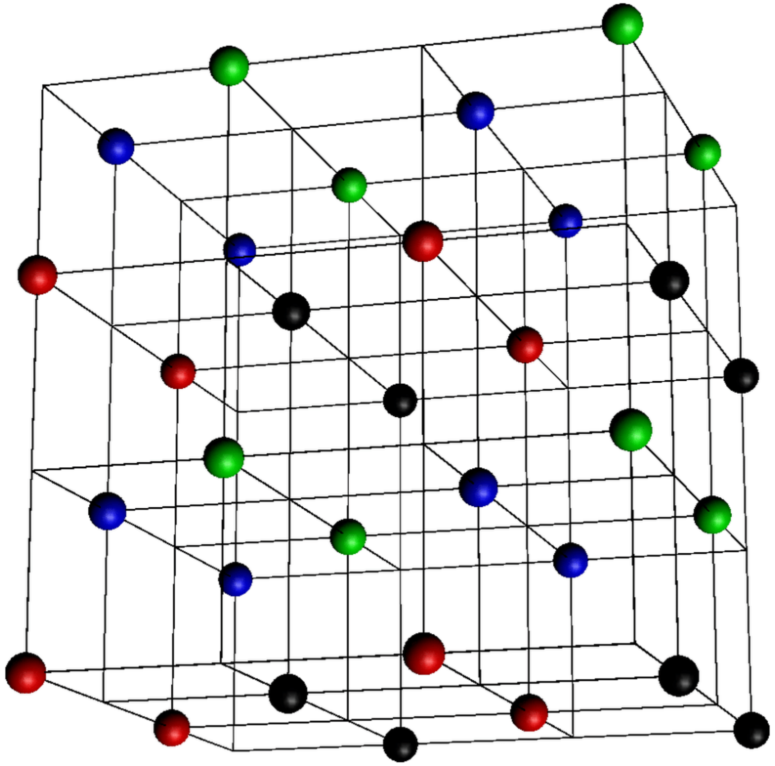
PD for the sublevelset filtration

- There is a 0-dimensional bar [10,12) in the PD



3D image

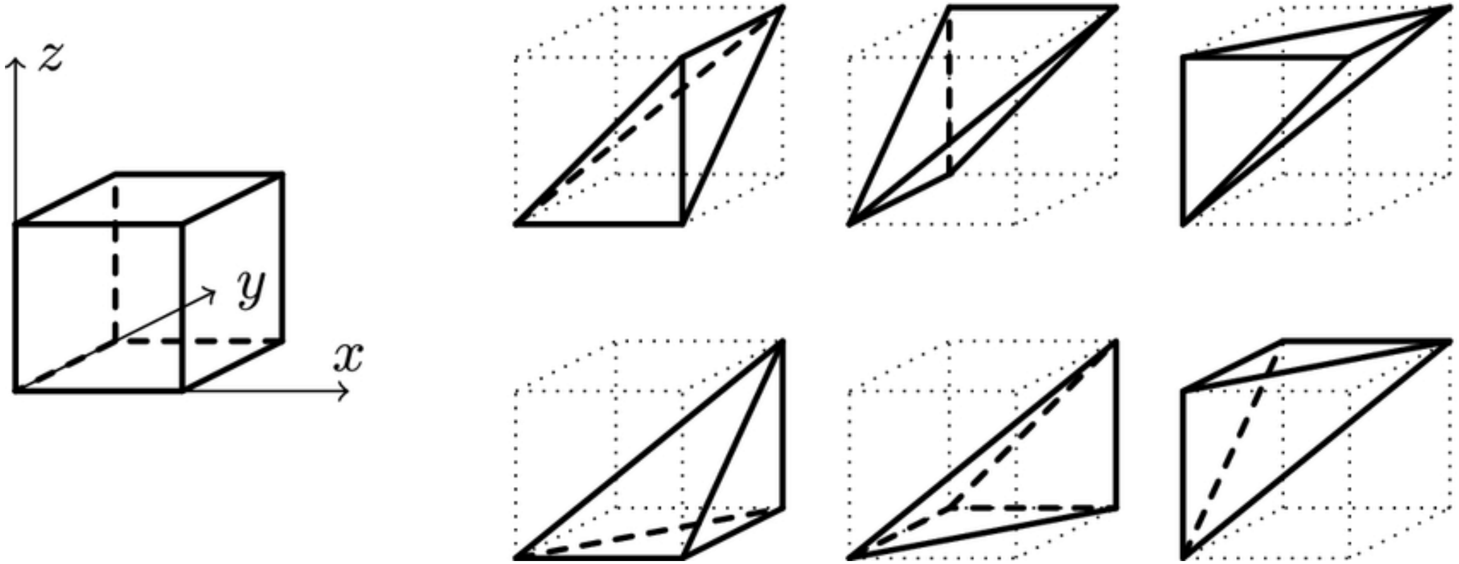
- We view the domain X for a 3D image as a 3D grid, and we have a function value on each grid point



Img source: Hamilton&Webb. Room Acoustics Modelling Using GPU-Accelerated Finite Difference and Finite Volume Methods on a Face-Centered Cubic Grid

3D image

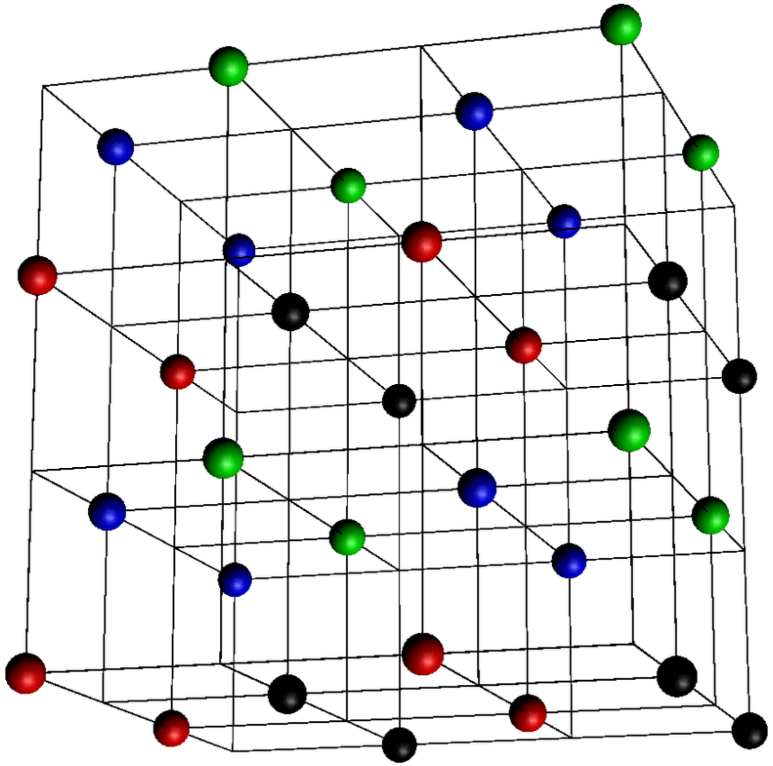
- We also need to subdivide the cube into (six) tetrahedra to make the domain a simplicial complex



de Crouy-Chanel, Simon. Random Knots in 3-Dimensional 3-Colour Percolation: Numerical Results and Conjectures

3D image

- And then we only need to assign value to each edge, triangle, tetrahedron based on the maximum values of their vertices
- The sublevelset filtration can then be defined similarly



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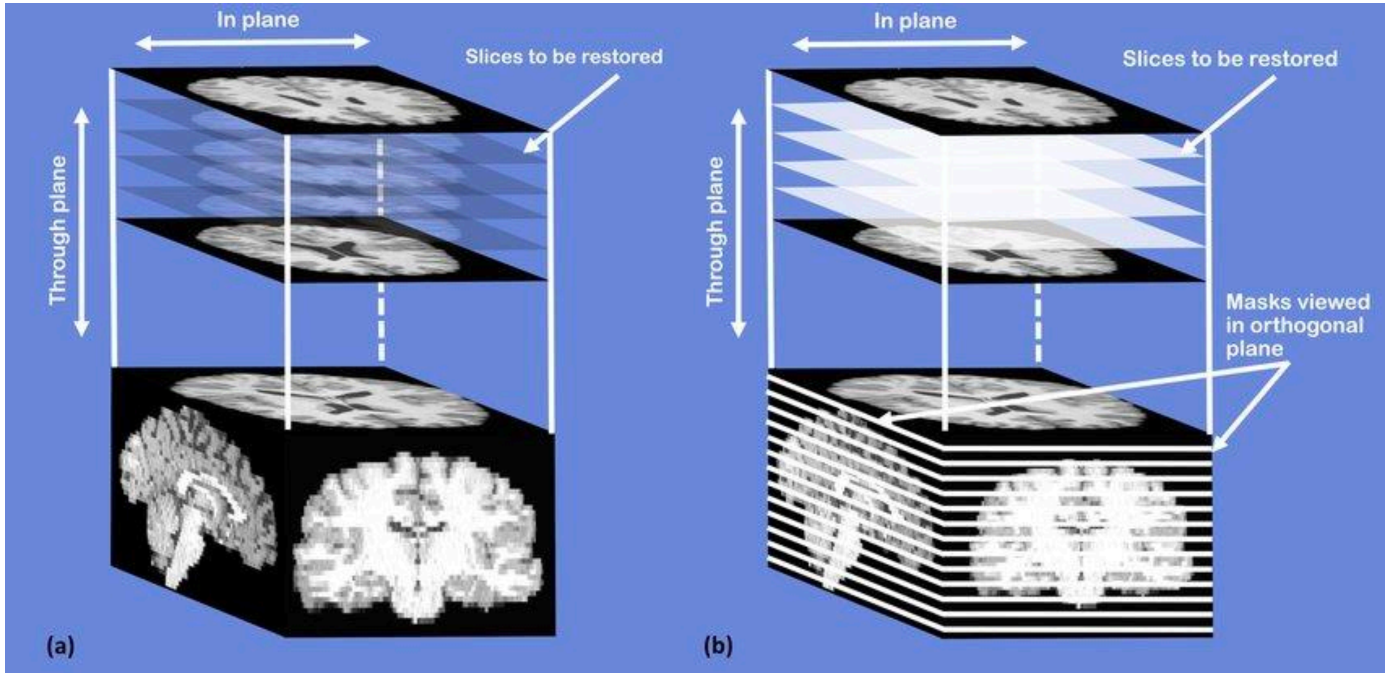
More about 3D images

- 3D images can be considered as a stacking of several 2D images, and are commonly used in medical imaging (e.g., CT-scans, MRI)



Img source:. Chai et al. MRI Restoration Using Edge-Guided Adversarial Learning

More about 3D images

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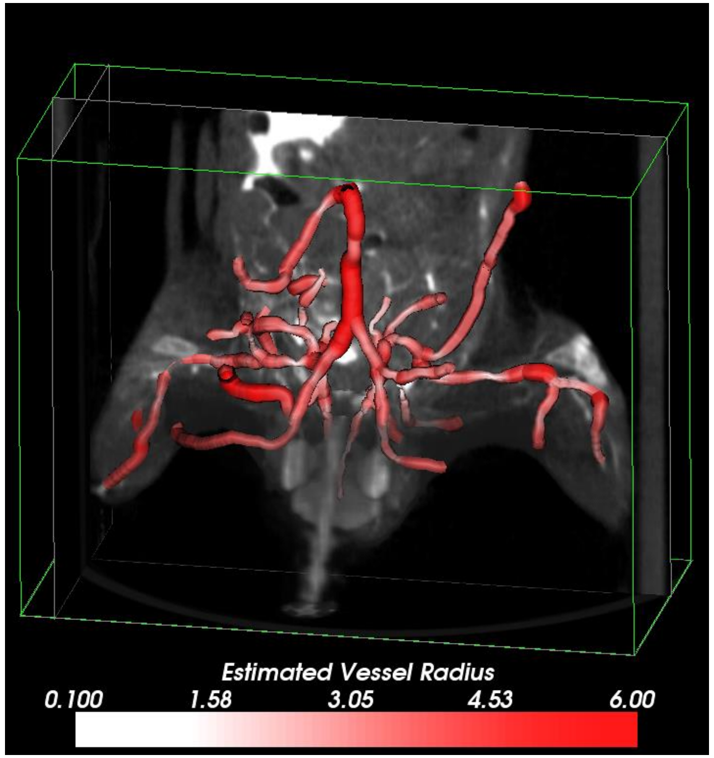
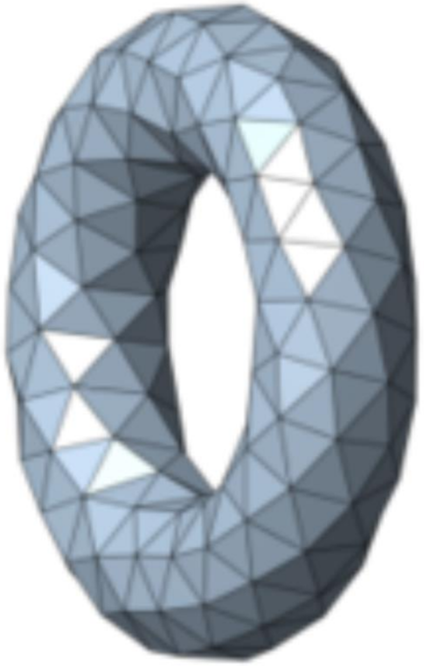
- Analyzing medical images is a hot and important in image processing



Img source: Jackowski, Papademetris, Dobrucki, Staib. Characterizing Vascular Connectivity from microCT Images

Triangular meshes

- Naturally, we could also define sublevelset filtrations on triangular meshes by assigning function values to the vertices (edges / triangles are then induced)



Img source: Lockerby. Integration over discrete closed surfaces using the Method of Fundamental Solutions

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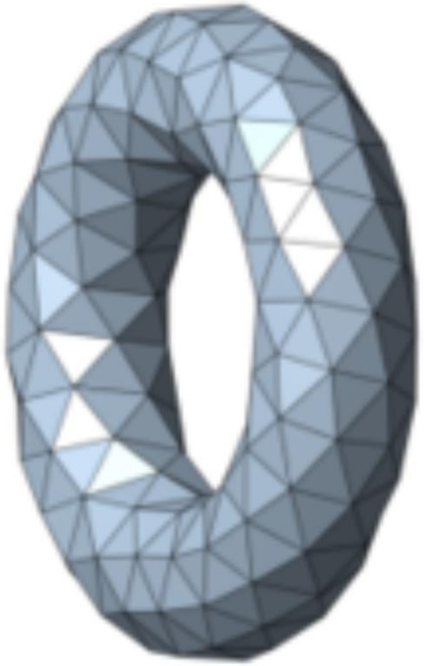
- There is a natural way to assign values to the vertices which is to use the "height function"



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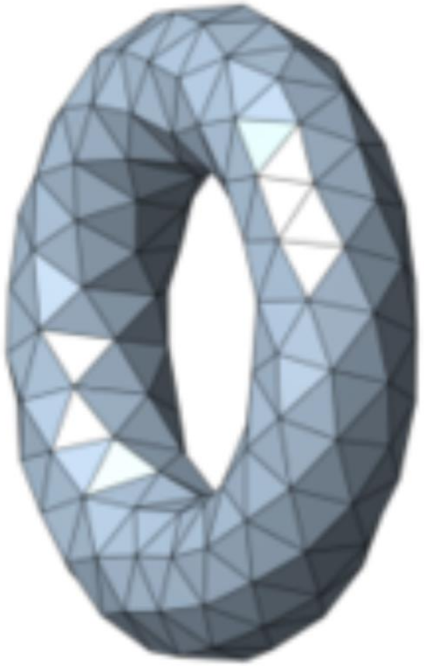
Triangular meshes

- For each vertex, we project the vertex to a certain direction and get its height value



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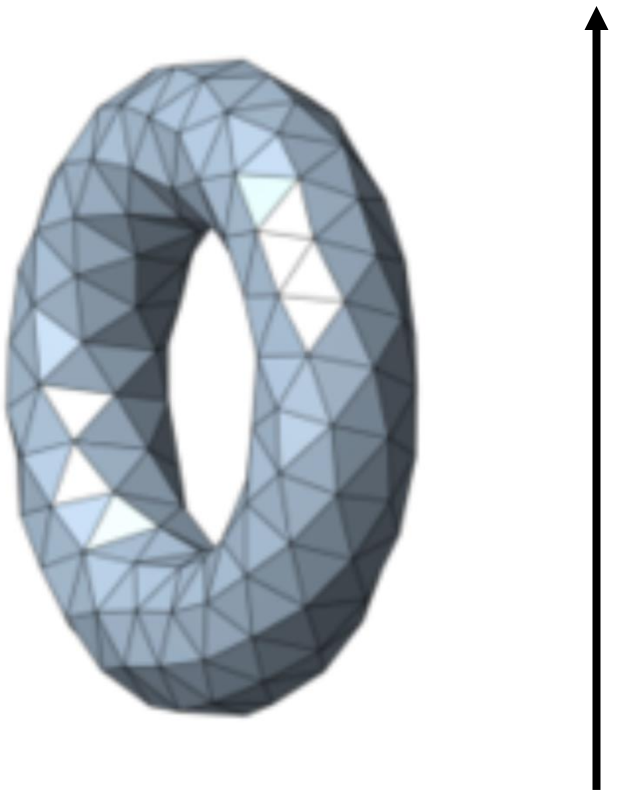

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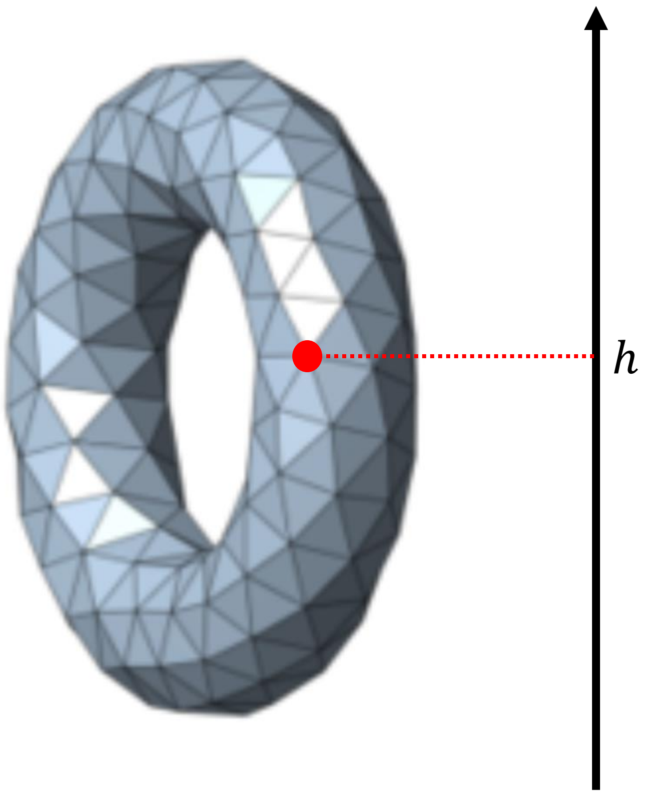
Triangular meshes

- For each vertex, we project the vertex to a certain direction and get its height value



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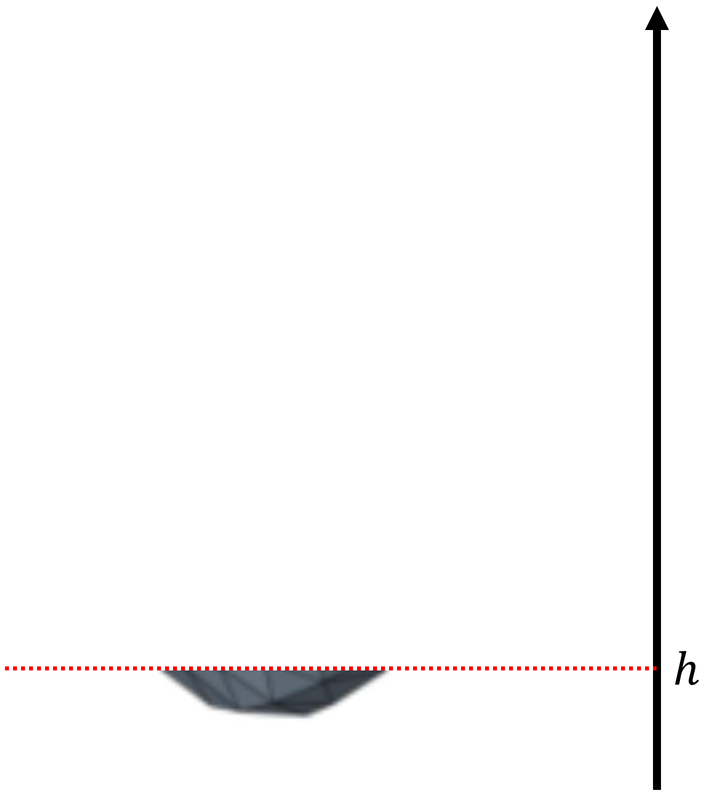

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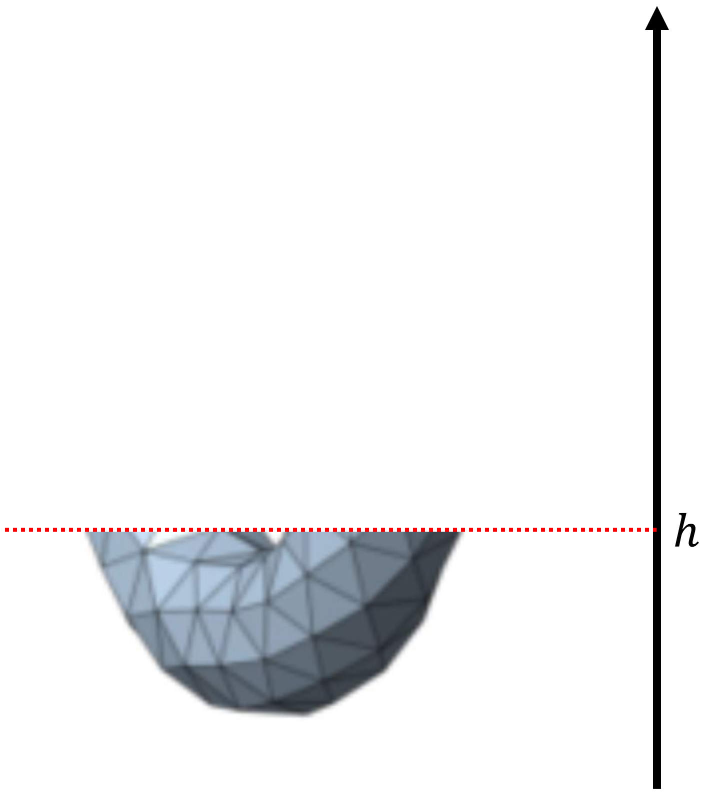

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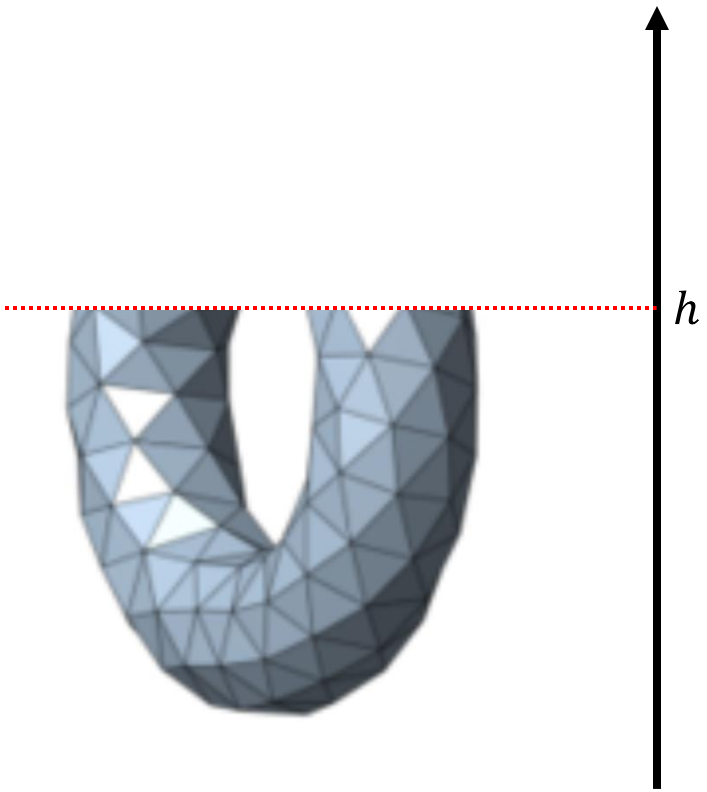

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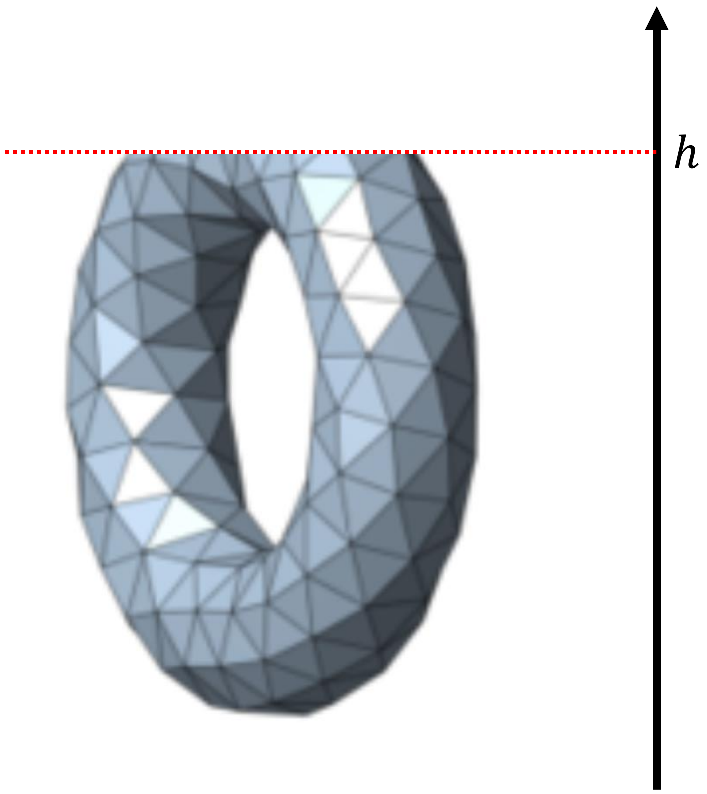

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More sublevelset filtrations

- Indeed we have also seen sublevelset filtrations in previous slides
- An interactive example: https://iuricichf.github.io/ICT/filtration.html

Superlevelset filtration

- There is a counterpart of sublevelset filtration called **super**levelset filtration
- A superlevelset of is the subset of X whose function values are **greater than or equal to** a value α, and we denote it as $f^{-1}[\alpha, \infty)$
- We then take all possible functions values and **descreasingly** sort them (i.e, start with the height value):

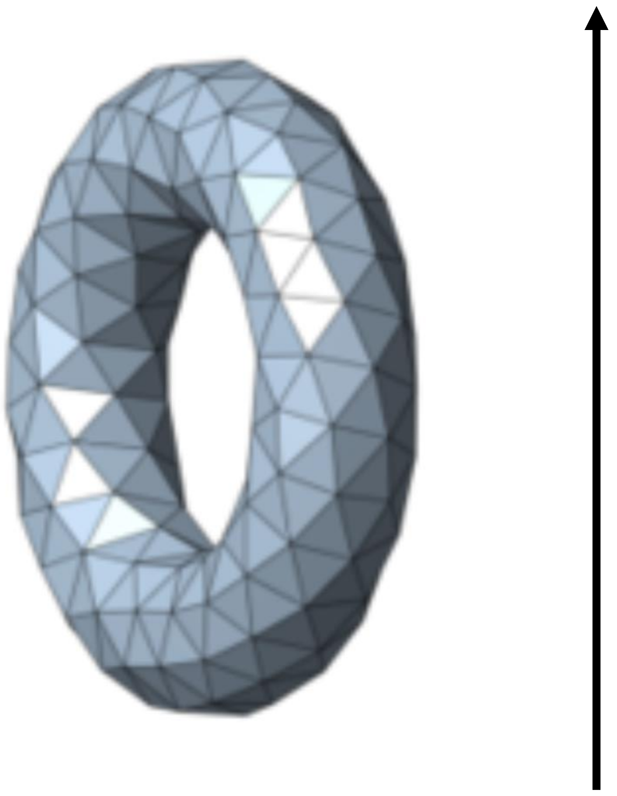
$$\alpha_0 > \alpha_1 > \cdots > \alpha_m$$

- The superlevelset filtration is then the superlevelsets over the above values:

$$f^{-1}[\alpha_0, \infty) \subseteq f^{-1}[\alpha_1, \infty) \subseteq \cdots \subseteq f^{-1}[\alpha_m, \infty)$$

Superlevelset filtration

- The superlevelset filtration for the previous height function on torus would be:



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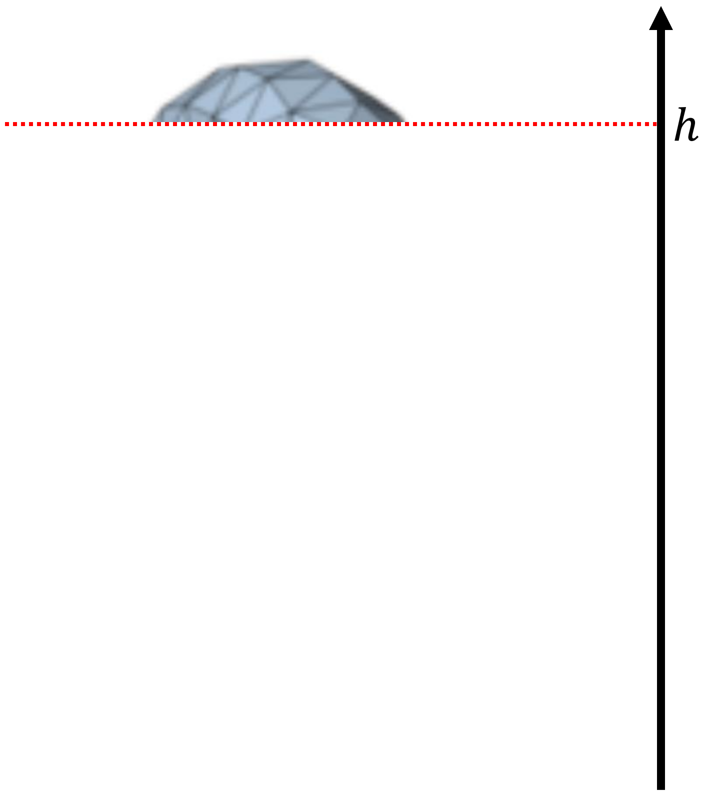

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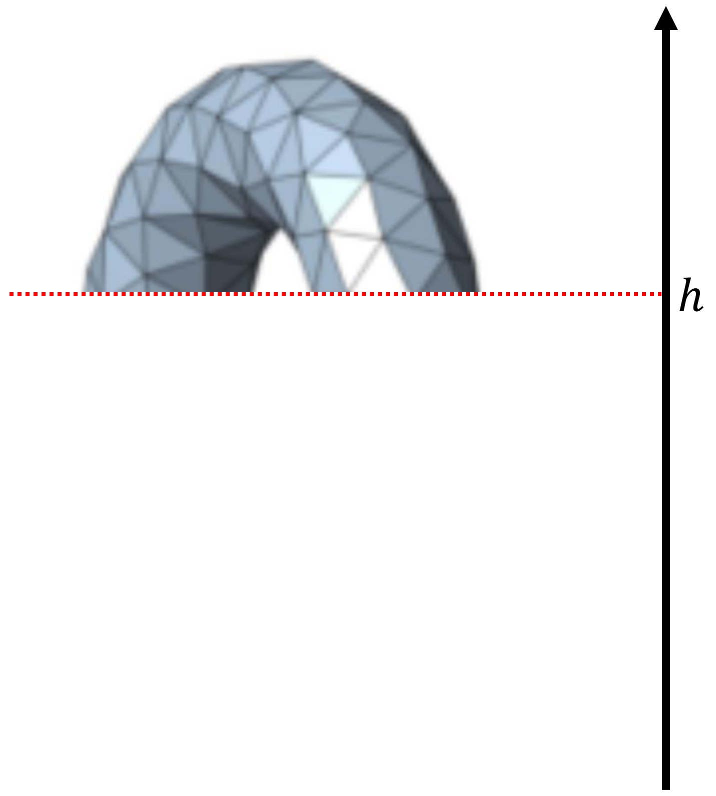

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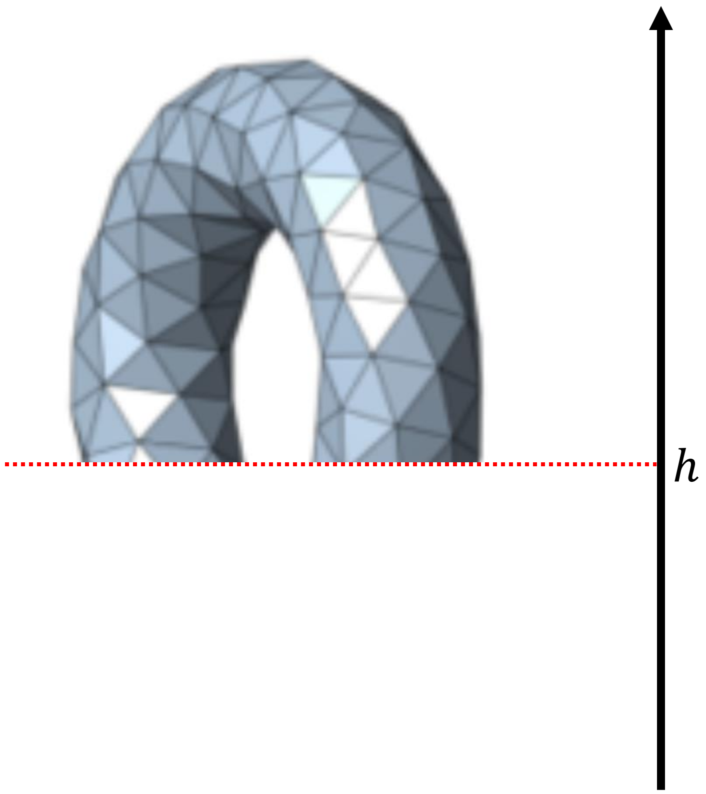

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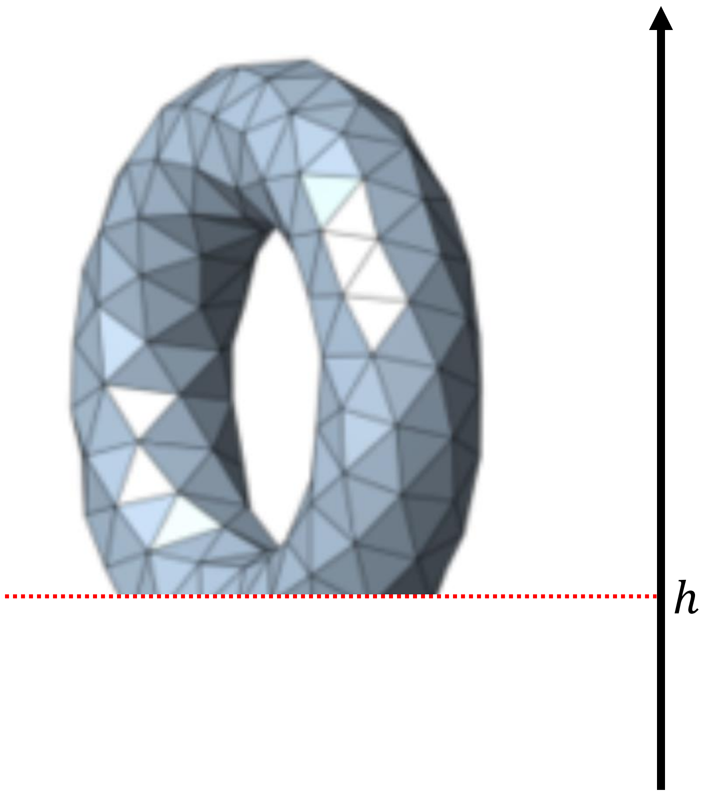

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Clarification on PD for different filtrations

- Previously when we define PD by computing it from a discrete filtration:

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

intervals in the PD are "integer intervals" (e.g., $[3, 6) = \{3, 4, 5\}$).

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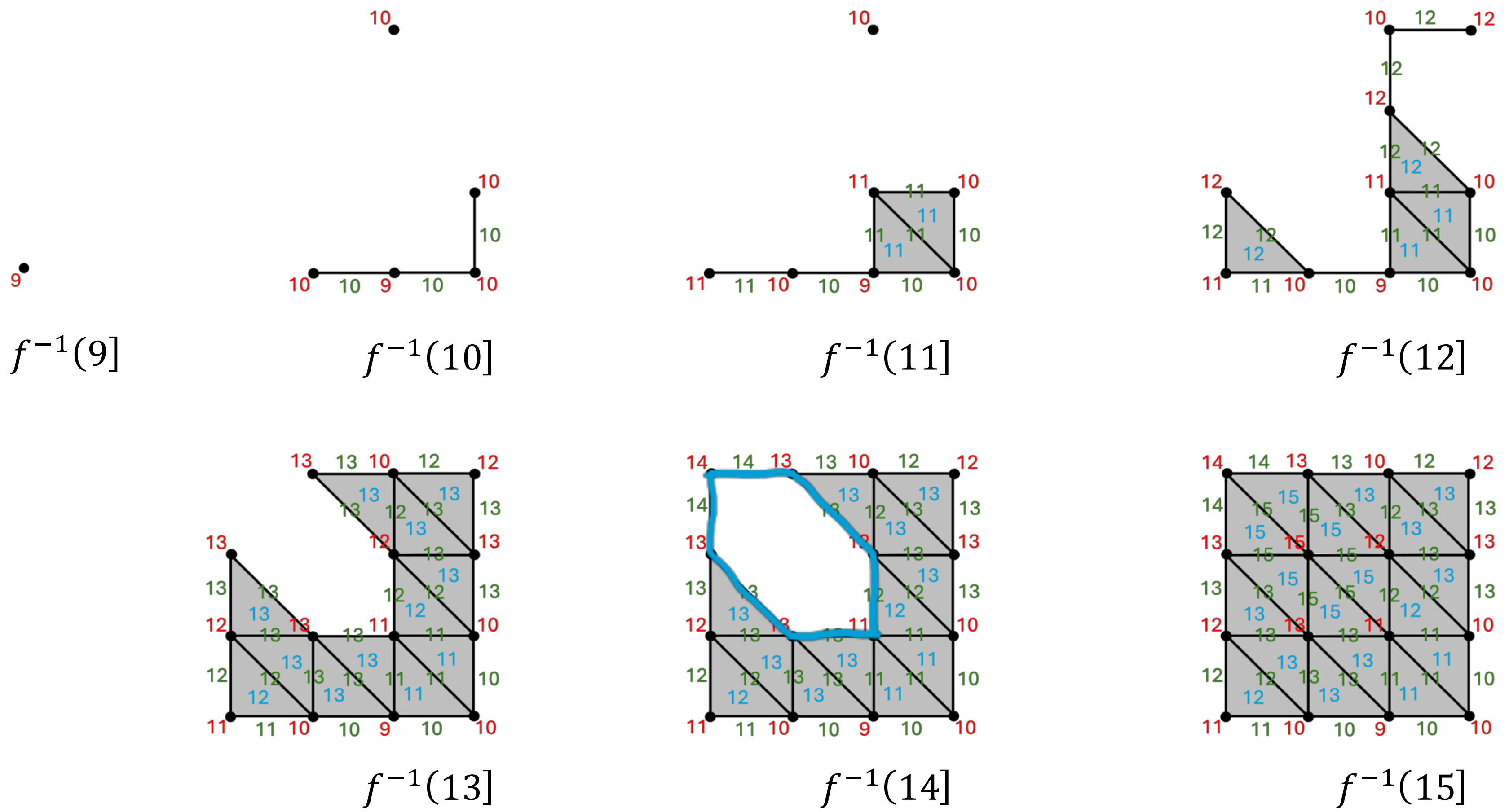
- This applies when it is not clear where the discrete filtration is built from
- In practice, filtrations are built from different types of data. Each complex in the discrete filtration is associate with a real value (or a bunch of them)
- Intervals in the PD for such a filtration (when we know source data) is then continuous intervals of real values (e.g., $[3.52, 6.37)$)

Clarification on PD for different filtrations

- For the previous sublevelset filtration for image, we can also number each complex in the filtration from 0 to 6



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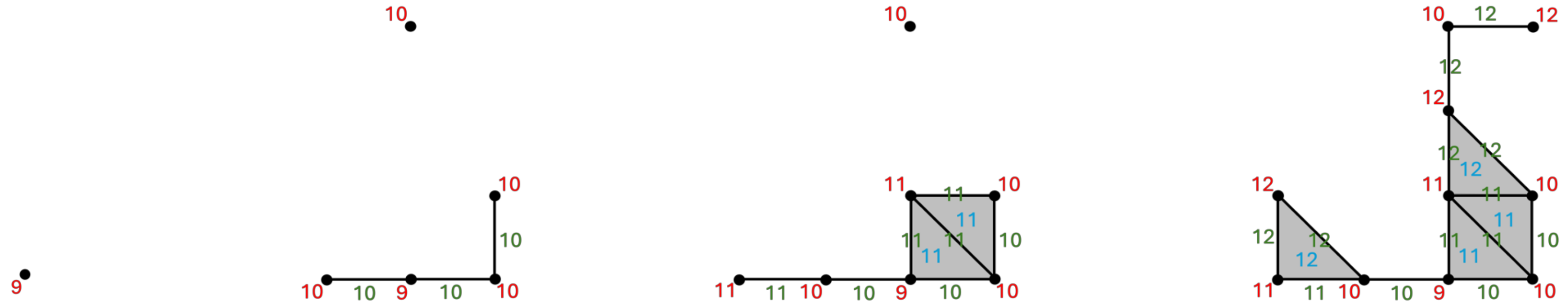
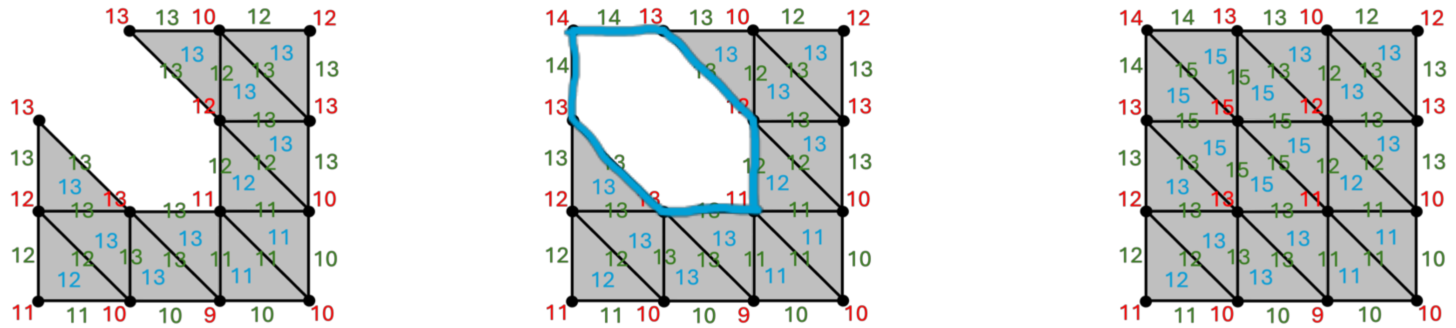


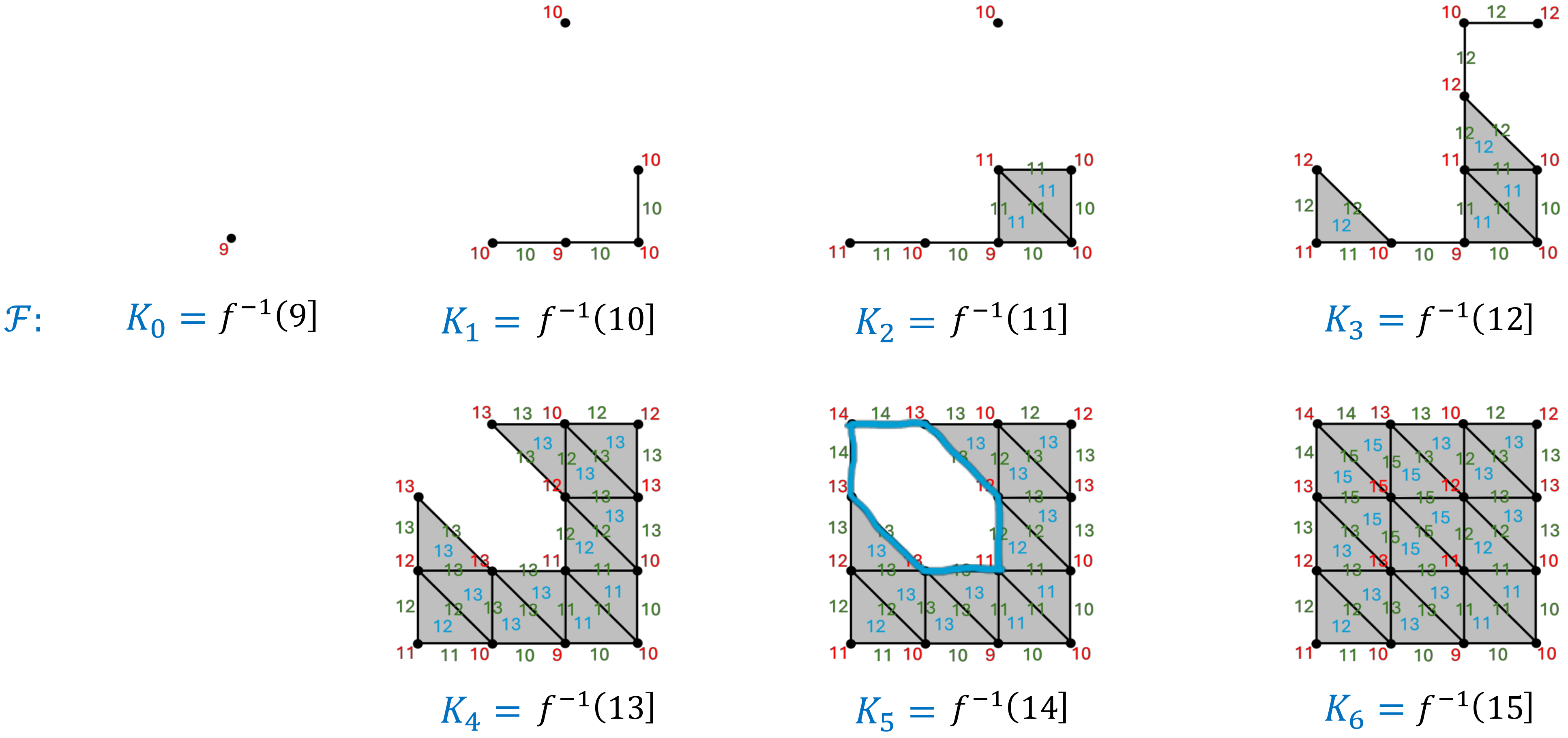
$\mathcal{F}$: $K_0 = f^{-1}(9]$ $K_1 = f^{-1}(10]$ $K_2 = f^{-1}(11]$ $K_3 = f^{-1}(12]$



$K_4 = f^{-1}(13]$ $K_5 = f^{-1}(14]$ $K_6 = f^{-1}(15]$

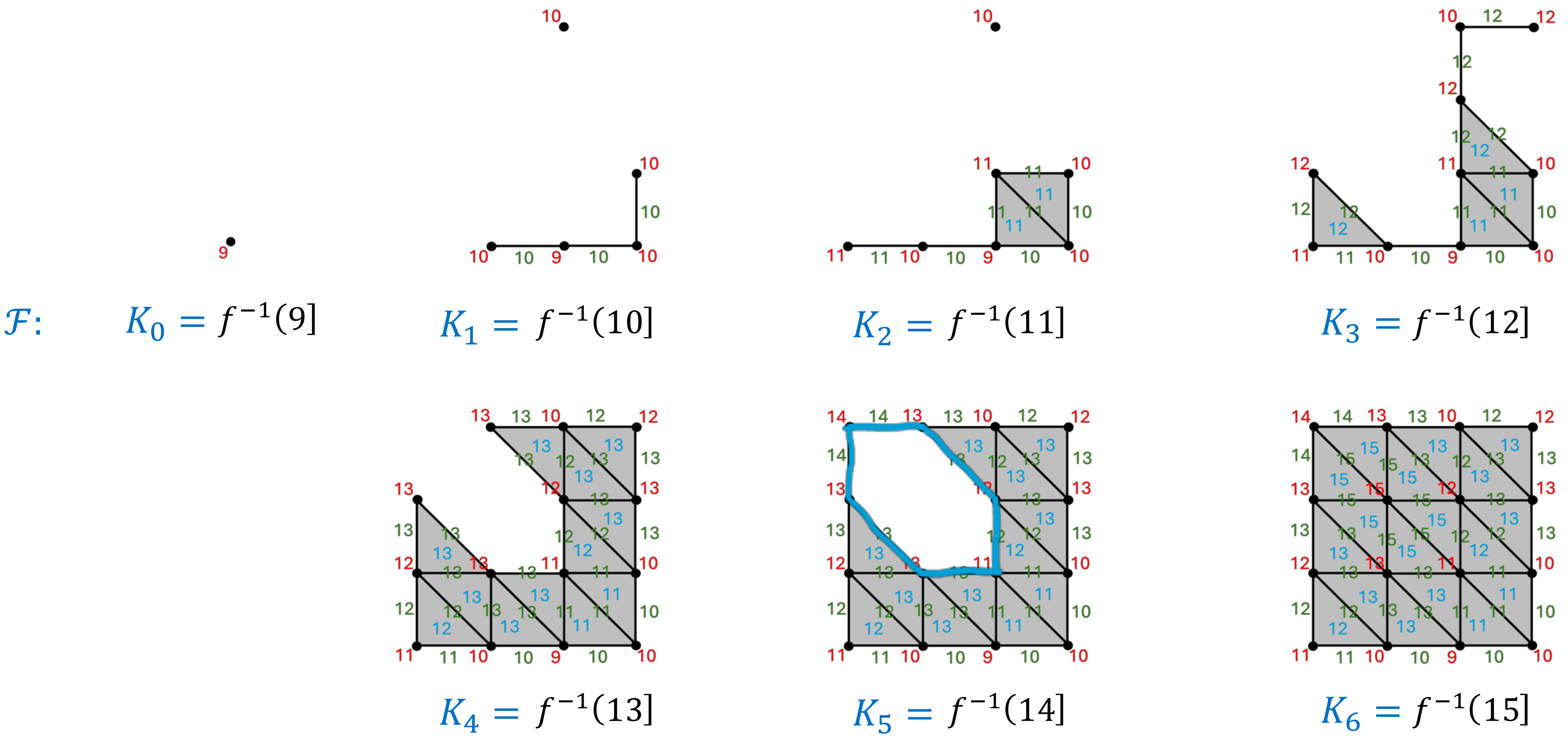
Clarification on PD for different filtrations

- For the previous sublevelset filtration for image, we can also number each complex in the filtration from 0 to 6
- But we use the pixel values (e.g., 9, 10, …) instead of the integer indices (e.g., 0, 1, …) for the PD



Clarification on PD for different filtrations

- E.g., the below 1d interval is $[14,15)$ rather than $[5,6)$



Clarification on PD for different filtrations

- The below 0d interval is $[10,12)$ rather than $[1,3)$