

# Geometry and Topology of Data

From point clouds through complexes to persistent homology

Ulrich Bauer

Technical University of Munich (TUM)

December 6, 2024

Forum for matematiske perler (og kuriositeter)

NTNU Trondheim

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SFB  
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Discretization  
In Geometry  
and Dynamics

Technical  
University  
of Munich



mcmL  
Munich Center for Machine Learning



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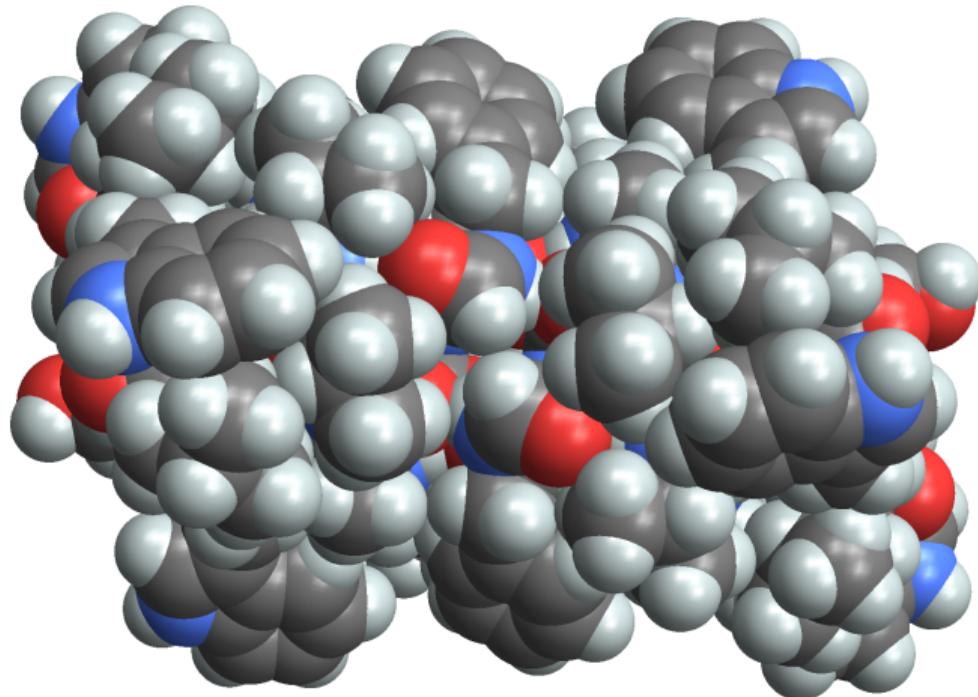


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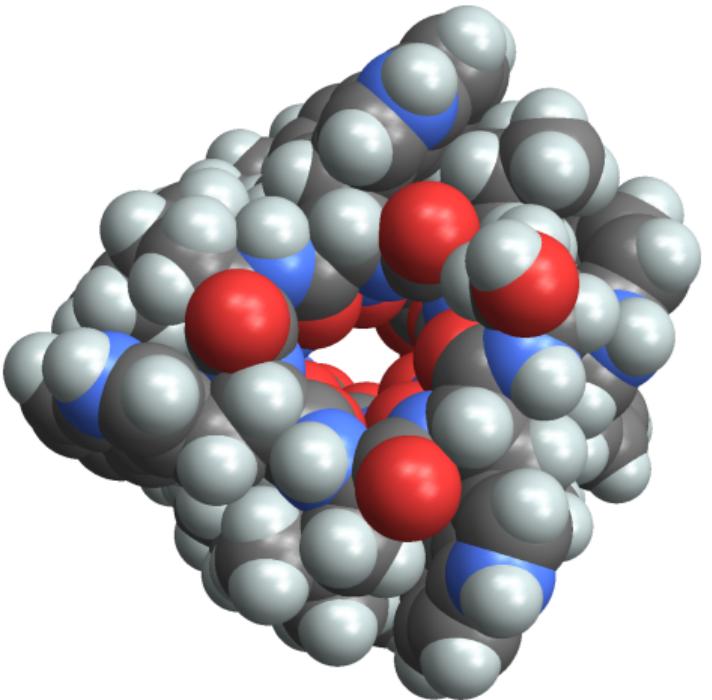
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# Biogeometry



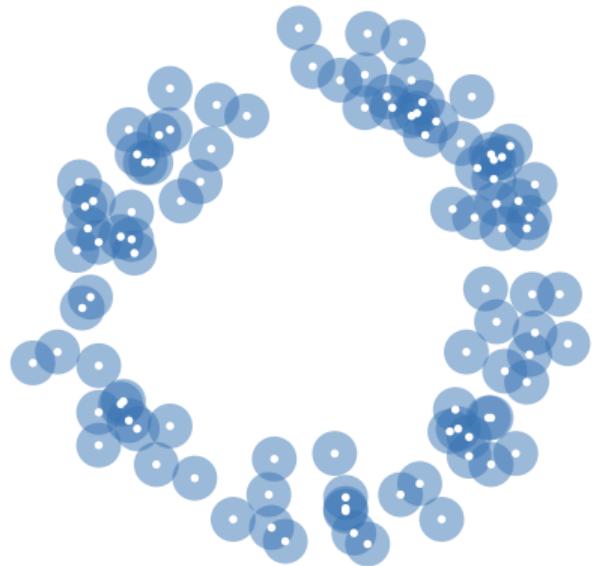
Gramicidin (an antibiotic functioning as an ion channel)

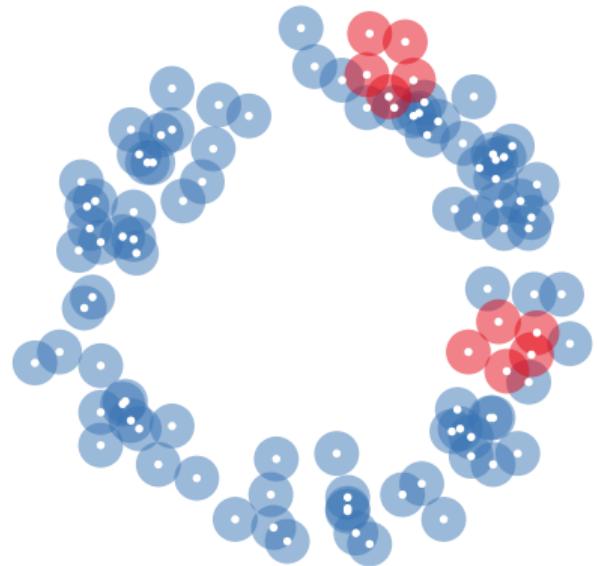
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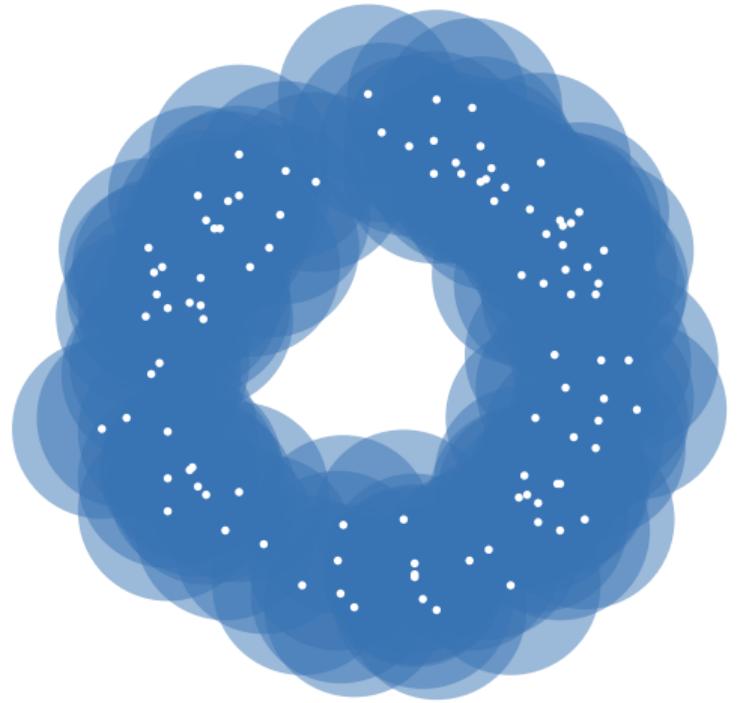
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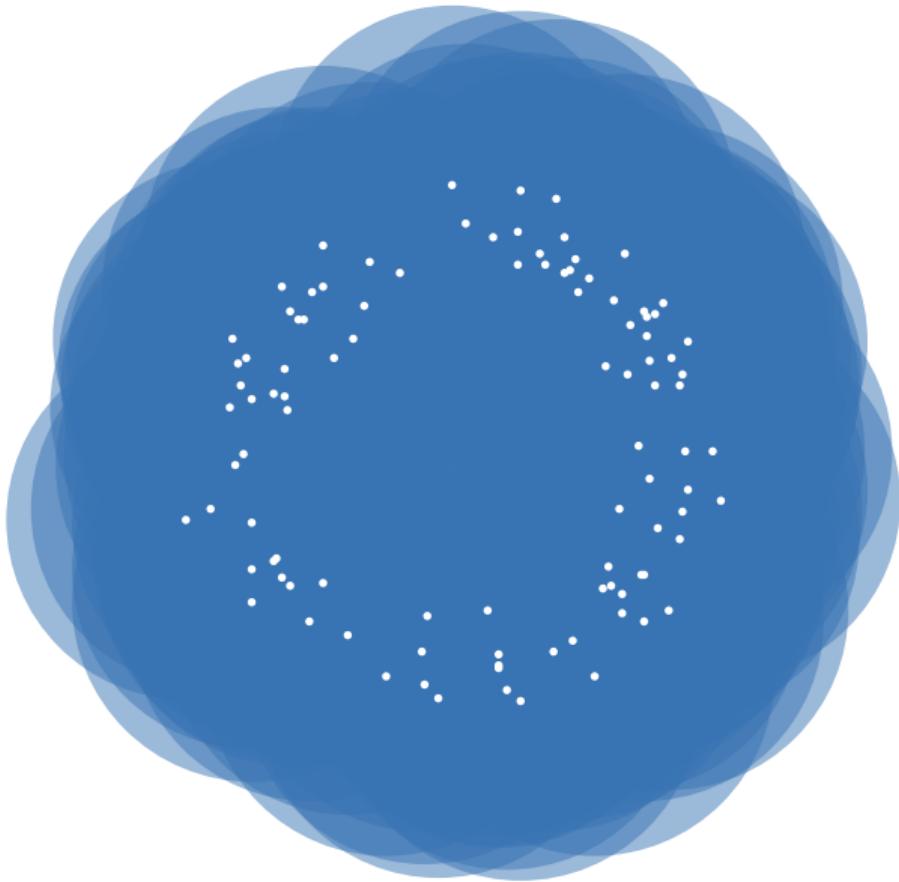


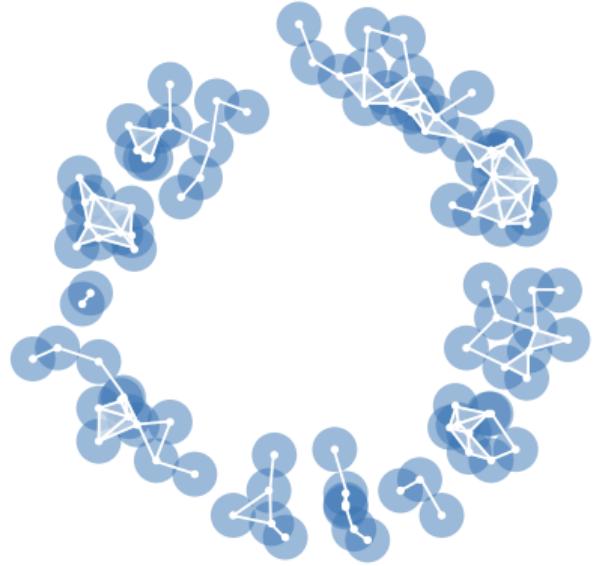


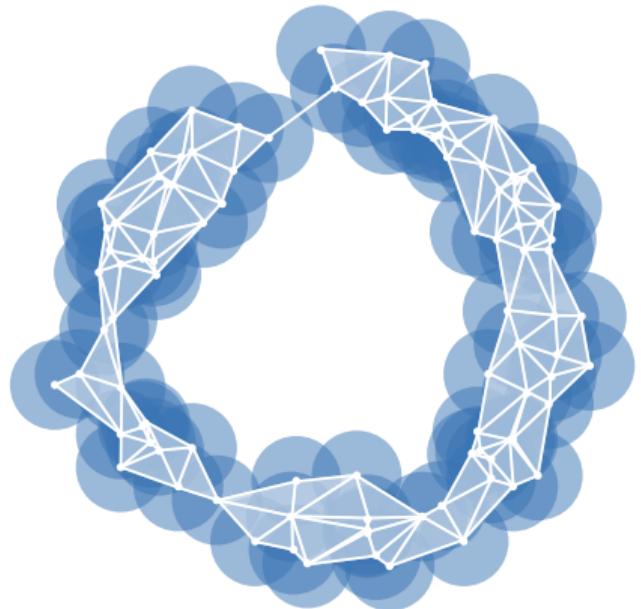


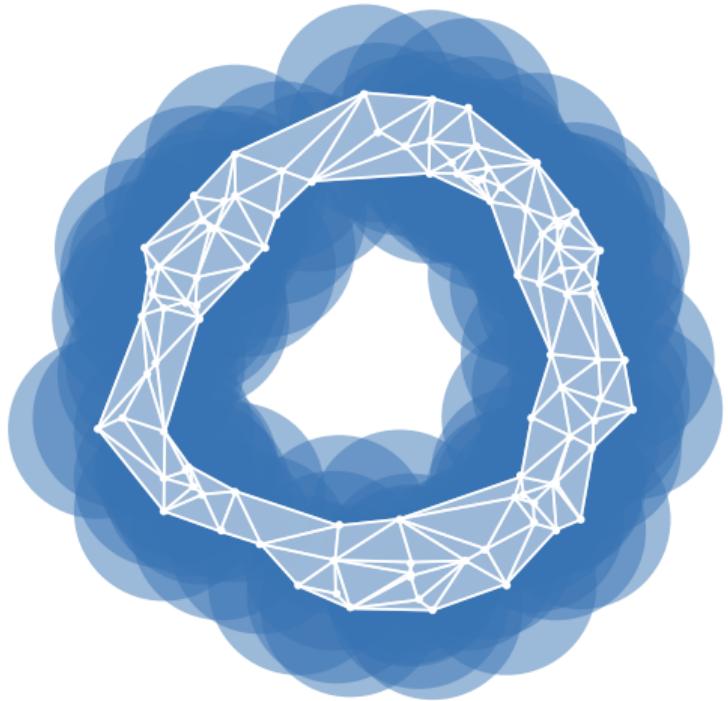


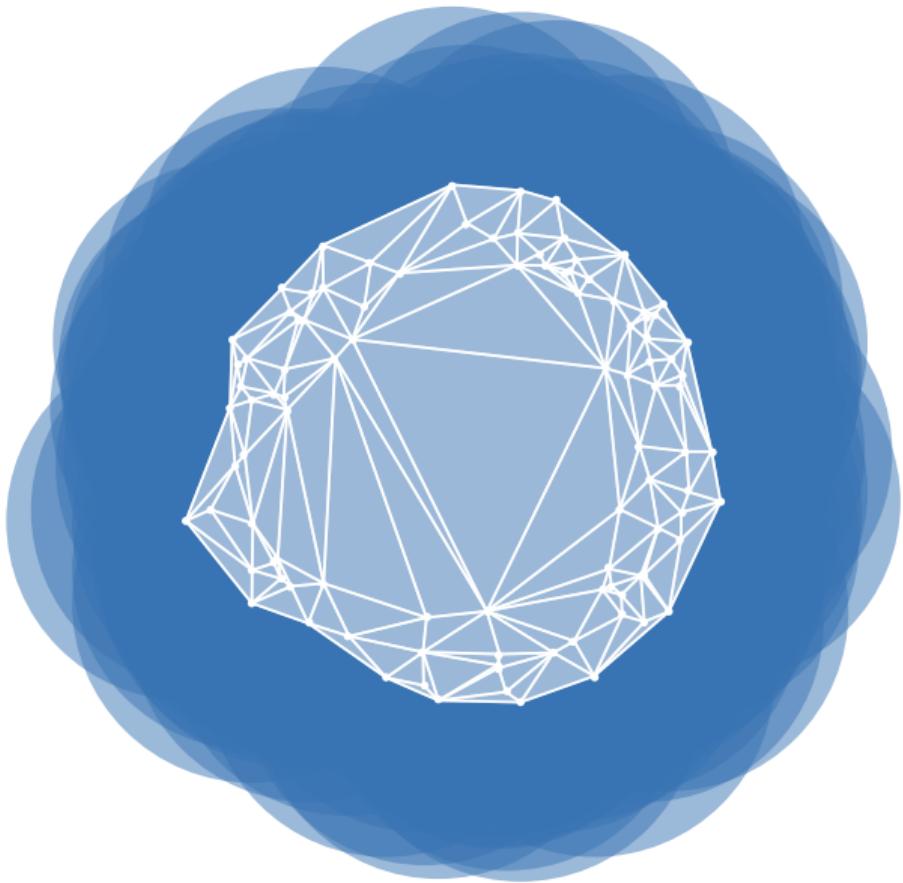






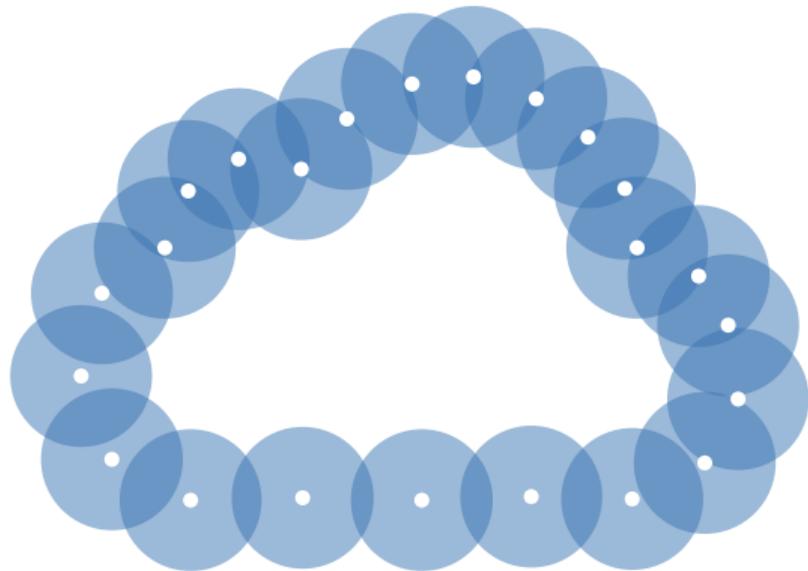




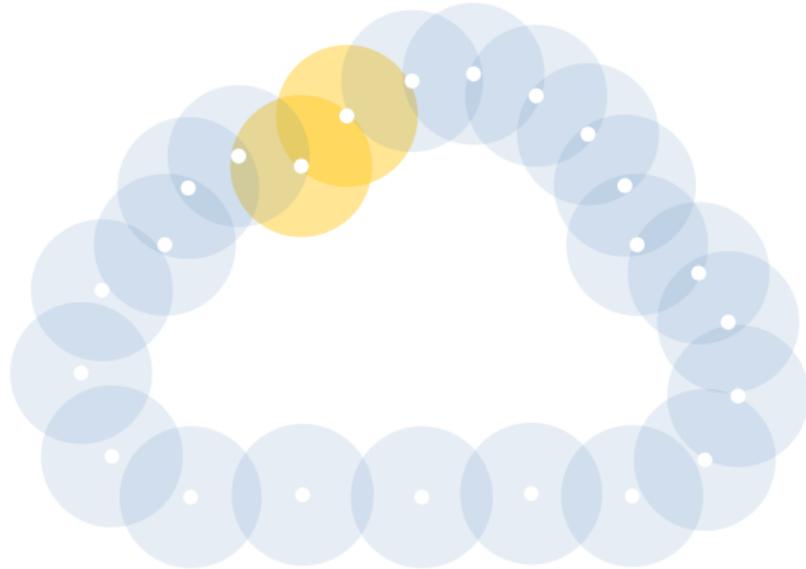


# Geometric complexes

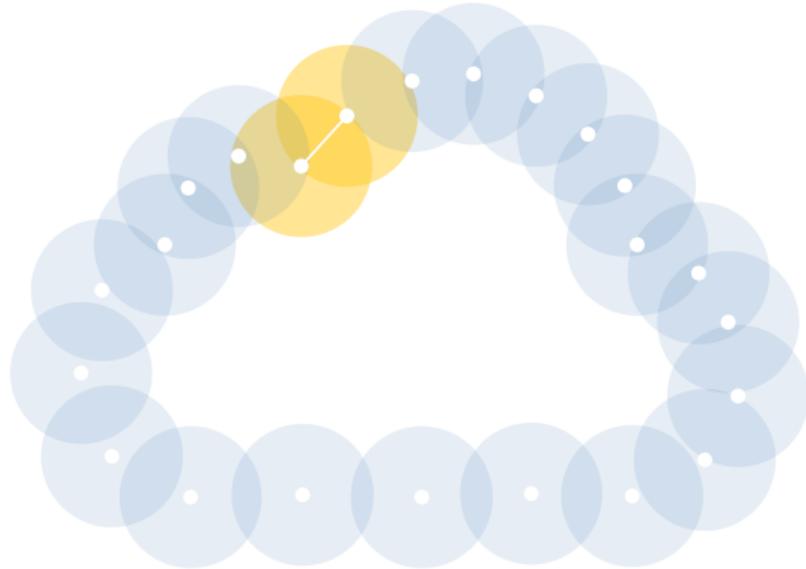
## Čech complexes



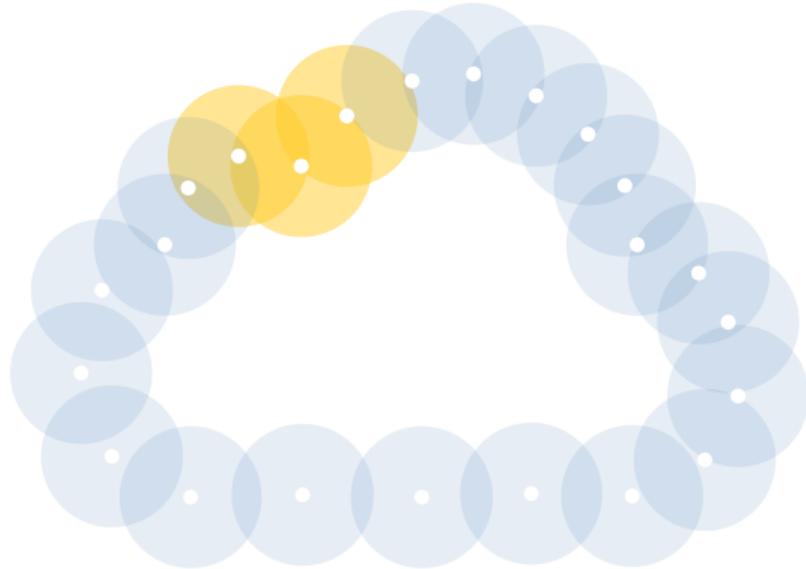
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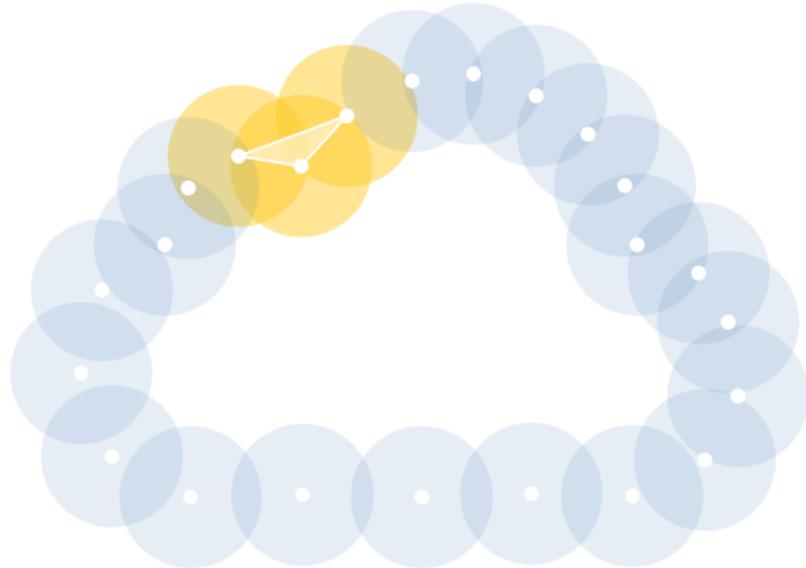
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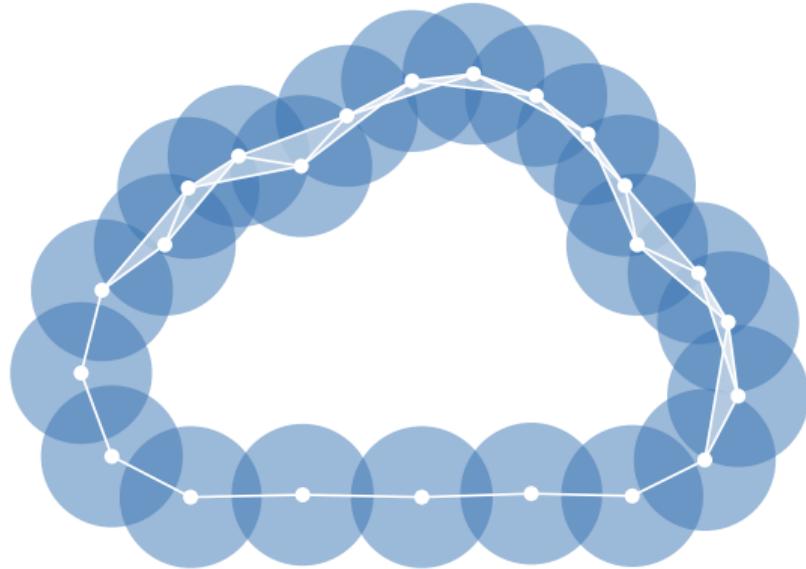
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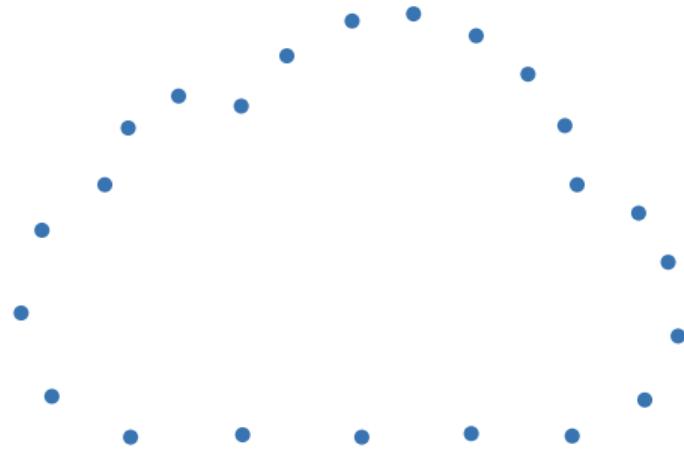
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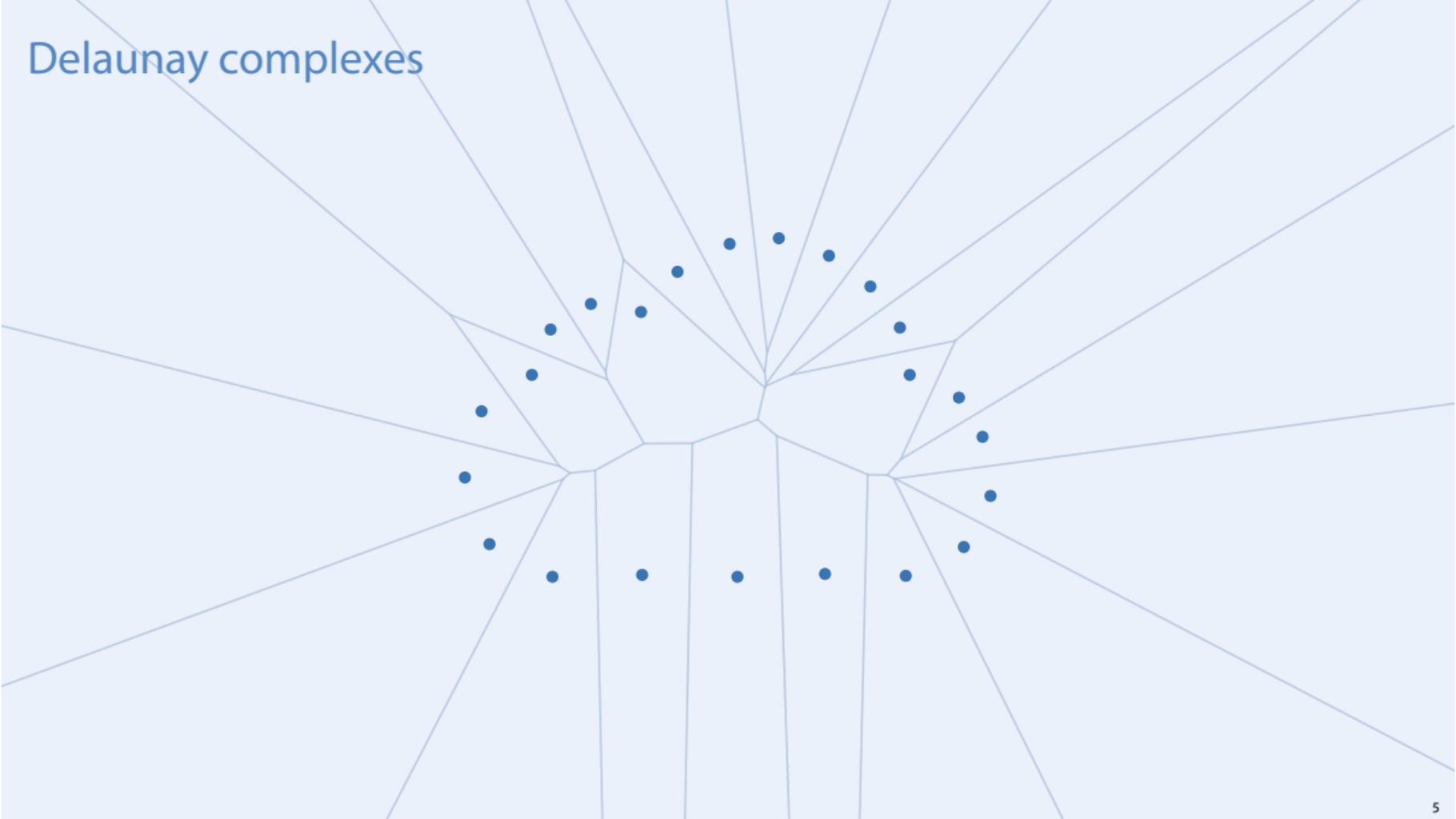
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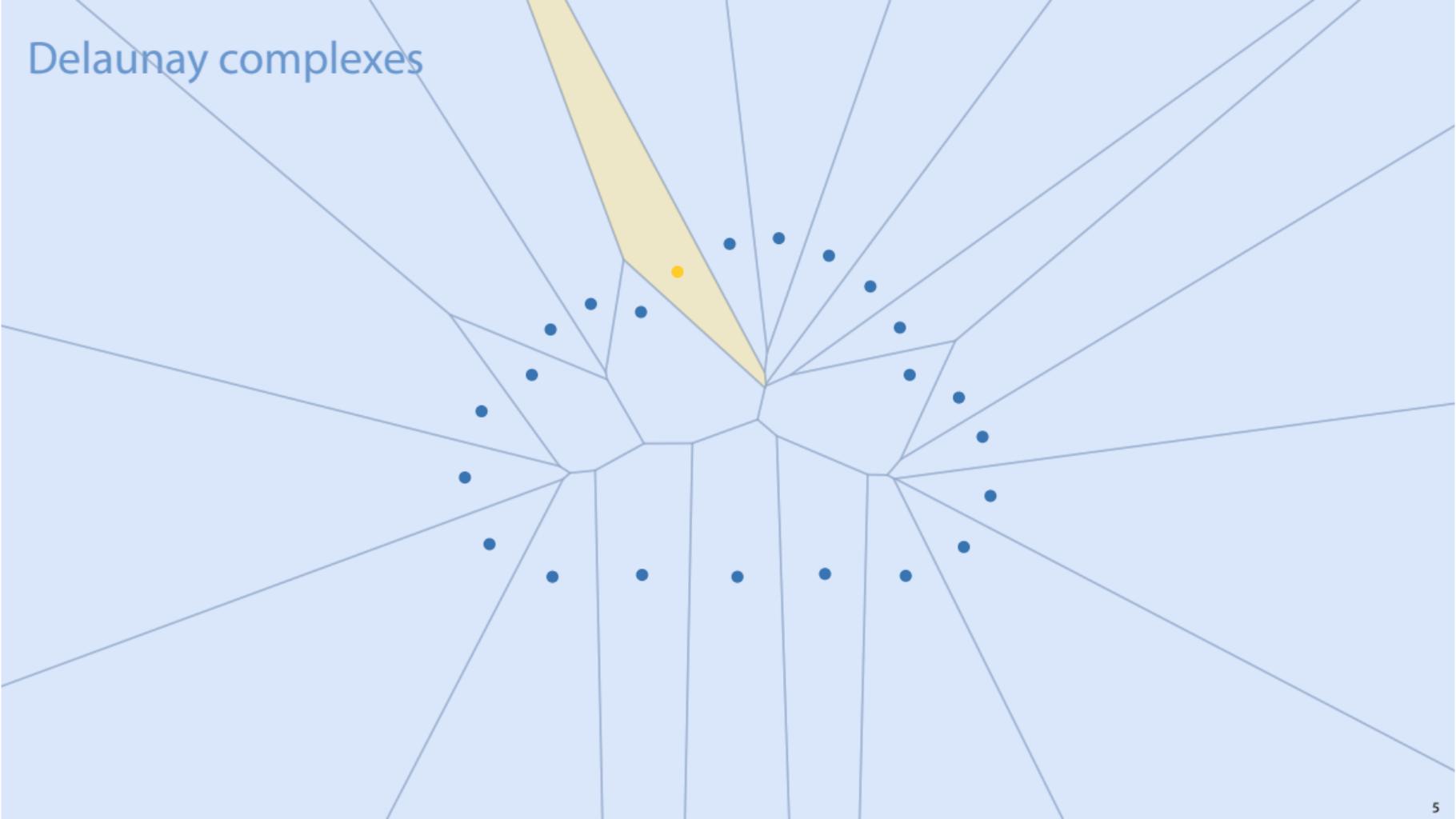
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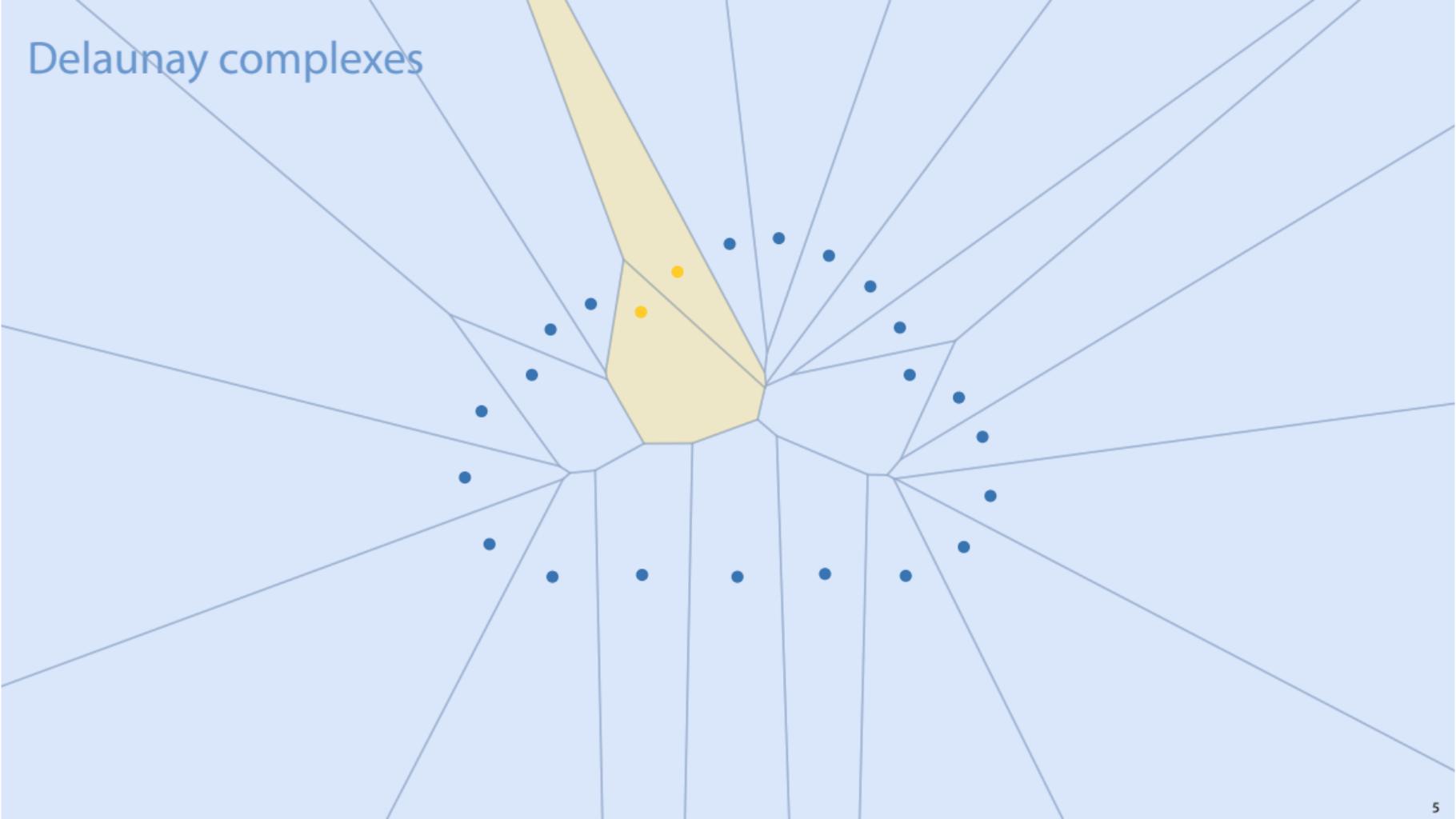
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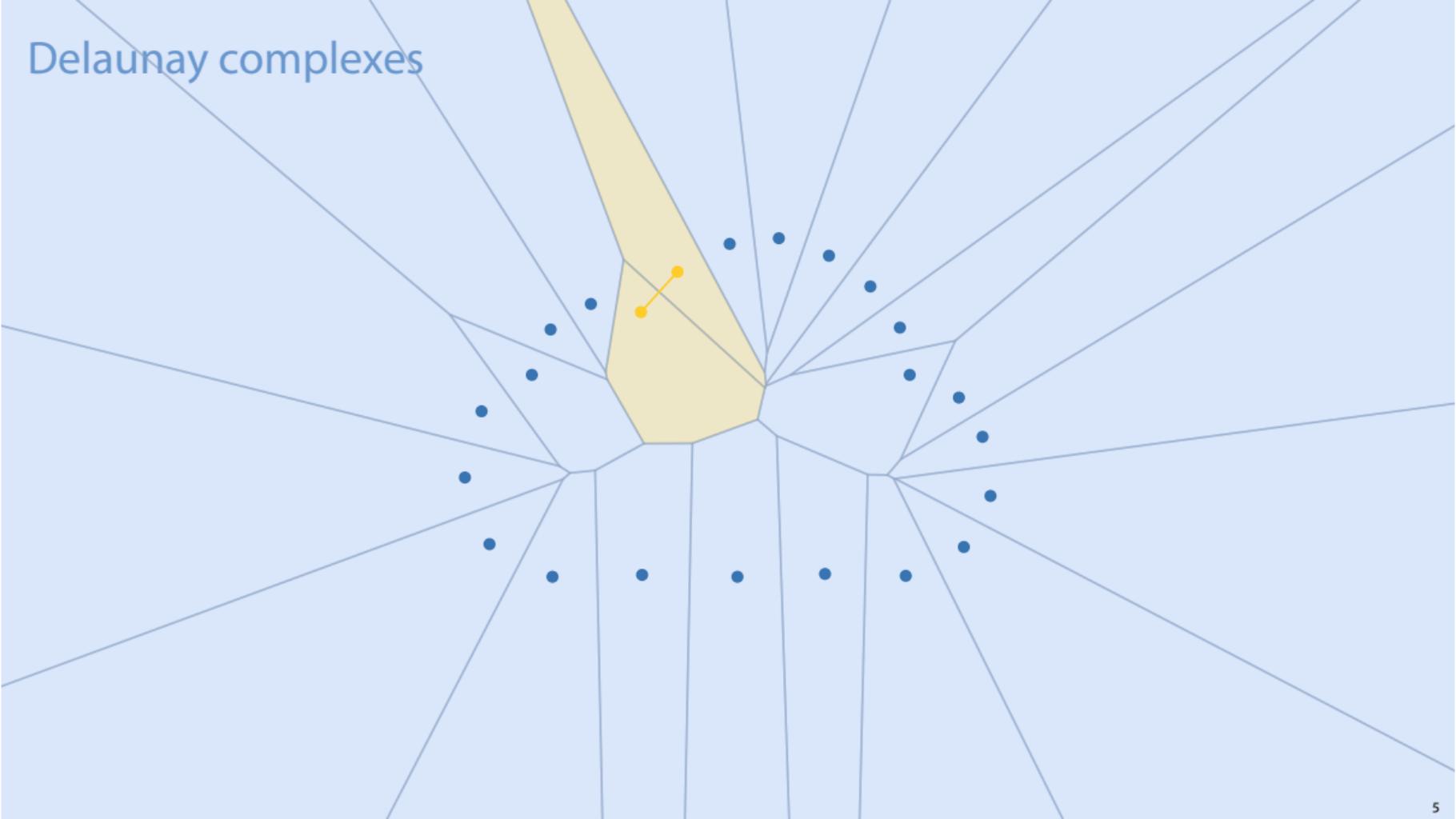
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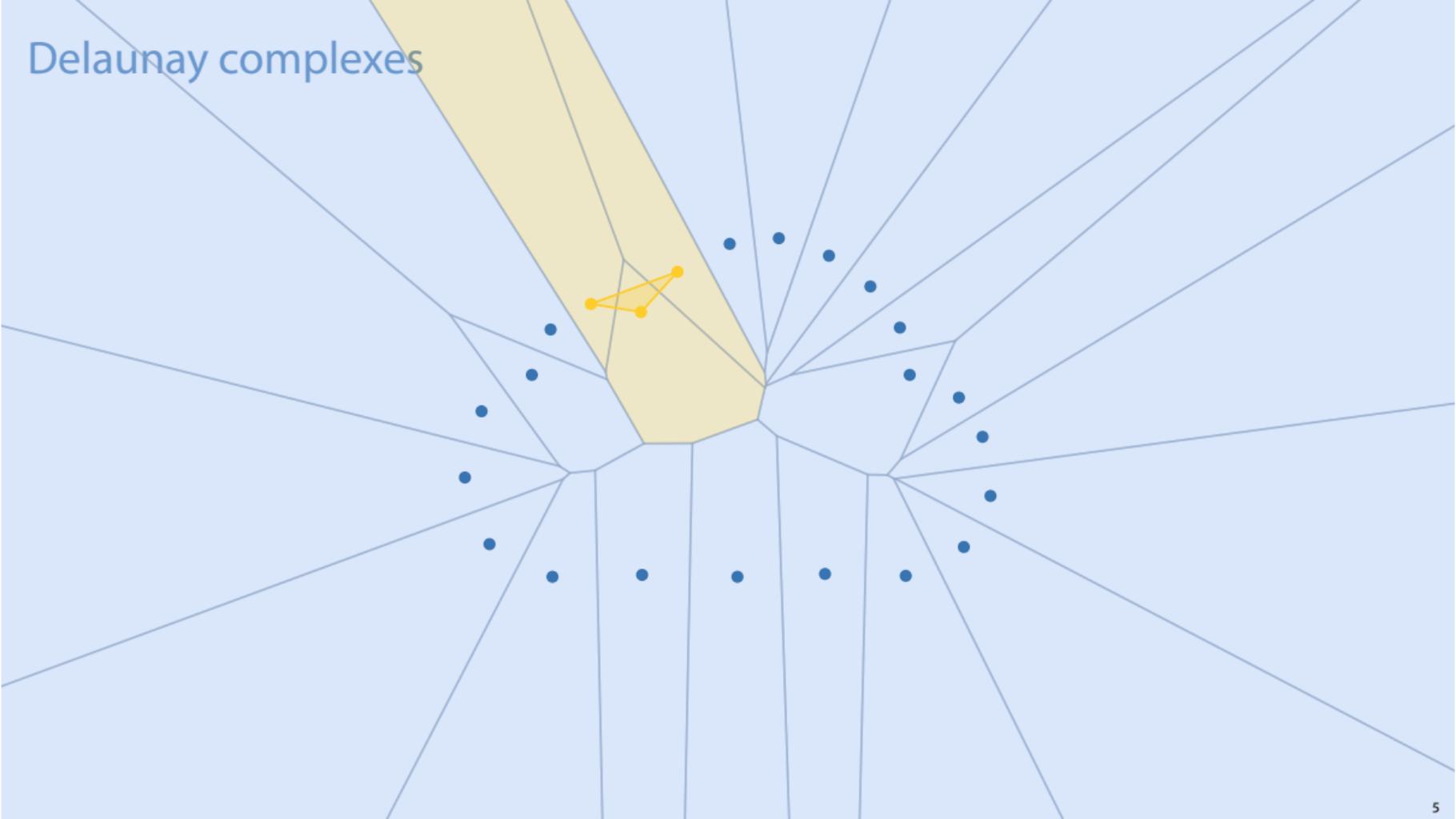
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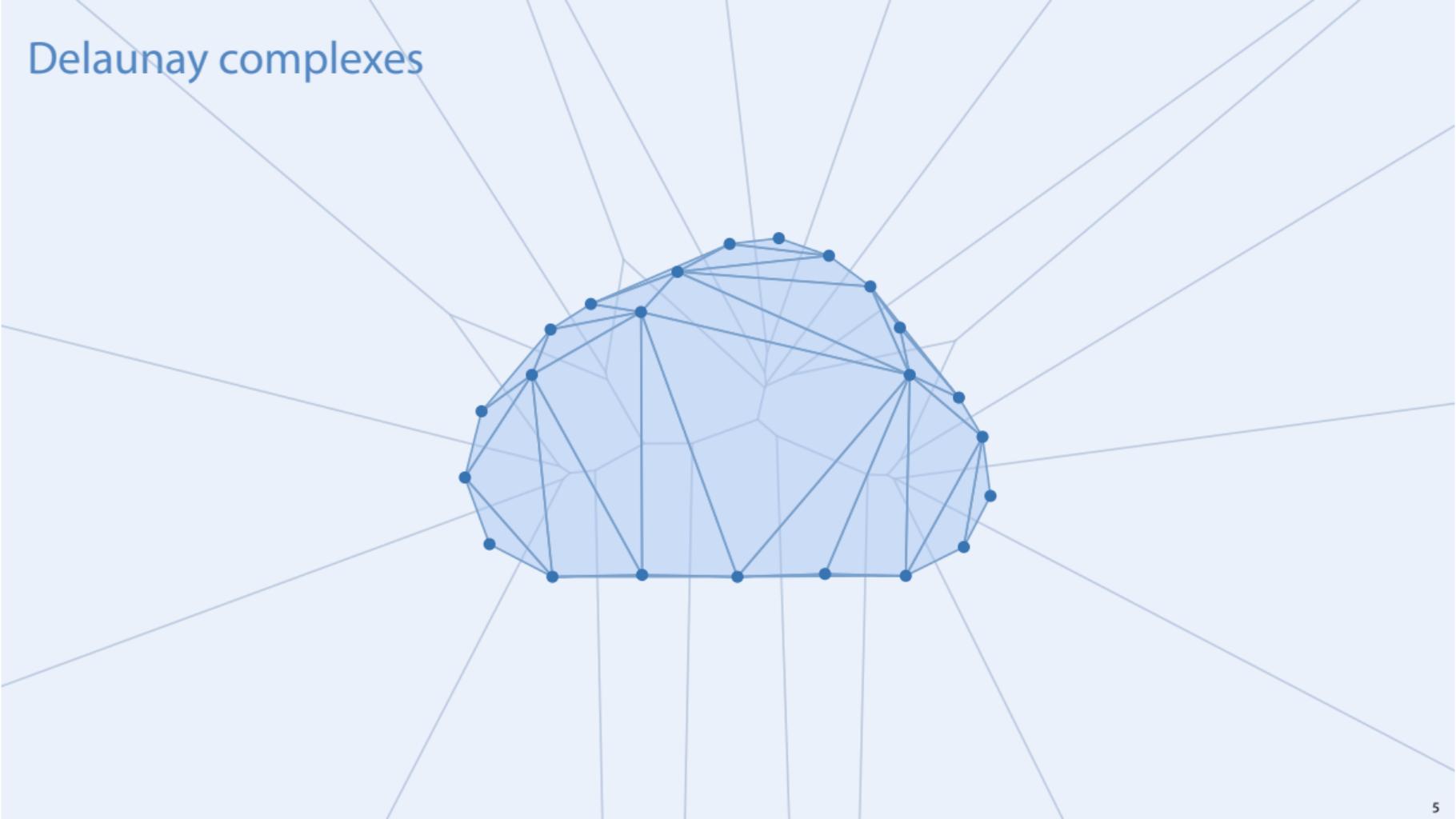
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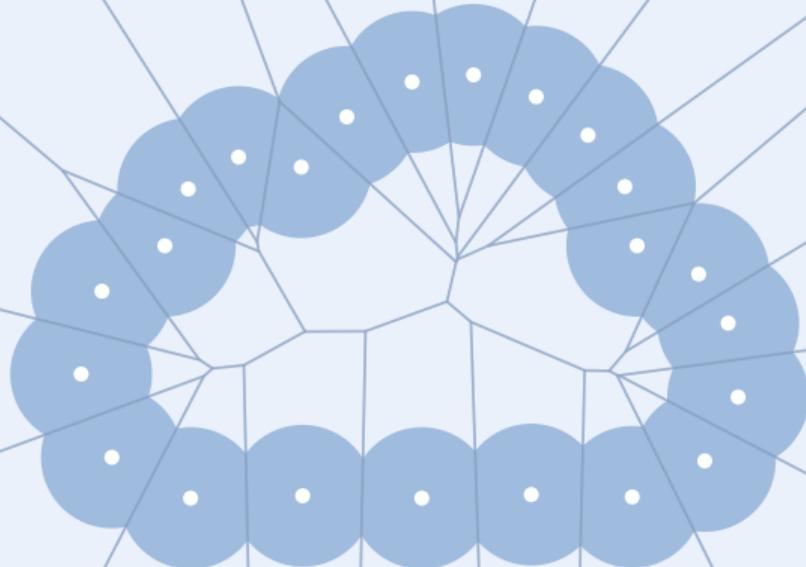
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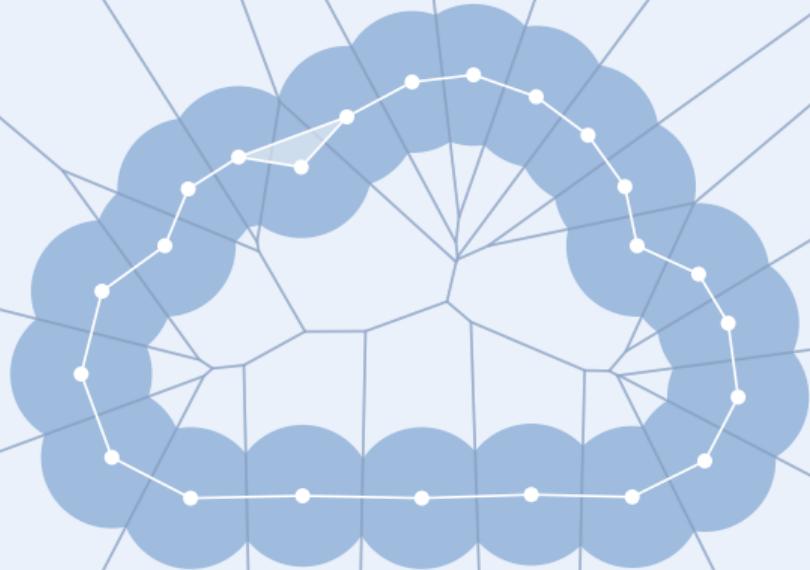
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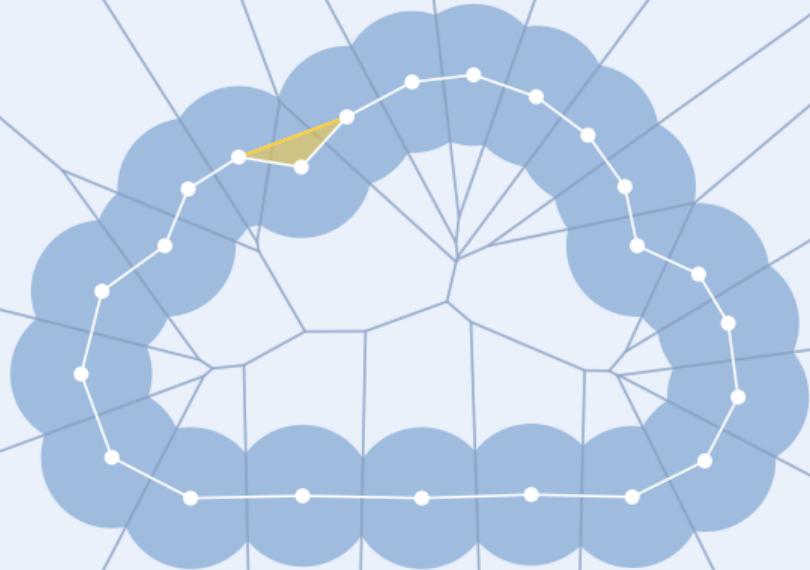
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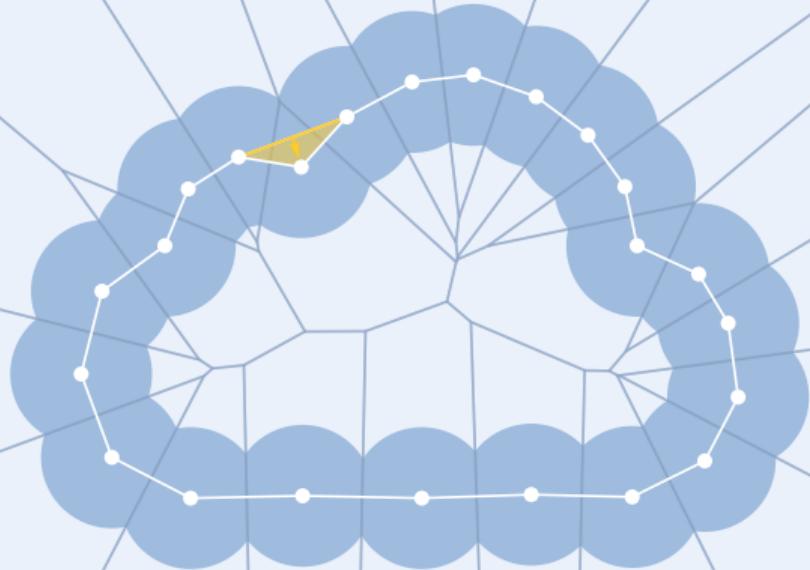
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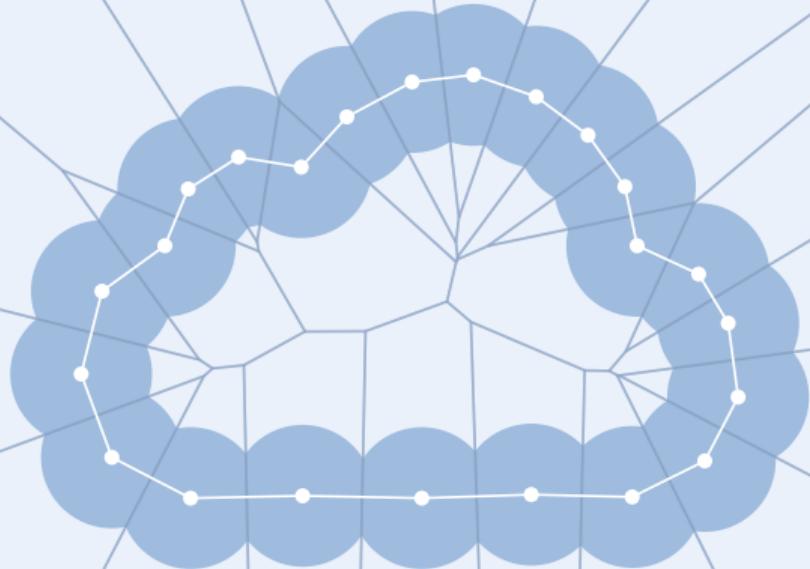
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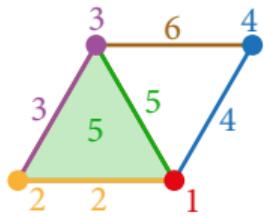
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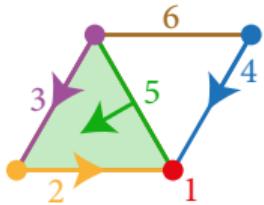
## Delaunay complexes



# Discrete Morse theory



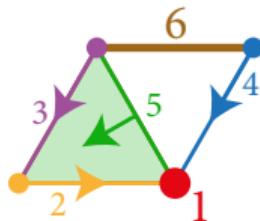
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## Theorem (Forman 1998)

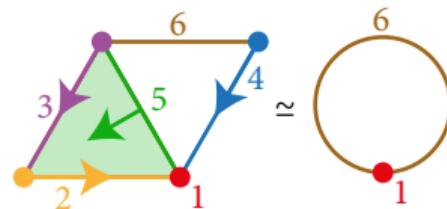
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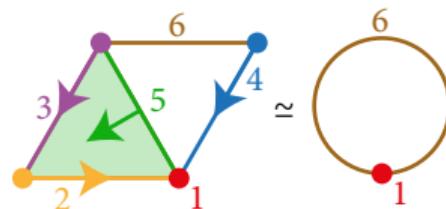
Discrete Morse functions – and their gradients – encode *collapses* of sublevel sets:



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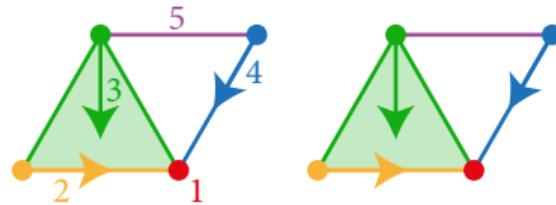


Discrete Morse functions – and their gradients – encode *collapses* of sublevel sets:



# Generalizing discrete Morse theory

Generalized gradients are a partition into intervals in the face poset (instead of just facet pairs):



# Morse theory for Čech and Delaunay complexes

## Proposition (B, Edelsbrunner 2014)

*For a point set in general position, the Čech and Delaunay complexes are sublevel sets of (generalized) discrete Morse functions.*

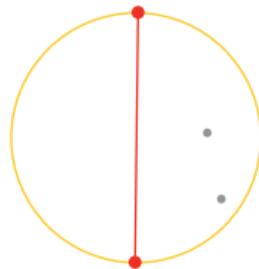


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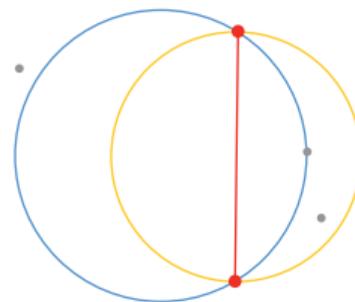


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- Čech: radius of smallest enclosing ball
- Delaunay: radius of smallest empty circumsphere

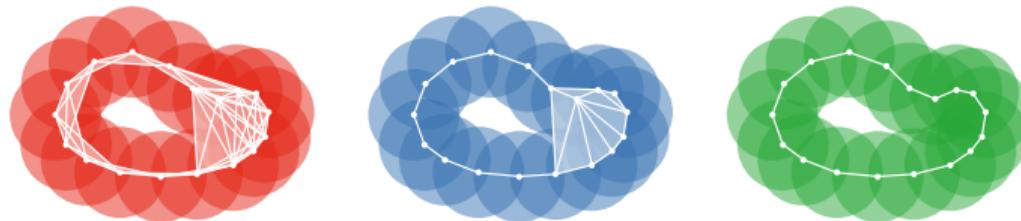


# From Čech to Delaunay to Wrap complexes

Theorem (B, Edelsbrunner 2017)

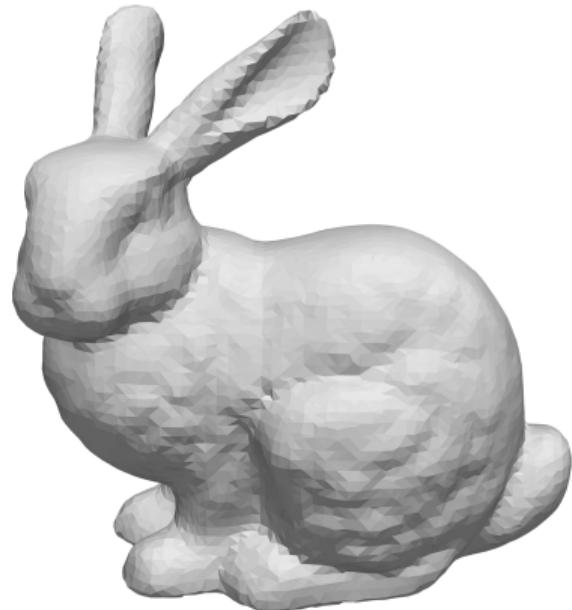
Čech, Delaunay, and Wrap complexes (at any scale  $r$ ) of a point set  $X \subset \mathbb{R}^d$  in general position are related by collapses encoded by a single discrete gradient field:

$$\text{Cech}_r X \searrow \text{Del}_r X \searrow \text{Wrap}_r X.$$



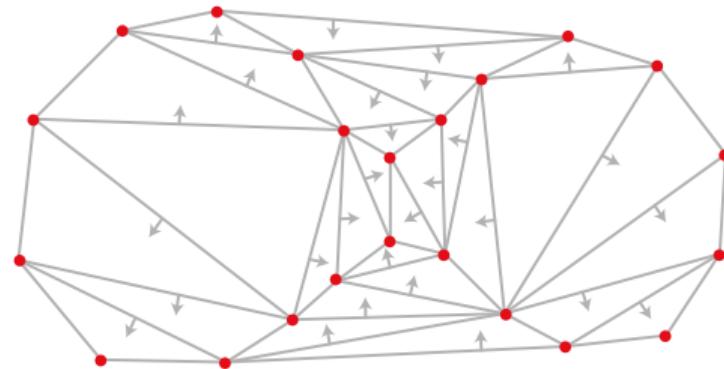
## Wrap complexes

Foundation of the surface reconstruction software *Wrap* (Edelsbrunner 1995, Geomagic)



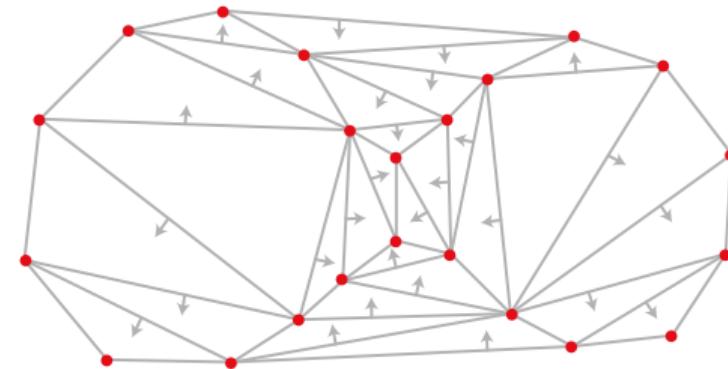
## Wrap complexes

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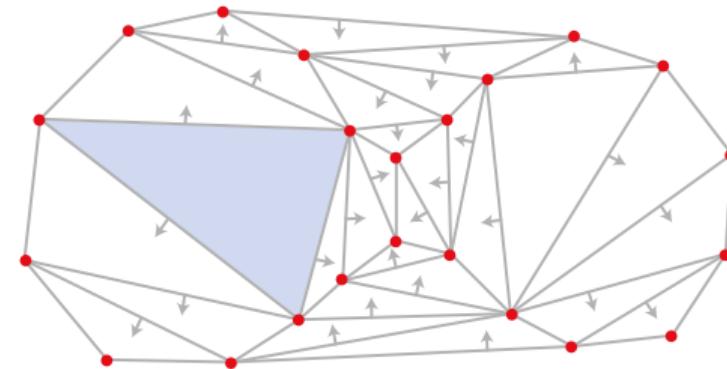
**Definition (Edelsbrunner 1995; B, Edelsbrunner 2017)**

$\text{Wrap}_r(X)$  is the *descending complex* of  $V$  on  $\text{Del}_r X$ :

- the smallest subcomplex of  $\text{Del}_r X$  that
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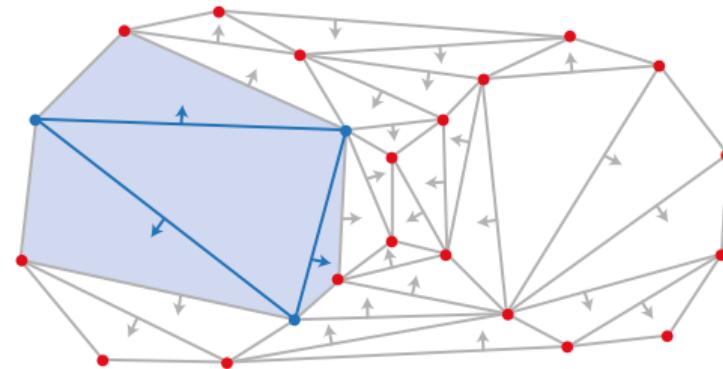
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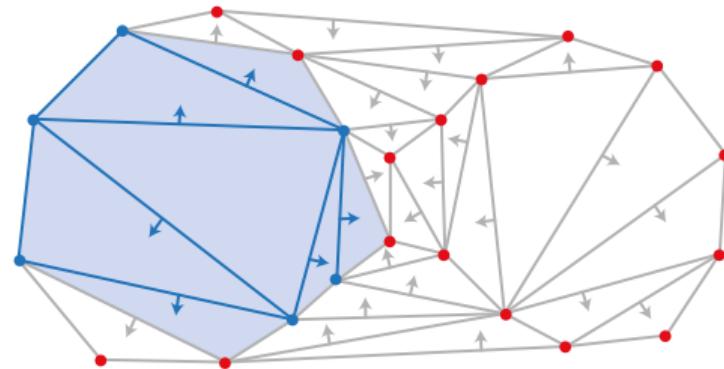
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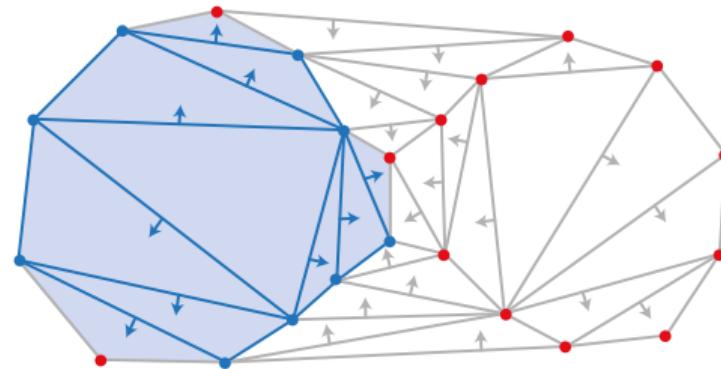
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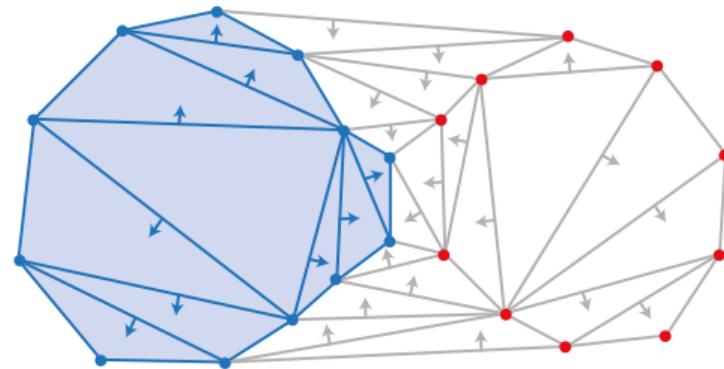
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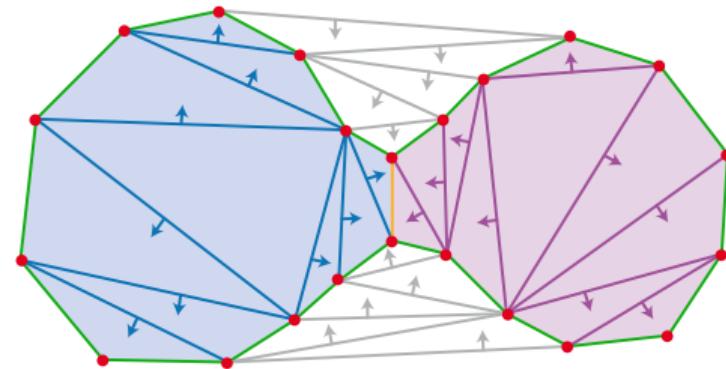
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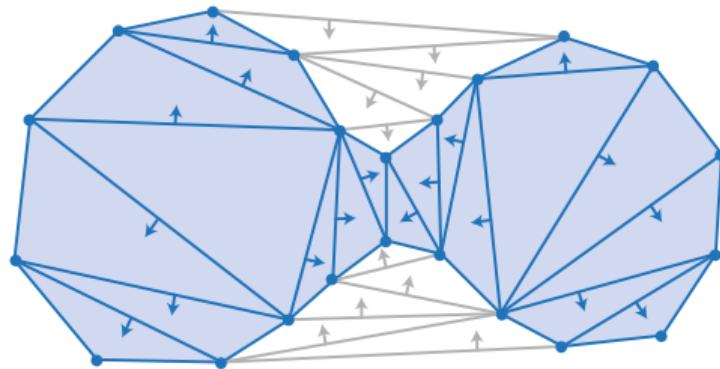
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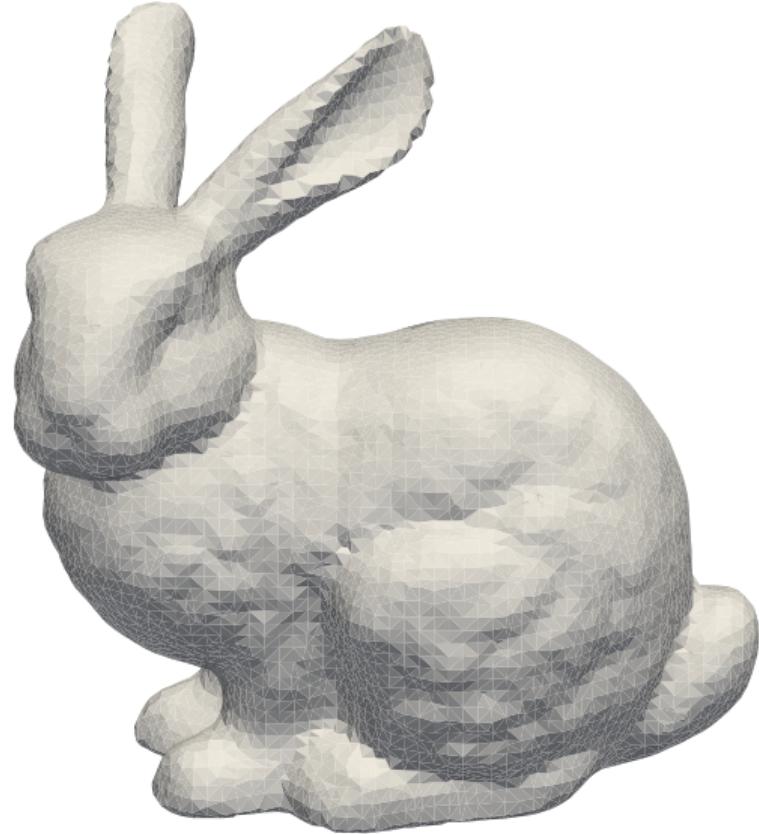
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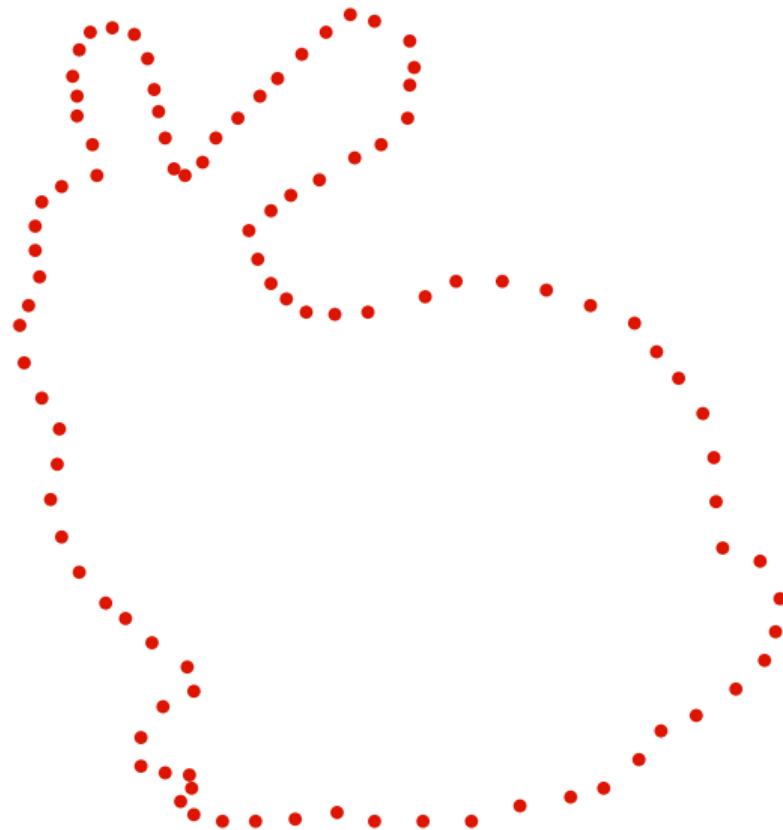
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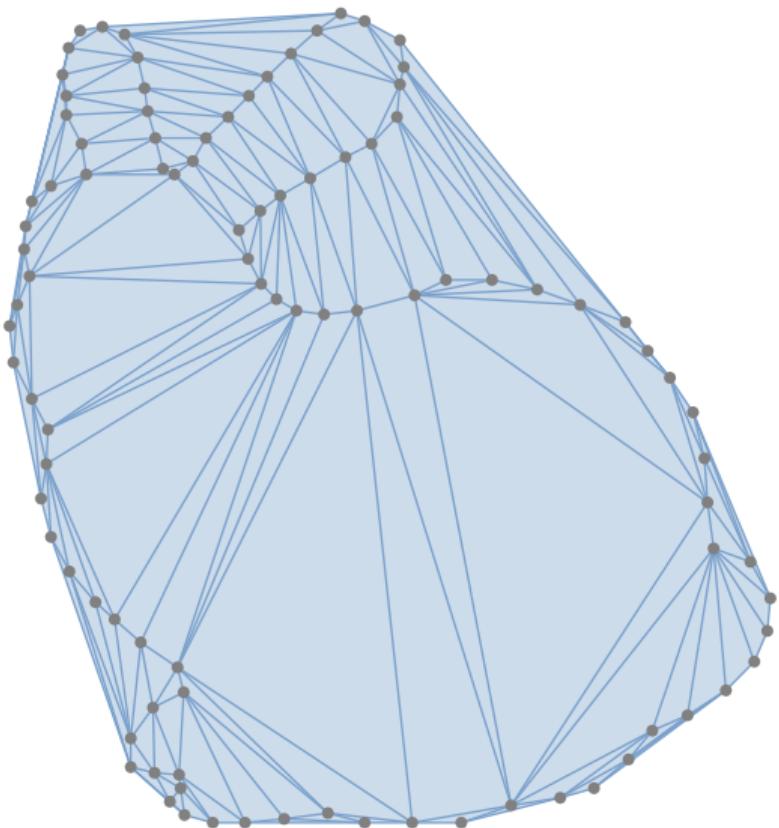
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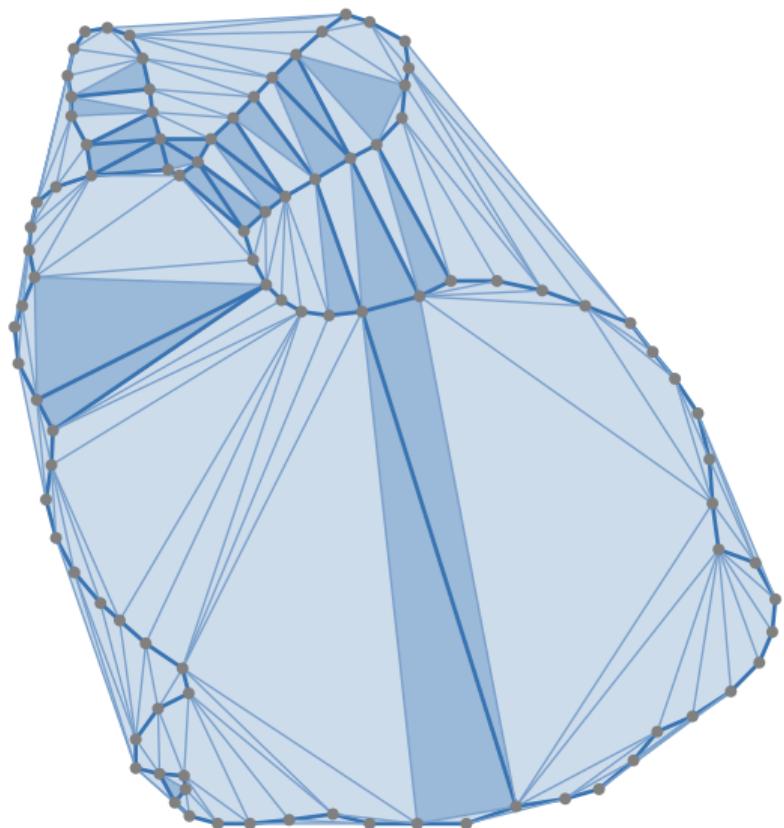
## Wrap complexes and lexicographically minimal cycles



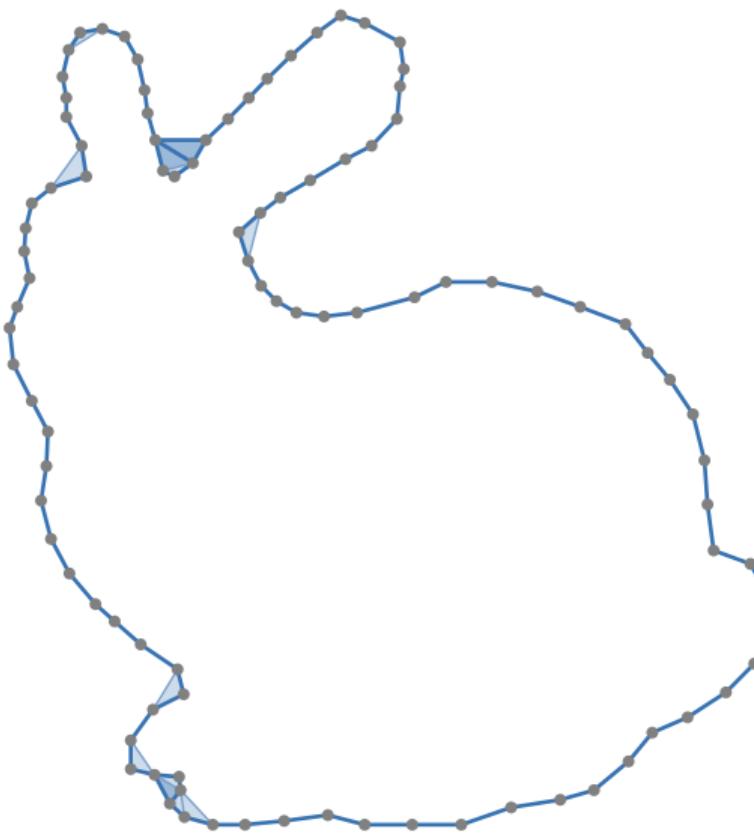
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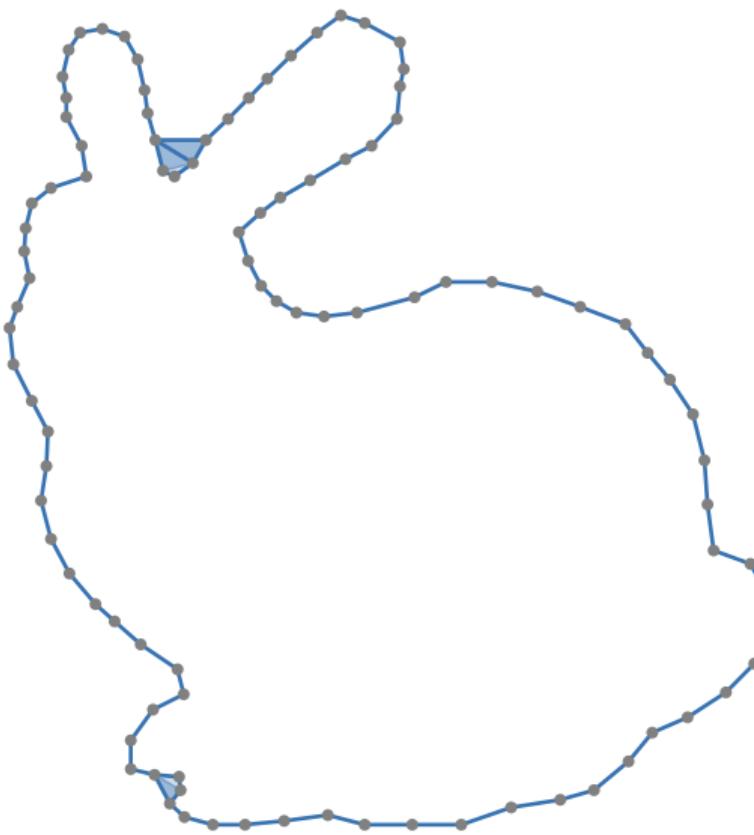
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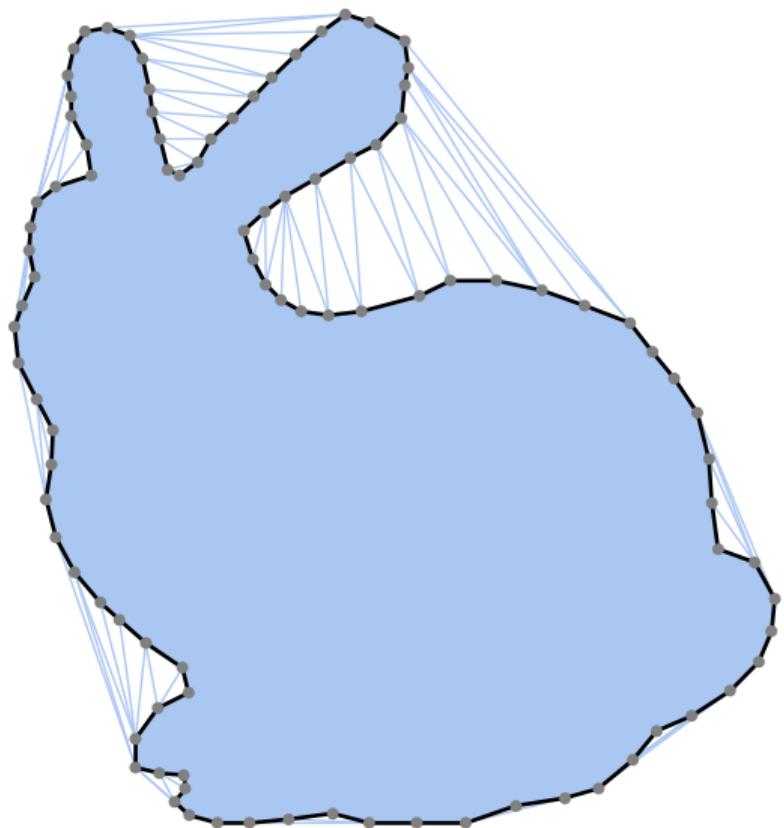
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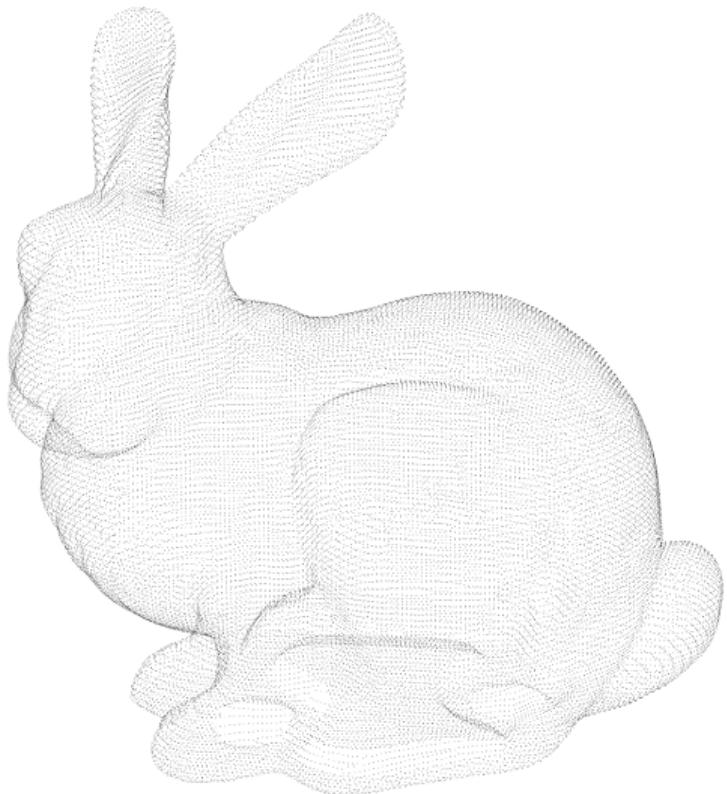
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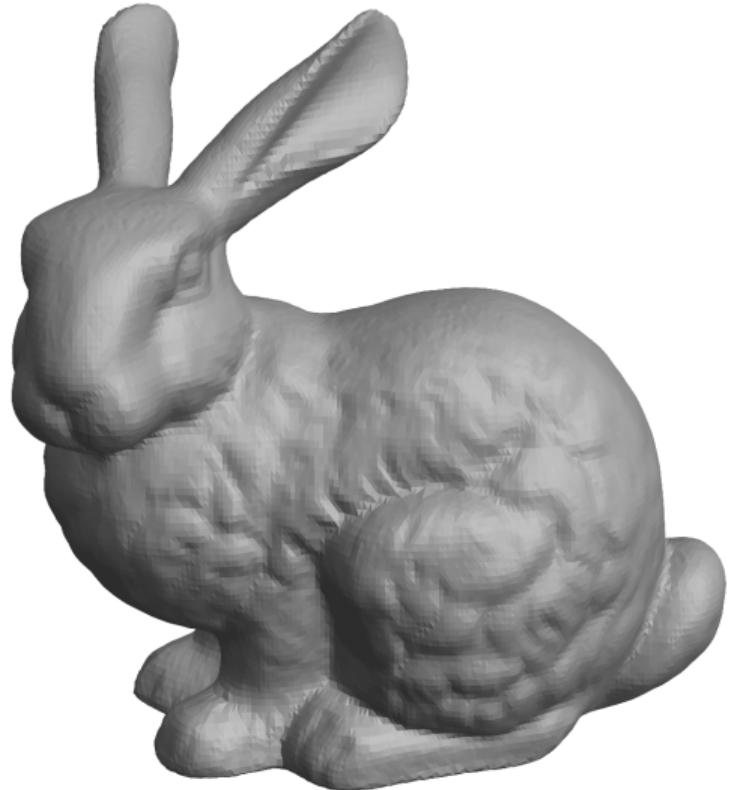
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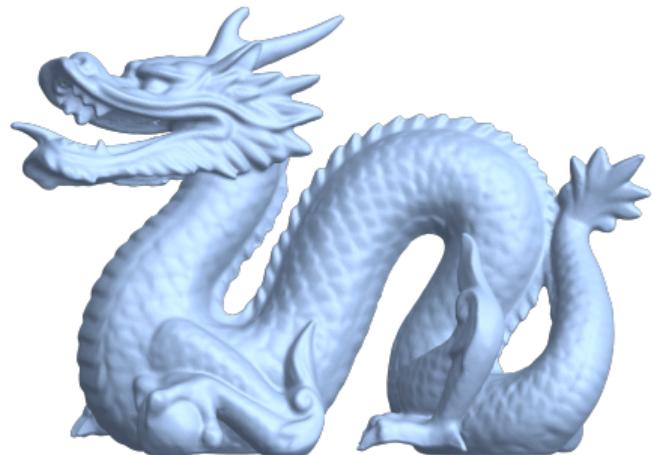
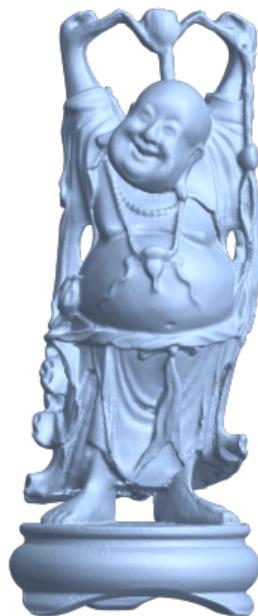
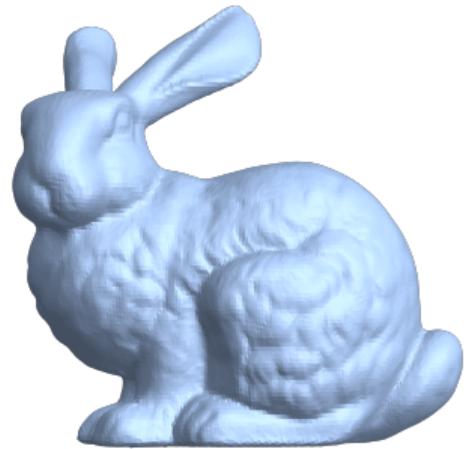
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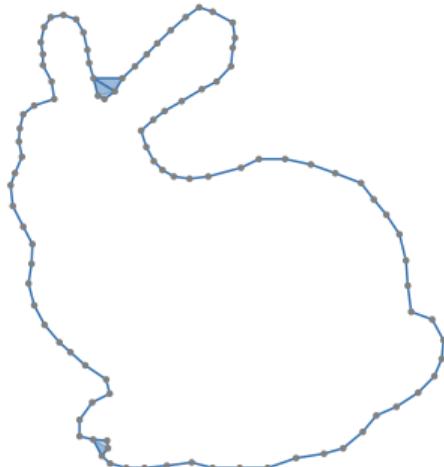
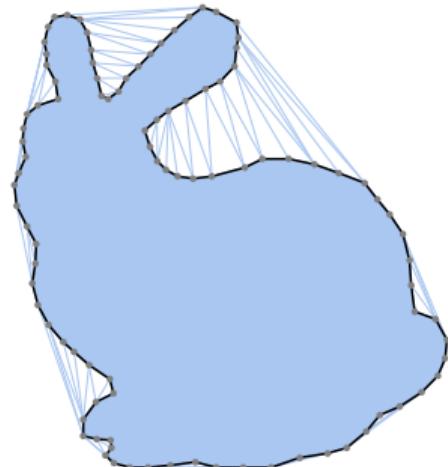
## Point cloud reconstruction with minimal cycles



# Minimal cycles within Wrap complexes

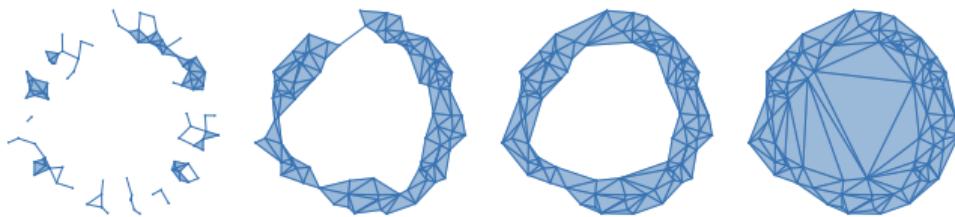
## Theorem (B, Roll 2024)

Let  $X \subset \mathbb{R}$  be a finite subset in general position and let  $r \in \mathbb{R}$ . Then the lexicographically minimal cycles of  $\text{Del}_r(X)$  are supported on  $\text{Wrap}_r(X)$ .

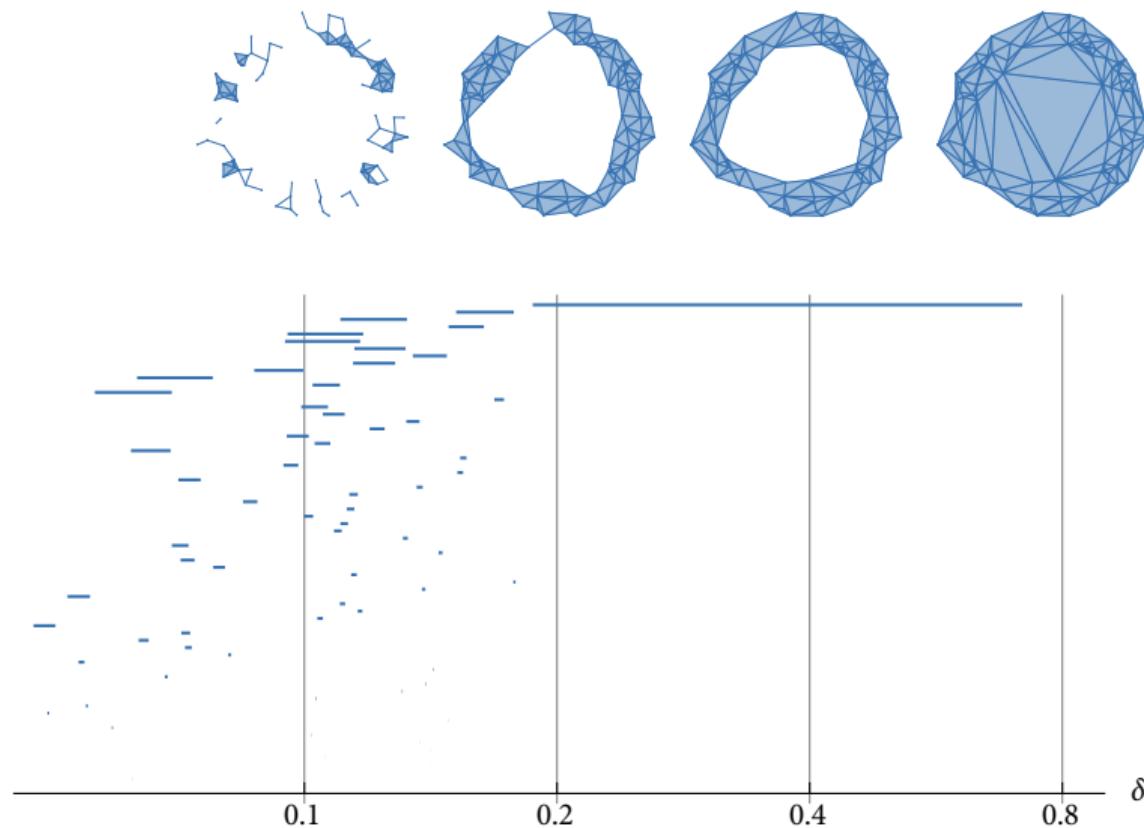


# Persistent homology

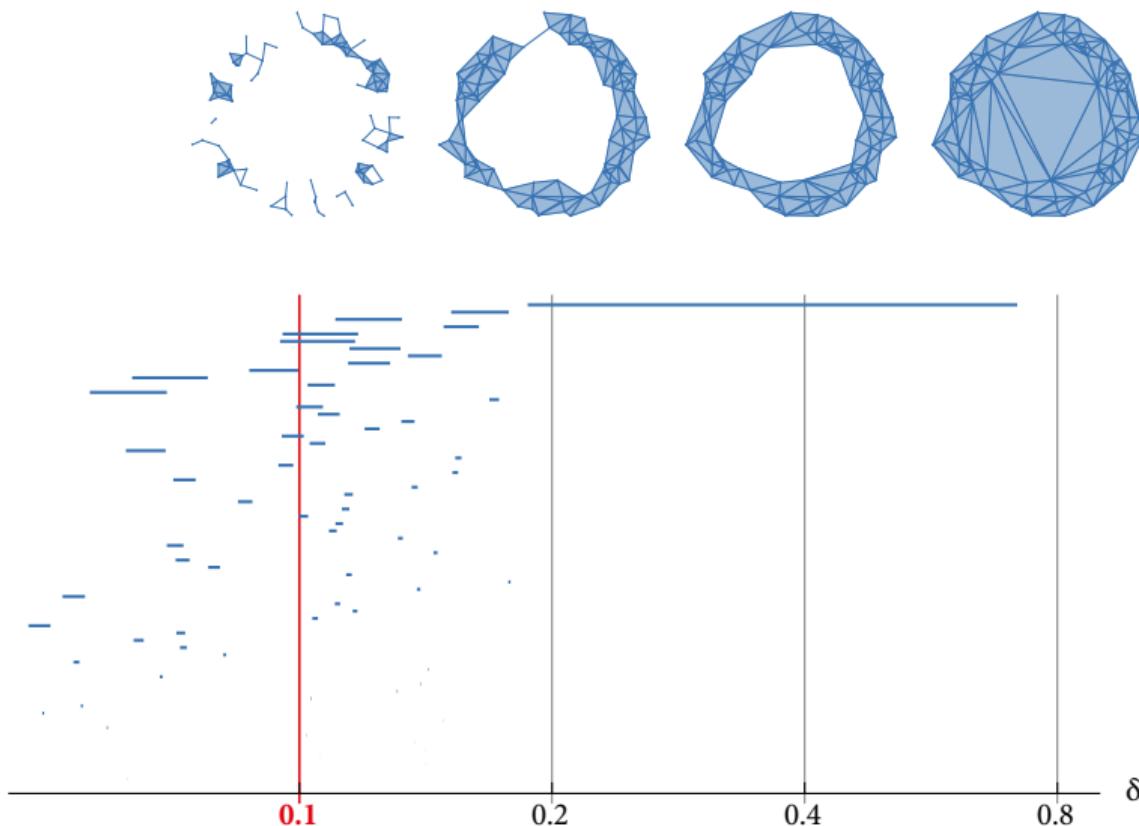
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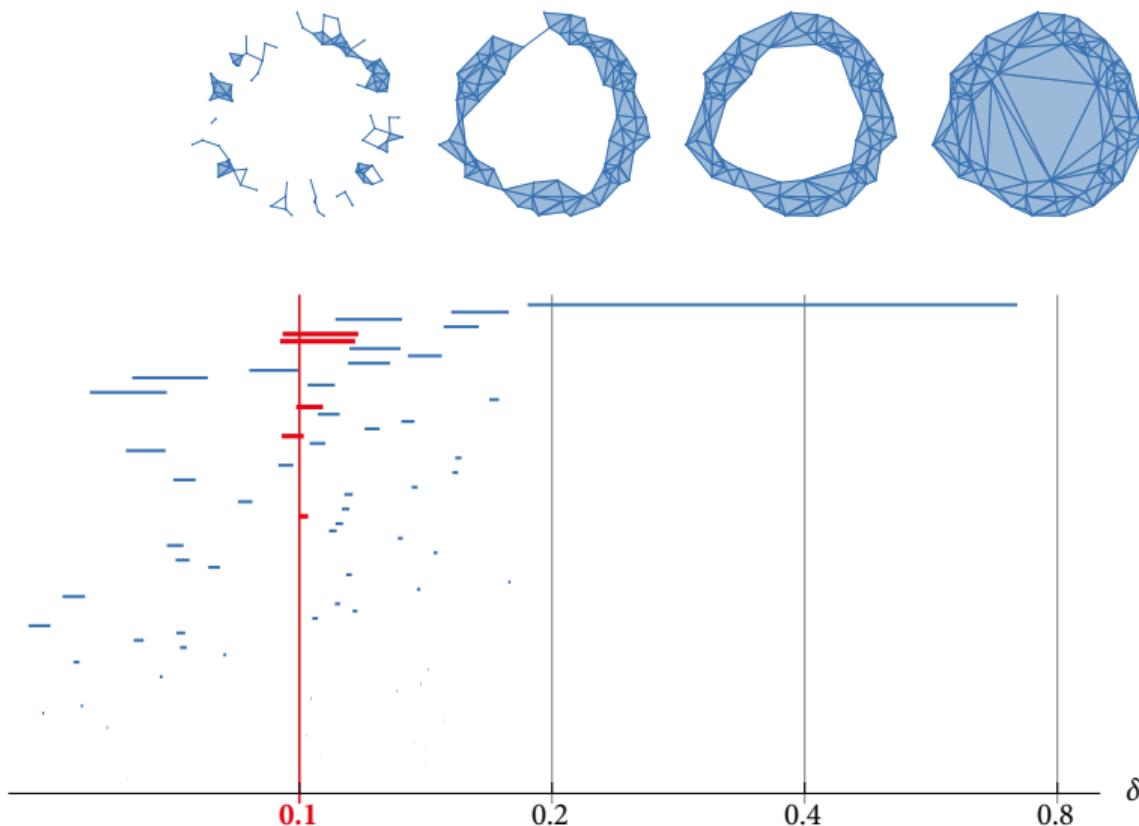
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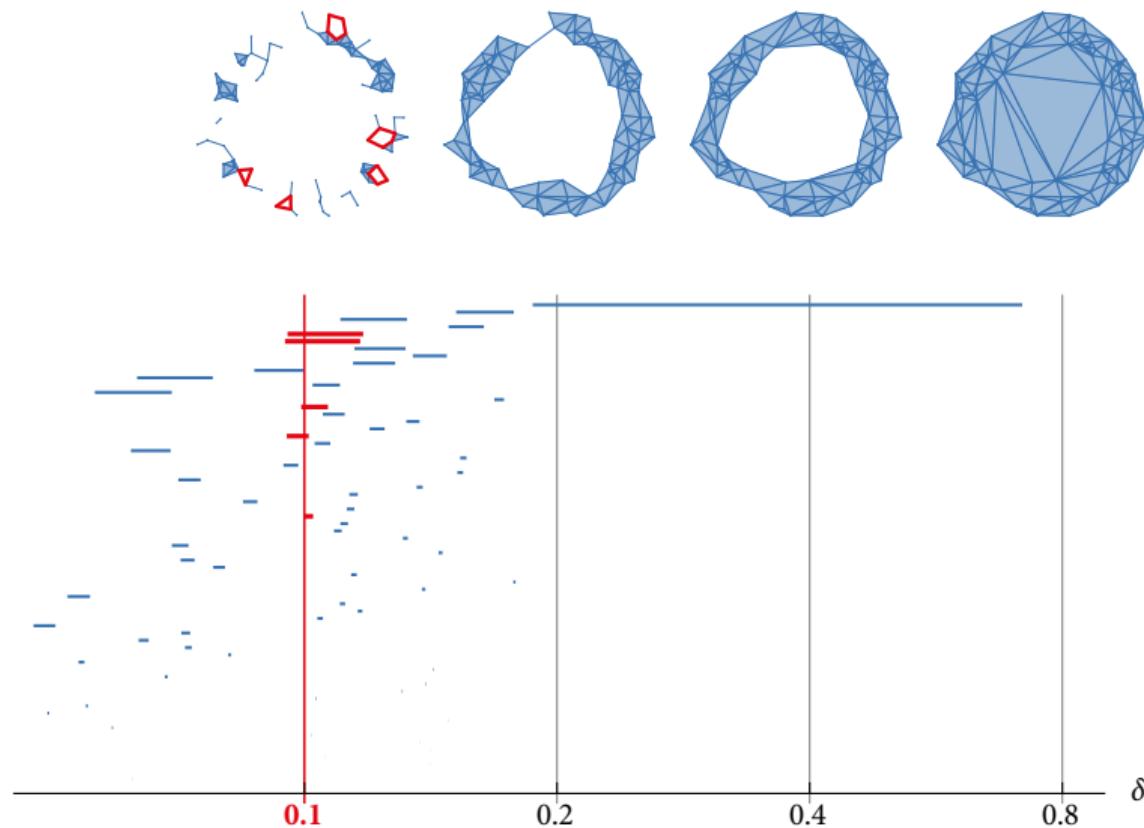
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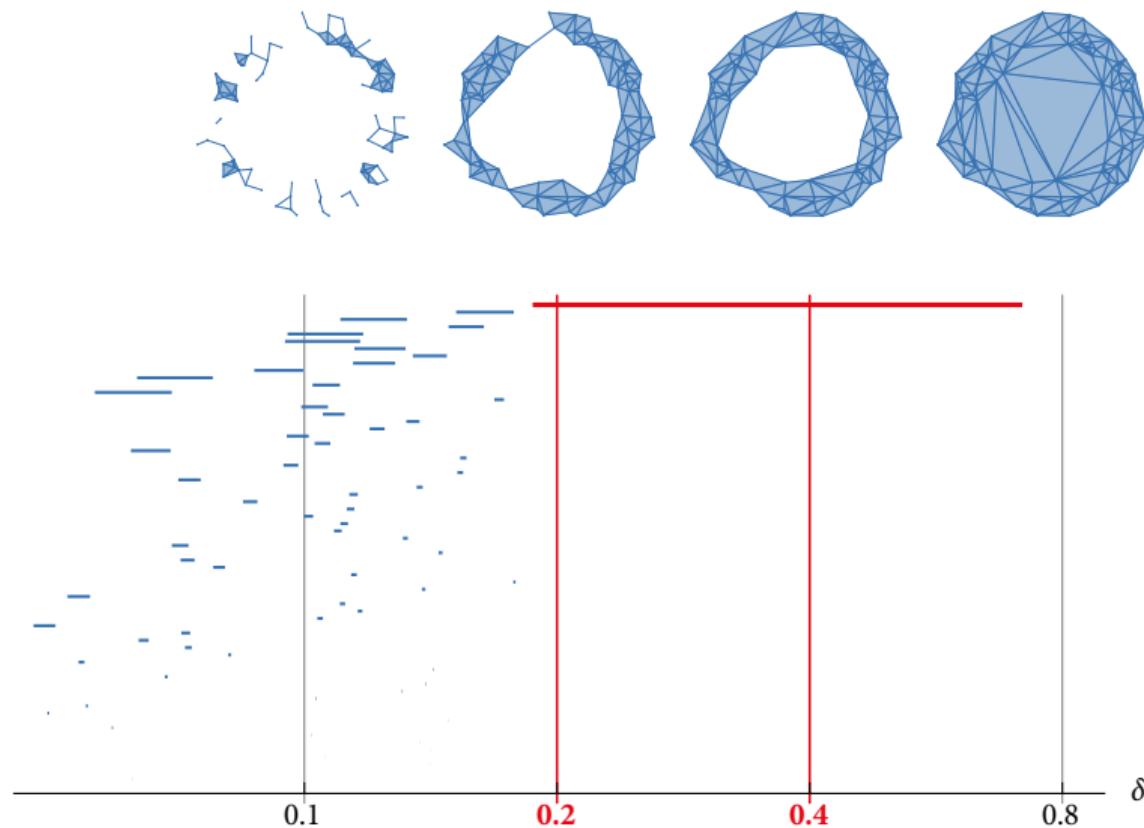
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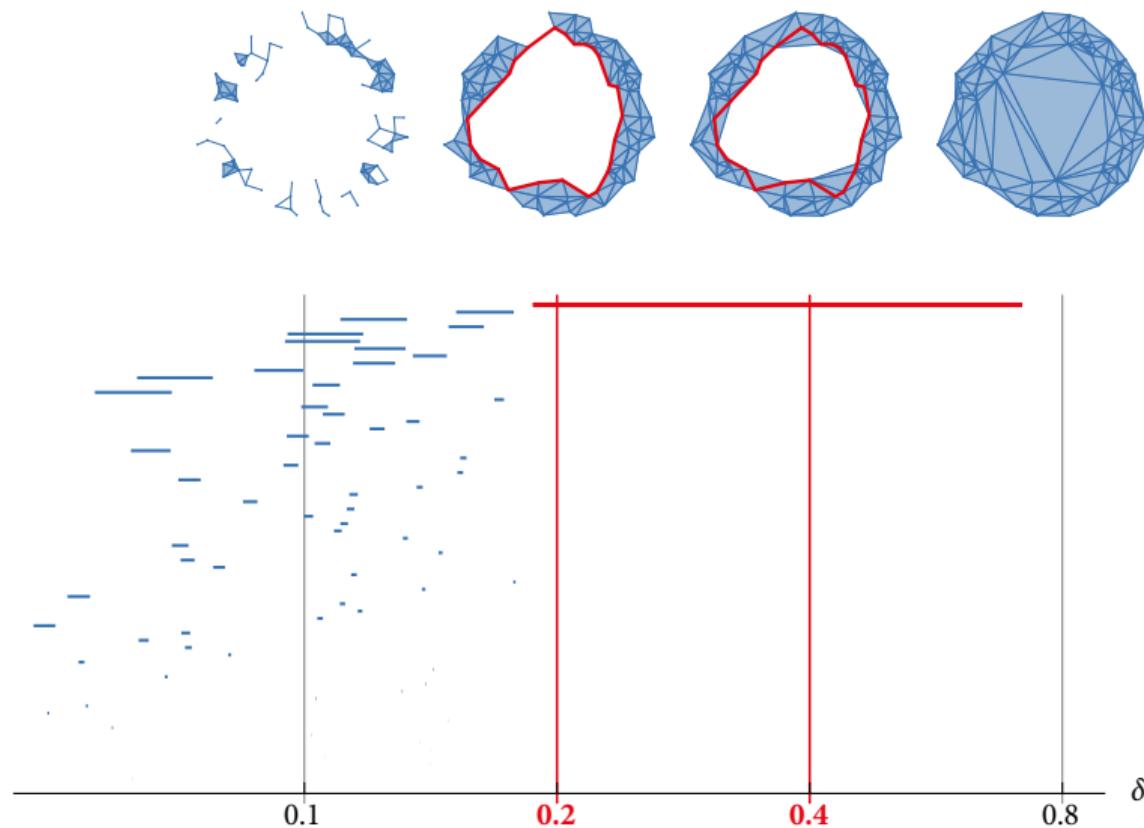
# What is persistent homology?



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# Structure

## The formalism of persistent homology

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- The maps  $K_s \hookrightarrow K_t$  for  $s \leq t \in \mathbb{R}$  are inclusions.
- Applying homology  $H_* : \mathbf{Top} \rightarrow \mathbf{Vect}$  yields a *persistence module*

$$M = H_* \circ K : \mathbf{R} \rightarrow \mathbf{Vect}$$





## Barcodes: the structure of persistence modules

### Theorem (Crawley-Boevey 2015)

*Any persistence module  $M : \mathbf{R} \rightarrow \mathbf{vect}$  (of finite dim. vector spaces over some field  $\mathbb{F}$ ) decomposes as a direct sum of interval modules*

$$\rightarrow \cdots \rightarrow 0 \rightarrow \mathbb{F} \rightarrow \cdots \rightarrow \mathbb{F} \rightarrow 0 \rightarrow \cdots \rightarrow$$

*(in an essentially unique way).*

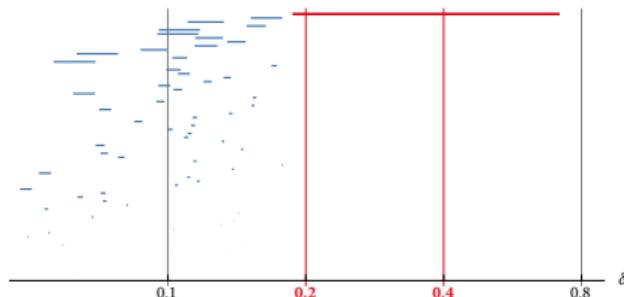
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- The supporting intervals form the *persistence barcode*. It describes  $M$  up to isomorphism.

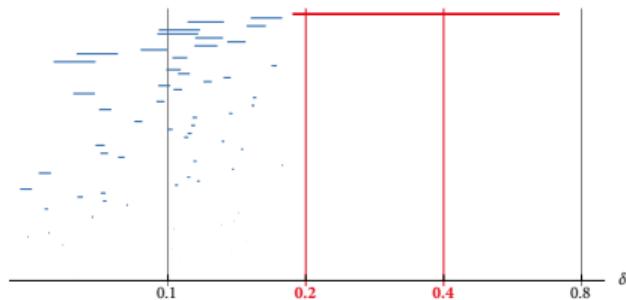
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(in an essentially unique way).



- The supporting intervals form the *persistence barcode*. It describes  $M$  up to isomorphism.
- We rarely have such a simple structure for other diagrams, like  $\mathbf{R}^2 \rightarrow \mathbf{vect}$  (2 parameters).

## Indecomposables abound in multi-parameter persistence

Theorem (B, Scoccola 2022)

*For  $n > 1$ , almost every finitely presentable  $n$ -parameter persistence module is indecomposable.*

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In other words:

- Indecomposability is a generic property.

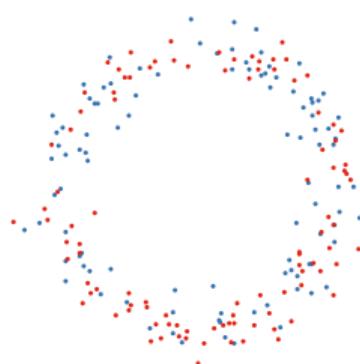
# Stability

## Stability of persistence barcodes

If two point clouds are close, then their barcodes are also close:

**Theorem (Cohen-Steiner, Edelsbrunner, Harer 2005)**

Let  $X, Y \subset \mathbb{R}^d$  be finite point sets with Hausdorff distance  $d_H(X, Y) = \delta$ .



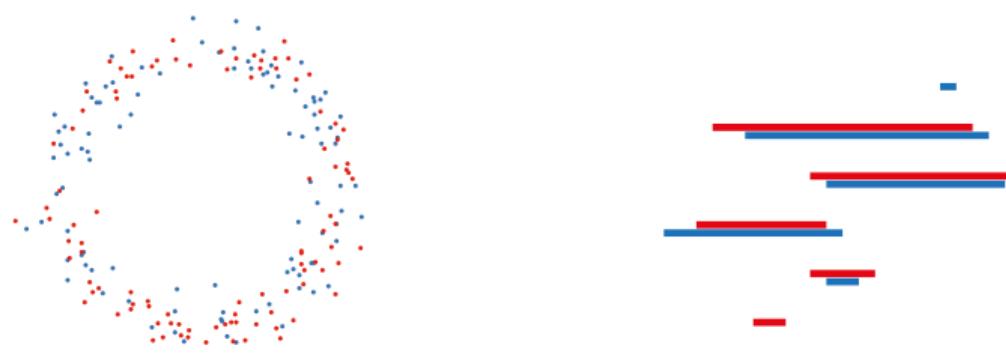
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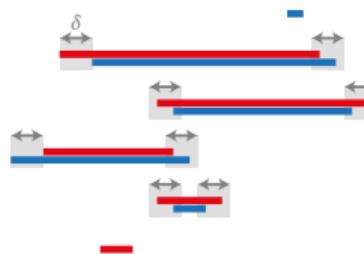
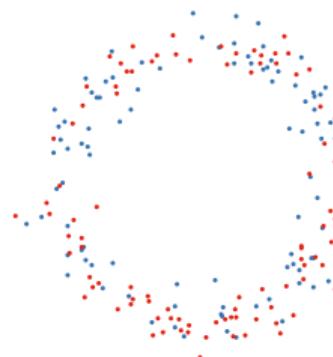
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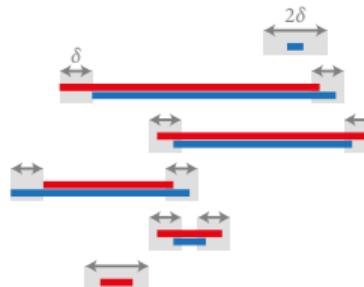
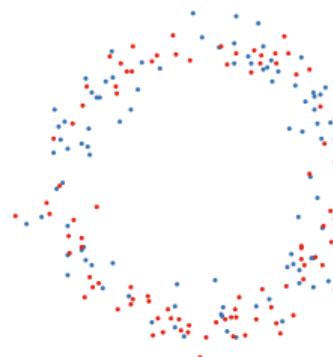
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- matched intervals have endpoints within distance  $\leq \delta$ , and
- unmatched intervals have length  $\leq 2\delta$ .



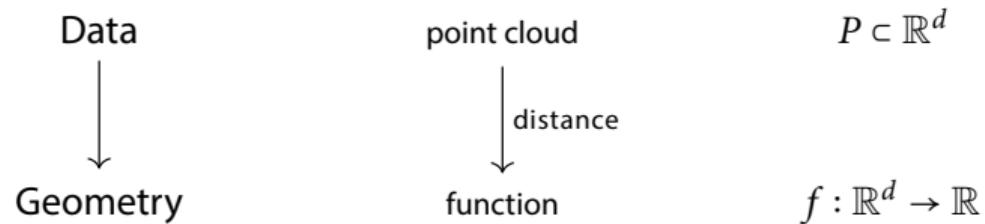
# Persistence and stability: the big picture

Data

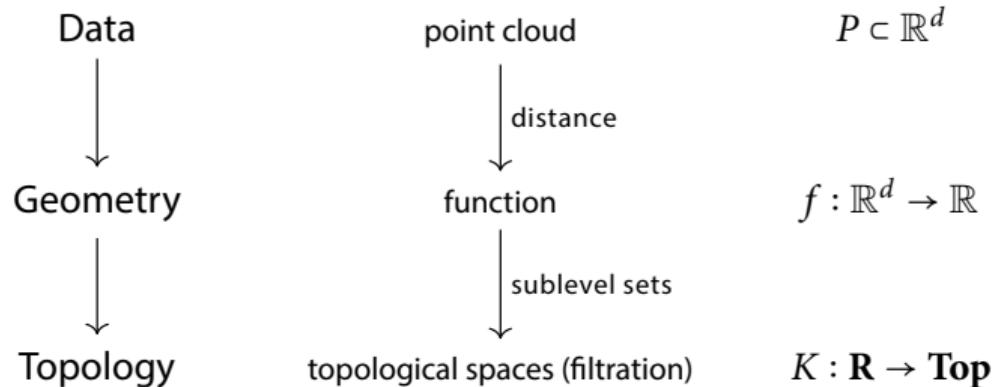
point cloud

$$P \subset \mathbb{R}^d$$

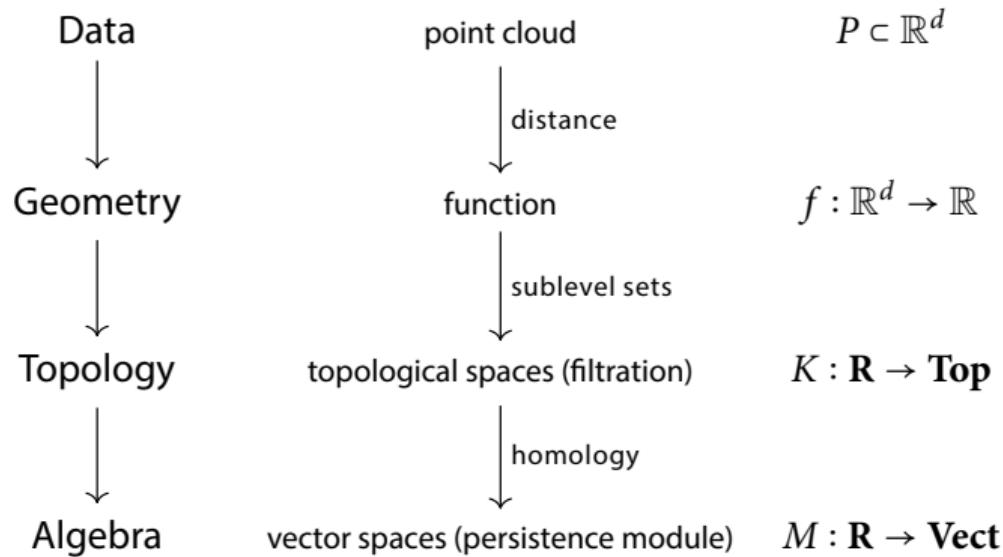
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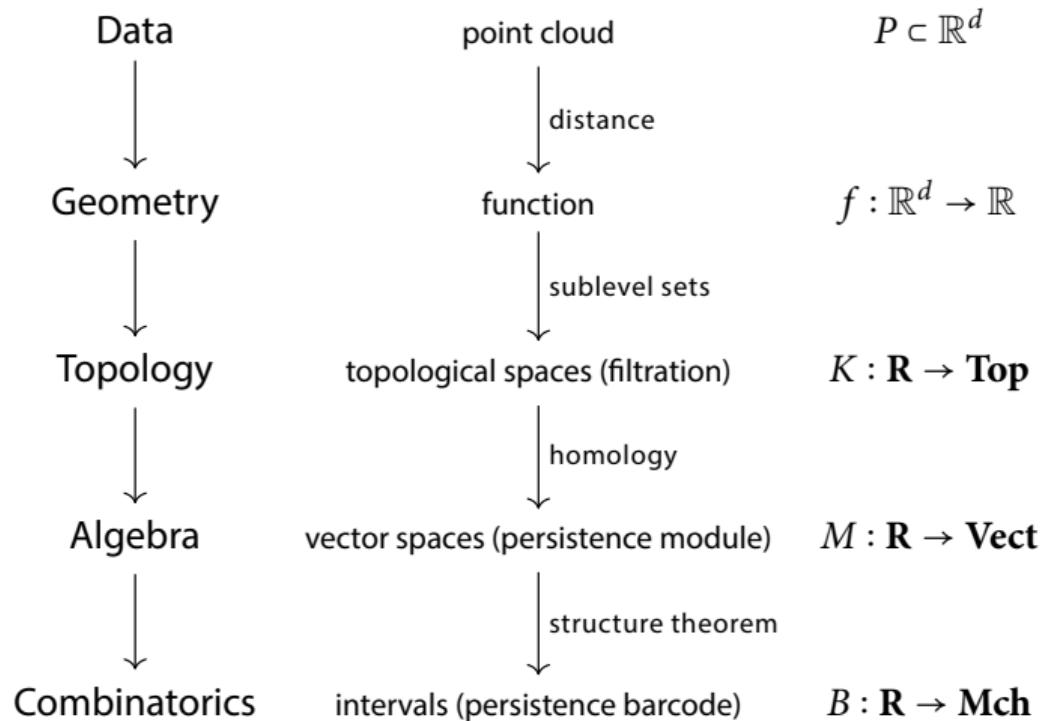
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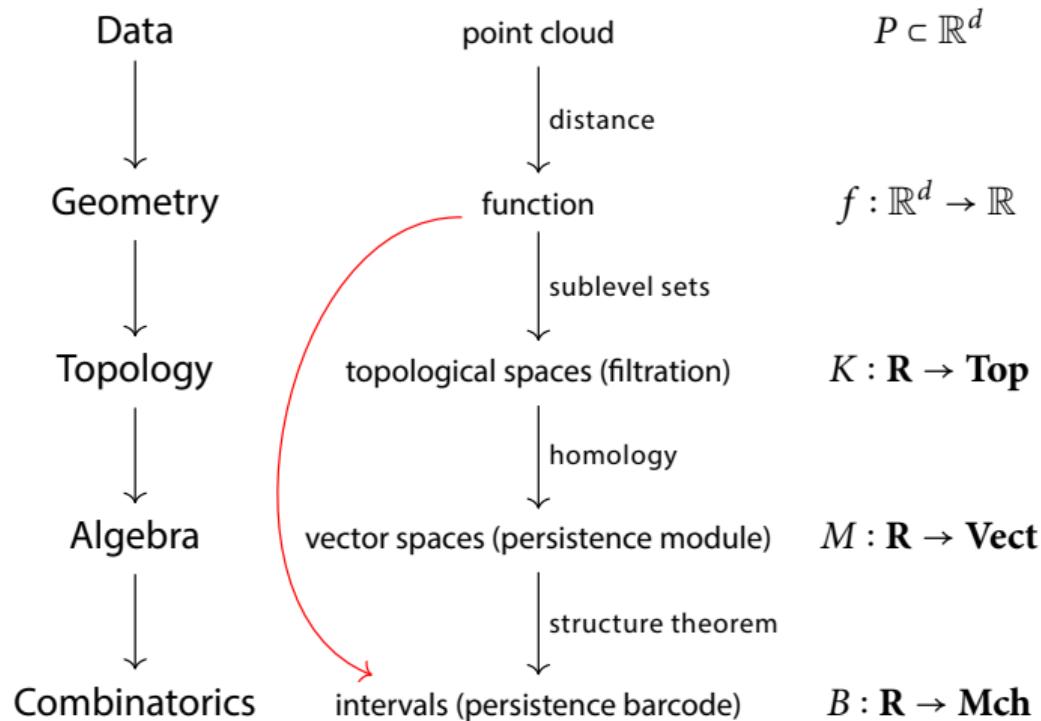
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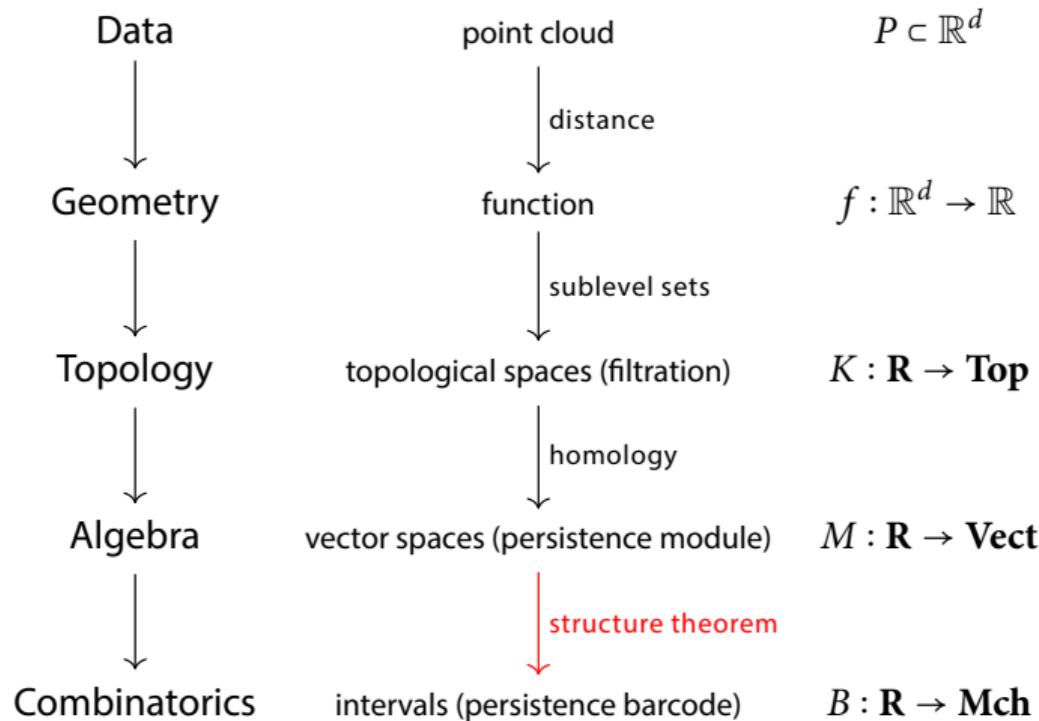
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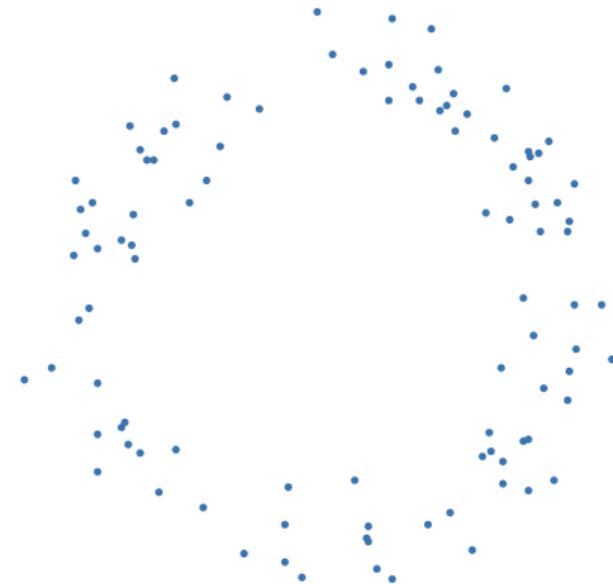


# Vietoris–Rips persistence

## Vietoris–Rips complexes

For a metric space  $X$ , the *Vietoris–Rips complex* at  $t > 0$  is the simplicial complex

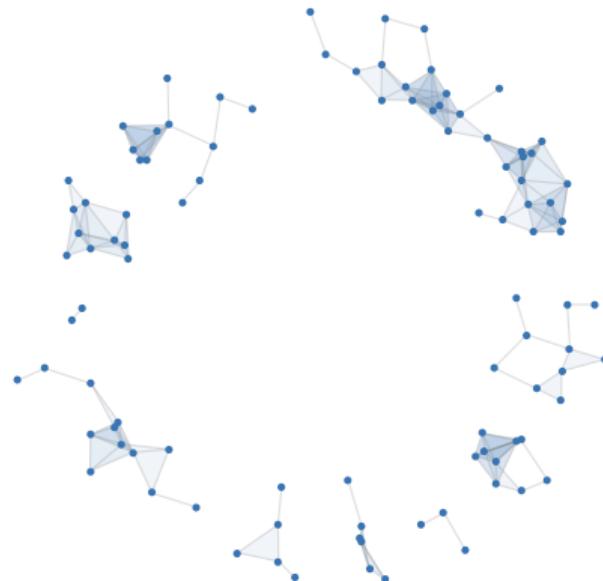
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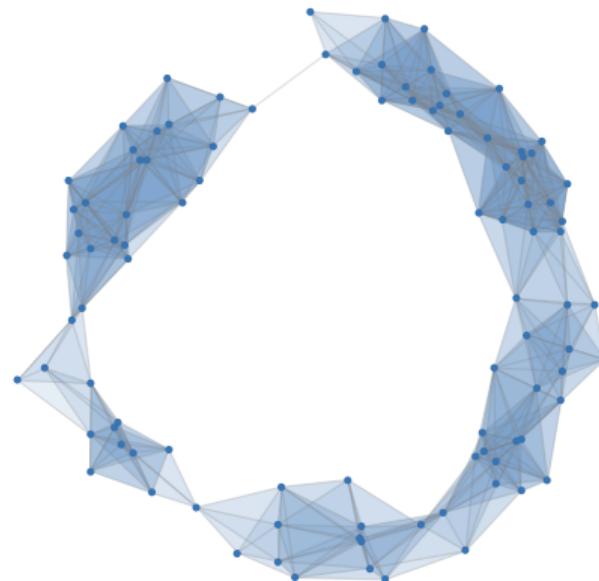
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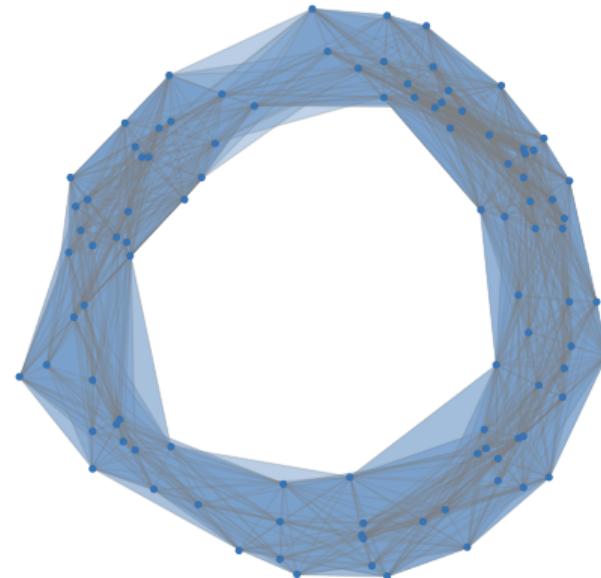
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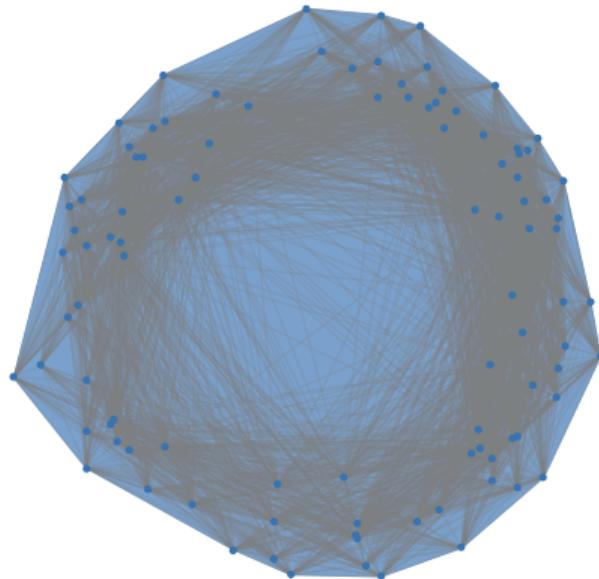
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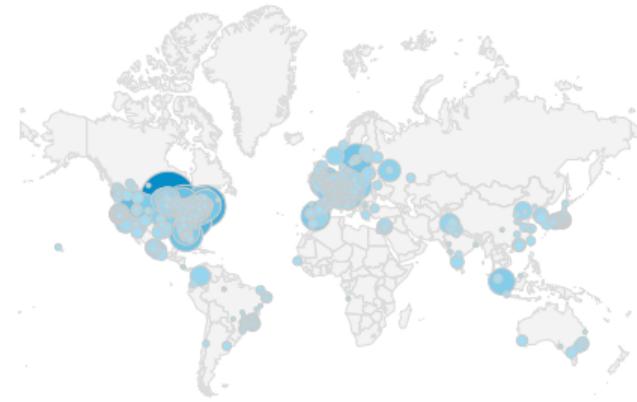
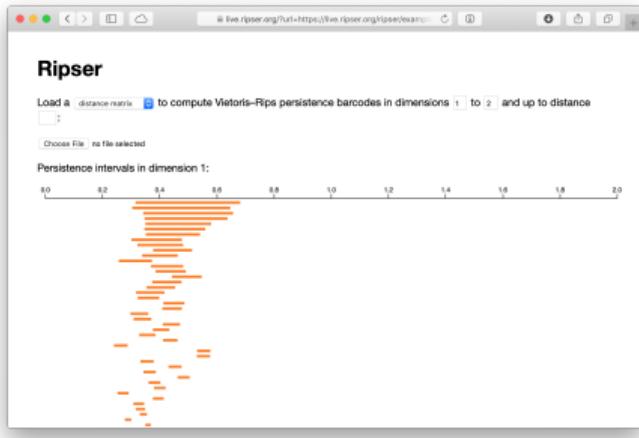
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# Ripser: software for computing Vietoris–Rips persistence barcodes

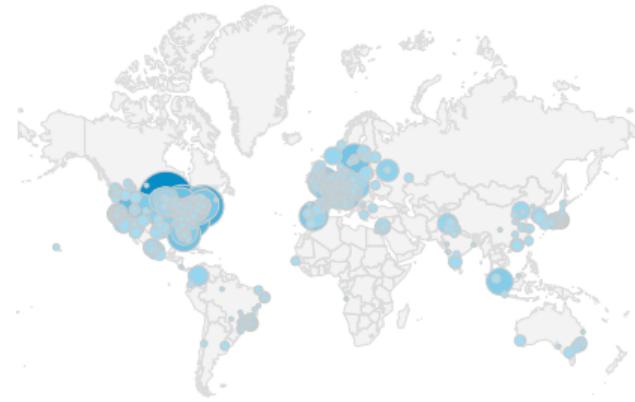
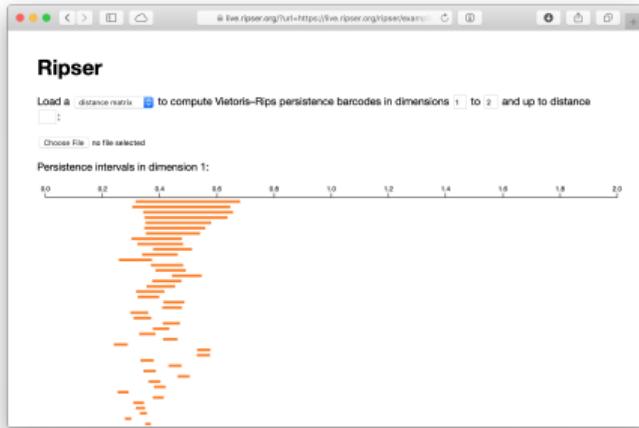
Open source software ([ripser.org](http://ripser.org))



Ripser users across the globe

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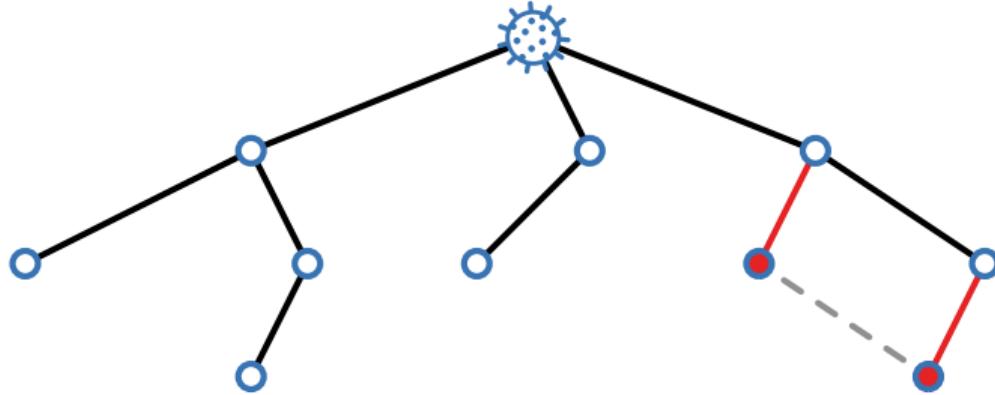


Ripser users across the globe

Computational improvements based on

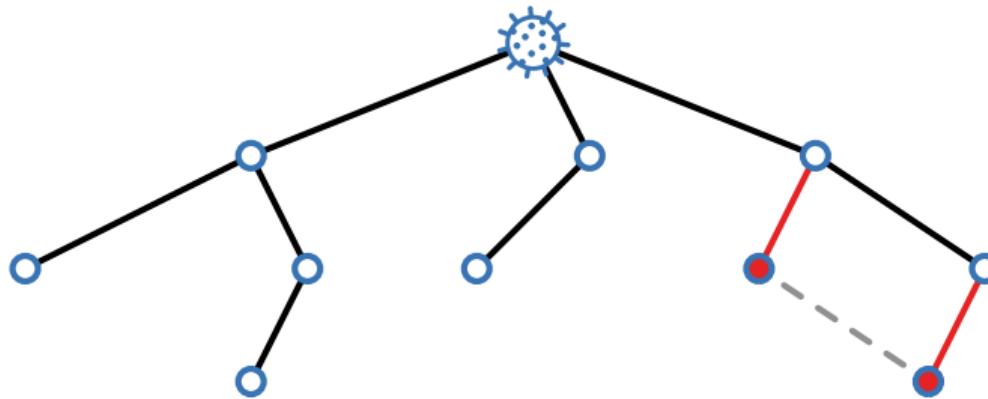
- *implicit matrix representations*
- *apparent pairs*, connecting persistence to discrete Morse theory

# Topology of viral evolution



Joint work with: A. Ott, M. Bleher, L. Hahn (Heidelberg), R. Rabadan, J. Patiño-Galindo (Columbia), M. Carrière (INRIA)

# Topology of viral evolution



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Observation: Ripser runs unusually fast on genetic distance data

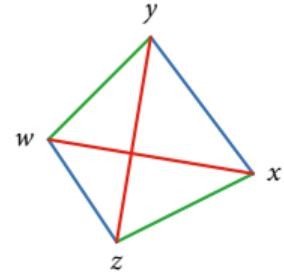
- SARS-CoV2 RNA sequences (spike protein)
- 25556 data points ( $2.8 \times 10^{12}$  simplices in 2-skeleton)
- 120 s computation time (with data points ordered appropriately)

# Gromov-hyperbolicity

## Definition (Gromov 1988)

A metric space  $X$  is  $\delta$ -hyperbolic (for  $\delta \geq 0$ ) if for all  $w, x, y, z \in X$  we have

$$d(w, x) + d(y, z) \leq \max\{d(w, y) + d(x, z), d(w, z) + d(x, y)\} + 2\delta.$$

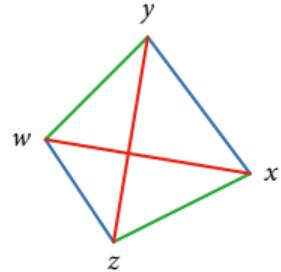


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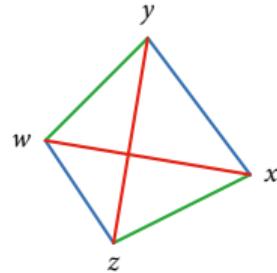


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- The hyperbolic plane is  $(\ln 2)$ -hyperbolic.



- The 0-hyperbolic spaces are precisely the metric trees and their subspaces.



## Rips Contractibility

Theorem (Rips; Gromov 1988)

*Let  $X$  be a  $\delta$ -hyperbolic geodesic metric space. Then  $\text{Rips}_t(X)$  is contractible for all  $t \geq 4\delta$ .*

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*Let  $X$  be a finite  $\delta$ -hyperbolic space. Then there is a single discrete gradient encoding the collapses*

$$\text{Rips}_u(X) \searrow \text{Rips}_t(X) \searrow \{\ast\}$$

*for all  $u > t \geq 4\delta + 2\nu$ , where  $\nu$  is the geodesic defect of  $X$ .*

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*If  $X$  is a sample of a metric tree, then  $H_d(\text{Rips}_t(X))$  is trivial for  $d > 0$ .*

# Origins

When was persistent homology discovered first?

# When was persistent homology discovered first?

ANNALS OF MATHEMATICS  
Vol. 41, No. 2, April, 1940

## RANK AND SPAN IN FUNCTIONAL TOPOLOGY

BY MARSTON MORSE

(Received August 9, 1939)

### 1. Introduction.

The analysis of functions  $F$  on metric spaces  $M$  of the type which appear in variational theories is made difficult by the fact that the critical limits, such as absolute minima, relative minima, minimax values etc., are in general infinite in number. These limits are associated with relative  $k$ -cycles of various dimensions and are classified as 0-limits, 1-limits etc. The number of  $k$ -limits suitably counted is called the  $k^{\text{th}}$  type number  $m_k$  of  $F$ . The theory seeks to establish relations between the numbers  $m_k$  and the connectivities  $p_k$  of  $M$ . The numbers  $p_k$  are finite in the most important applications. It is otherwise with the numbers  $m_k$ .

The theory has been able to proceed provided one of the following hypotheses is satisfied. The critical limits cluster at most at  $1/n$ ; the critical points are

# When was persistent homology discovered first?

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All citations	<b>Rank and span in functional topology</b>	
Articles	<input type="checkbox"/> Search within citing articles	
Case law	<b>Exact homomorphism sequences in homology theory</b>	<a href="#">ed.ac.uk [PDF]</a>
My library	JL Kelley, E Pitcher - <i>Annals of Mathematics</i> , 1947 - JSTOR	
Any time	The developments of this paper stem from the attempts of one of the authors to deduce relations between homology groups of a complex and homology groups of a complex which is its image under a simplicial map. Certain relations were deduced (see [EP 1] and [EP 2] ...	
Since 2016	Cited by 46 Related articles All 3 versions Cite Save More	
Since 2015		
Since 2012		
Custom range...	<b>Marston Morse and his mathematical works</b>	<a href="#">ams.org [PDF]</a>
Sort by relevance	R Bott - <i>Bulletin of the American Mathematical Society</i> , 1980 - ams.org	
Sort by date	American Mathematical Society. Thus Morse grew to maturity just at the time when the subject of Analysis Situs was being shaped by such masters <sup>2</sup> as Poincaré, Veblen, LEJ Brouwer, GD Birkhoff, Lefschetz and Alexander, and it was Morse's genius and destiny to ...	
<input checked="" type="checkbox"/> include citations	Cited by 24 Related articles All 4 versions Cite Save More	
<input checked="" type="checkbox"/> Create alert	<b>Unstable minimal surfaces of higher topological structure</b>	
	M Morse, CB Tompkins - <i>Duke Math. J.</i> 1941 - projecteuclid.org	
	1. Introduction. We are concerned with extending the calculus of variations in the large to multiple integrals. The problem of the existence of minimal surfaces of unstable type contains many of the typical difficulties, especially those of a topological nature. Having studied this ...	
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	<a href="#">U Bauer - 2011 - Citeseer</a>	

# When was persistent homology discovered first?

BULLETIN (New Series) OF THE  
AMERICAN MATHEMATICAL SOCIETY  
Volume 3, Number 3, November 1980

## MARSTON MORSE AND HIS MATHEMATICAL WORKS

BY RAOUL BOTT<sup>1</sup>

**1. Introduction.** Marston Morse was born in 1892, so that he was 33 years old when in 1925 his paper *Relations between the critical points of a real-valued function of n independent variables* appeared in the Transactions of the American Mathematical Society. Thus Morse grew to maturity just at the time when the subject of Analysis Situs was being shaped by such masters<sup>2</sup> as Poincaré, Veblen, L. E. J. Brouwer, G. D. Birkhoff, Lefschetz and Alexander, and it was Morse's genius and destiny to discover one of the most beautiful and far-reaching relations between this fledgling and Analysis; a relation which is now known as *Morse Theory*.

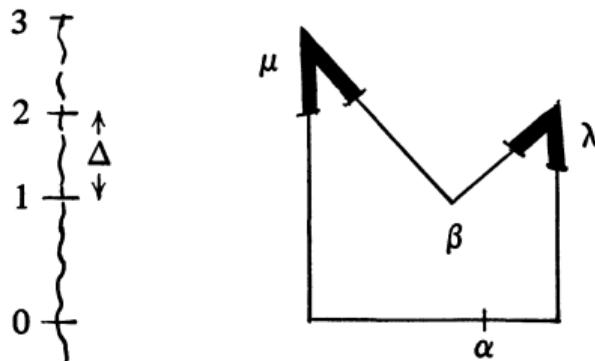
In retrospect all great ideas take on a certain simplicity and inevitability, partly because they shape the whole subsequent development of the subject. And so to us, today, Morse Theory seems natural and inevitable. However one only has to glance at these early papers to see what a tour de force it was in the 1920's to prove the main principles of Birkhoff's theory. Moreover,

## When was persistent homology discovered first?

inequalities pertain between the dimensions of the  $A_i$  and those of  $H(A_i)$ . Thus the Morse inequalities already reflect a certain part of the “Spectral Sequence magic”, and a modern and tremendously general account of Morse’s work on rank and span in the framework of Leray’s theory was developed by Deheuvels [D] in the 50’s.

Unfortunately both Morse’s and Deheuvel’s papers are not easy reading. On the other hand there is no question in my mind that the papers [36] and [44] constitute another tour de force by Morse. Let me therefore illustrate rather than explain some of the ideas of the rank and span theory in a very simple and tame example.

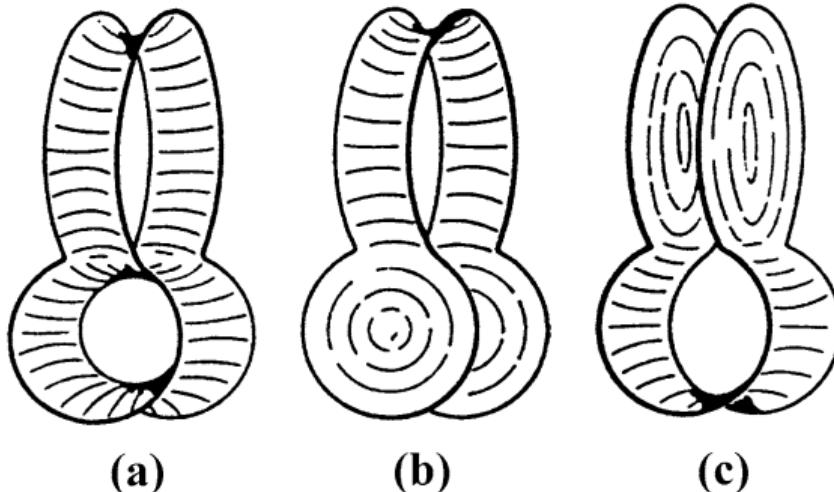
In the figure which follows I have drawn a homeomorph of  $M = S^1$  in the plane, and I will be studying the height function  $F = y$  on  $M$ .



# Motivation and application: minimal surfaces

## Problem (Plateau's problem)

*Find an immersed disk of least area spanned by a given closed Jordan curve.*

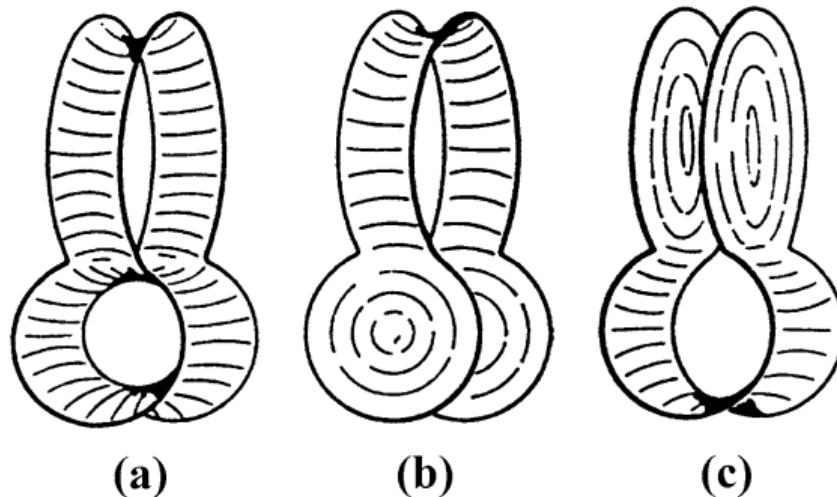


(from Dierkes et al.: *Minimal Surfaces*, 2010)

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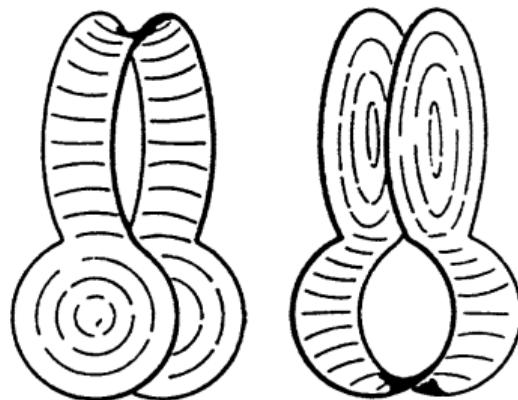
Solution by Douglas (1930; first Fields Medal 1936):

- identifies minimal surfaces with critical points of the *Douglas functional*

## Existence of unstable minimal surfaces

Theorem (Morse, Tompkins 1939; Shiffman 1939)

*Assume that a given curve bounds two separate stable minimal surfaces.*

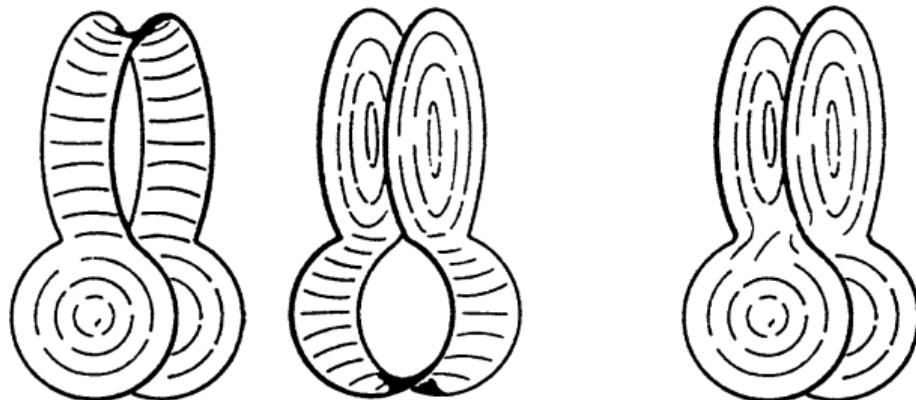


## Existence of unstable minimal surfaces

Theorem (Morse, Tompkins 1939; Shiffman 1939)

Assume that a given curve bounds two separate stable minimal surfaces.

Then that curve also bounds an unstable minimal surface (a critical point that is not a local minimum).



## Q-tame persistence modules

### Definition (Chazal et al. 2009)

A persistence module  $M : \mathbf{R} \rightarrow \mathbf{vect}$  is *q-tame* if all structure maps  $M_s \rightarrow M_t$  ( $s < t$ ) have finite rank.

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- A q-tame persistence module still admits a persistence barcode.

## Q-tame persistence modules

### Definition (Chazal et al. 2009)

A persistence module  $M : \mathbf{R} \rightarrow \mathbf{vect}$  is *q-tame* if all structure maps  $M_s \rightarrow M_t$  ( $s < t$ ) have finite rank.

- A q-tame persistence module still admits a persistence barcode.

Morse's main technical result, in modern language:

- The minimal surface functional has q-tame persistent Vietoris homology.

## Q-tameness from local connectivity

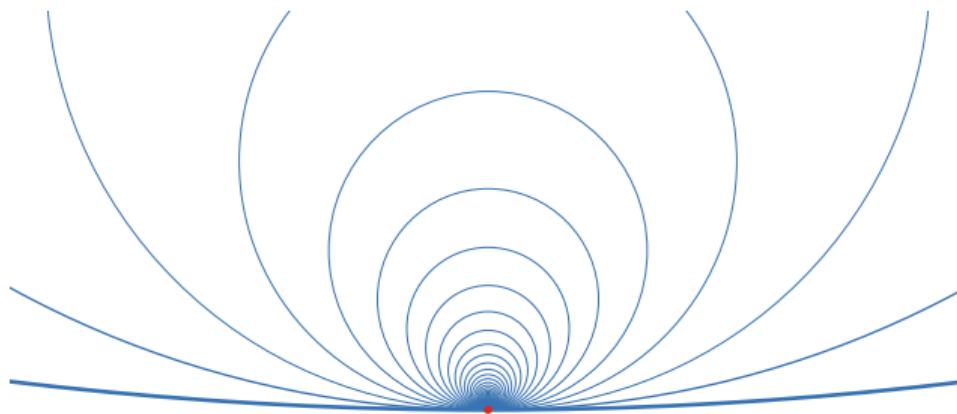
Theorem (Morse, 1937)

*If the sublevel set filtration off:  $X \rightarrow \mathbb{R}$  is compact and weakly locally connected, then it has q-tame persistent Vietoris homology.*

# Q-tameness from local connectivity

Theorem (Morse, 1937; incorrect)

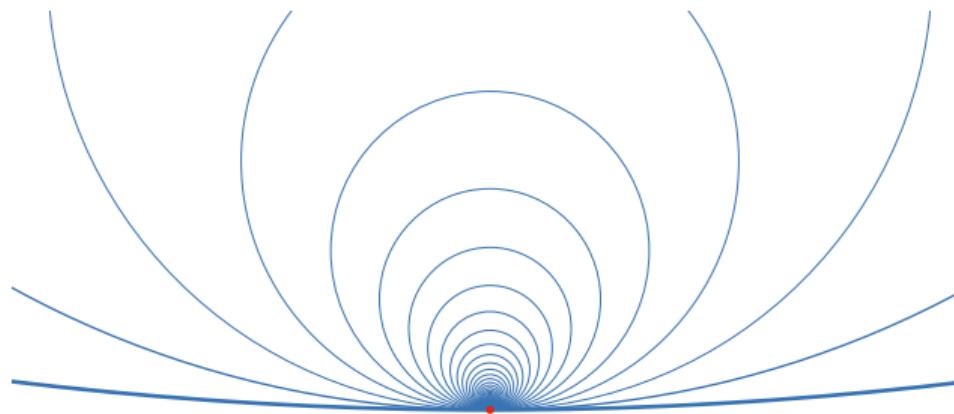
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# Q-tameness from local connectivity

Theorem (Morse, 1937; incorrect)

*If the sublevel set filtration off:  $X \rightarrow \mathbb{R}$  is compact and weakly locally connected, then it has  $q$ -tame persistent Vietoris homology.*



Theorem (B, Medina-Mardones, Schmahl 2021)

*If the sublevel set filtration off:  $X \rightarrow \mathbb{R}$  is compact and homologically locally connected, then it has  $q$ -tame persistent homology.*

# Simplification

# Topological simplification of functions

Consider the following problem:

## Problem (Topological simplification)

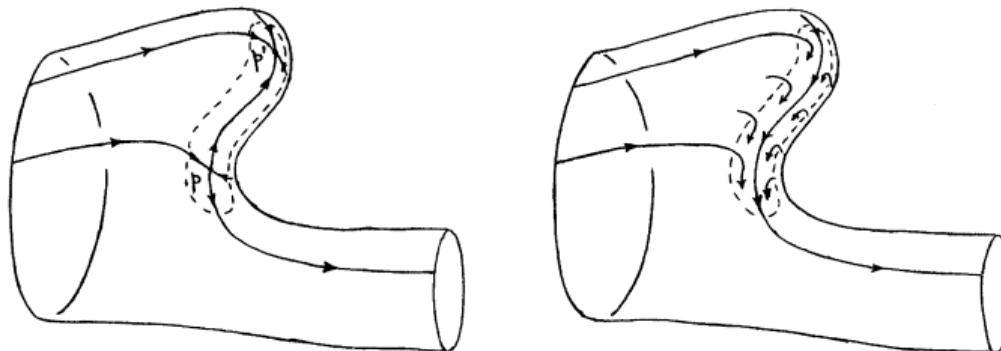
*Given a function  $f: X \rightarrow \mathbb{R}$  and a real number  $\delta \geq 0$ , find a function  $f_\delta$*

- *with the minimal number of critical points*
- *subject to  $\|f_\delta - f\|_\infty \leq \delta$ .*

# Persistence and Morse theory

Morse theory (smooth or discrete):

- Relates critical points to homology of sublevel sets
- Provides a method for *cancelling* pairs of critical points

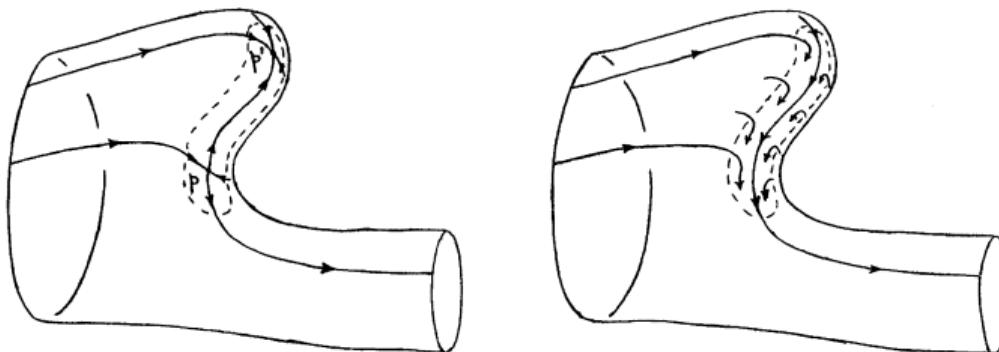


(from Milnor: *Lectures on the h-cobordism theorem*, 1965)

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Persistent homology of a Morse function:

- critical points correspond to endpoints of barcode intervals

## Canceling persistence pairs

By stability of persistence barcodes:

### Proposition

*The critical points of  $f$  with persistence  $> 2\delta$  provide a lower bound on the number of critical points of any function  $g$  with  $\|g - f\|_\infty \leq \delta$ .*

## Canceling persistence pairs

By stability of persistence barcodes:

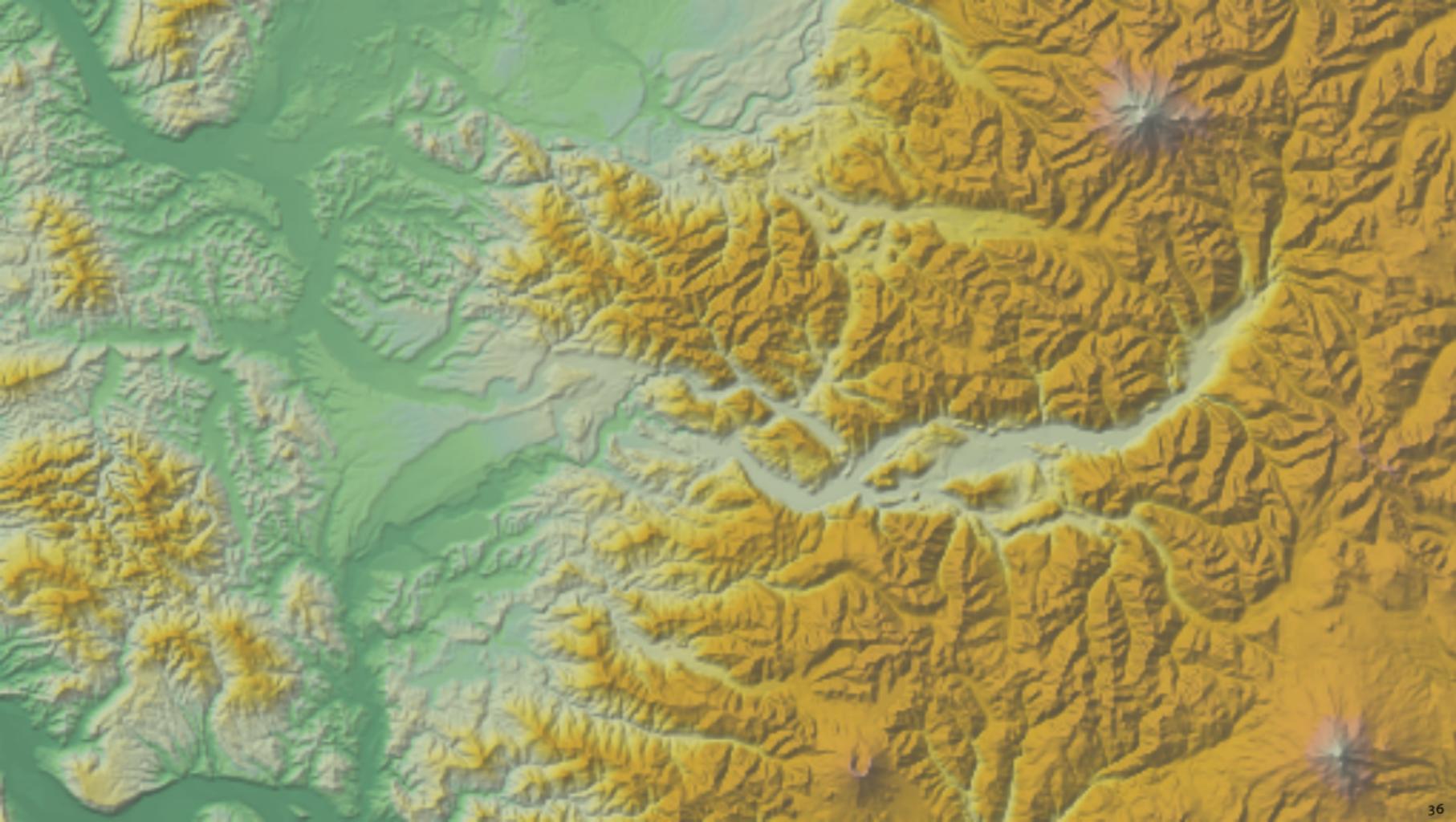
### Proposition

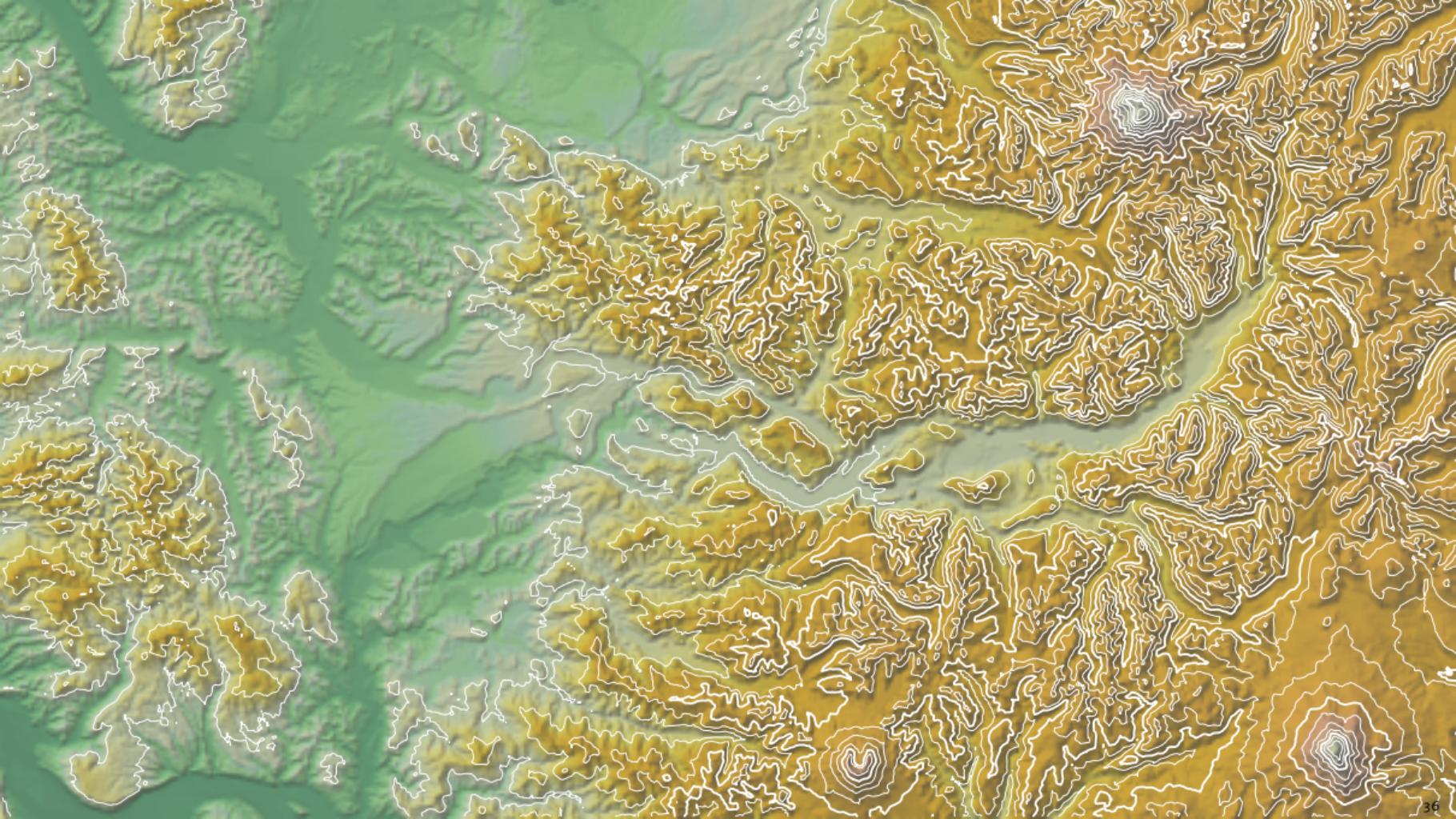
*The critical points of  $f$  with persistence  $> 2\delta$  provide a lower bound on the number of critical points of any function  $g$  with  $\|g - f\|_\infty \leq \delta$ .*

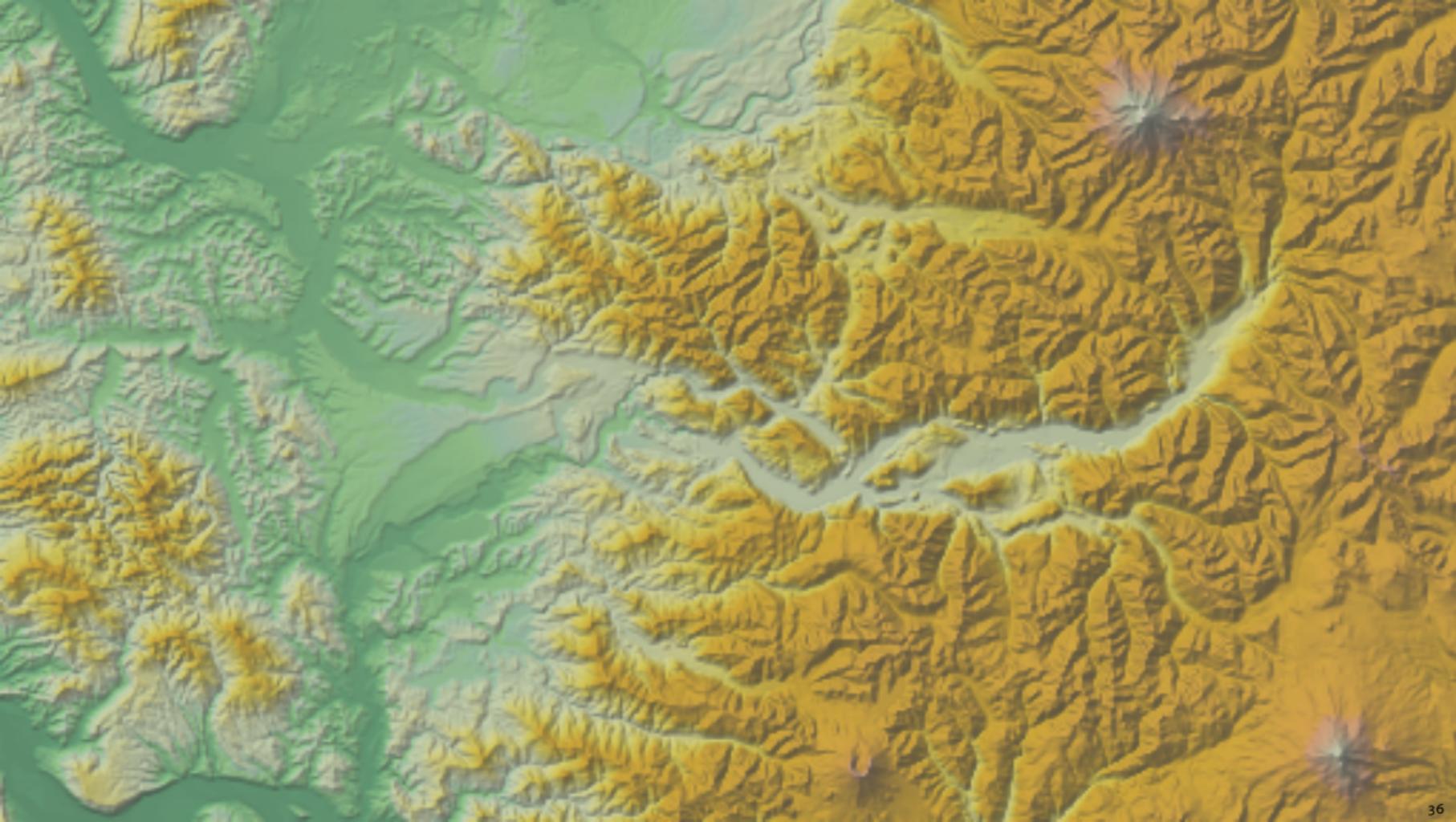
### Theorem (B, Lange, Wardetzky, 2011)

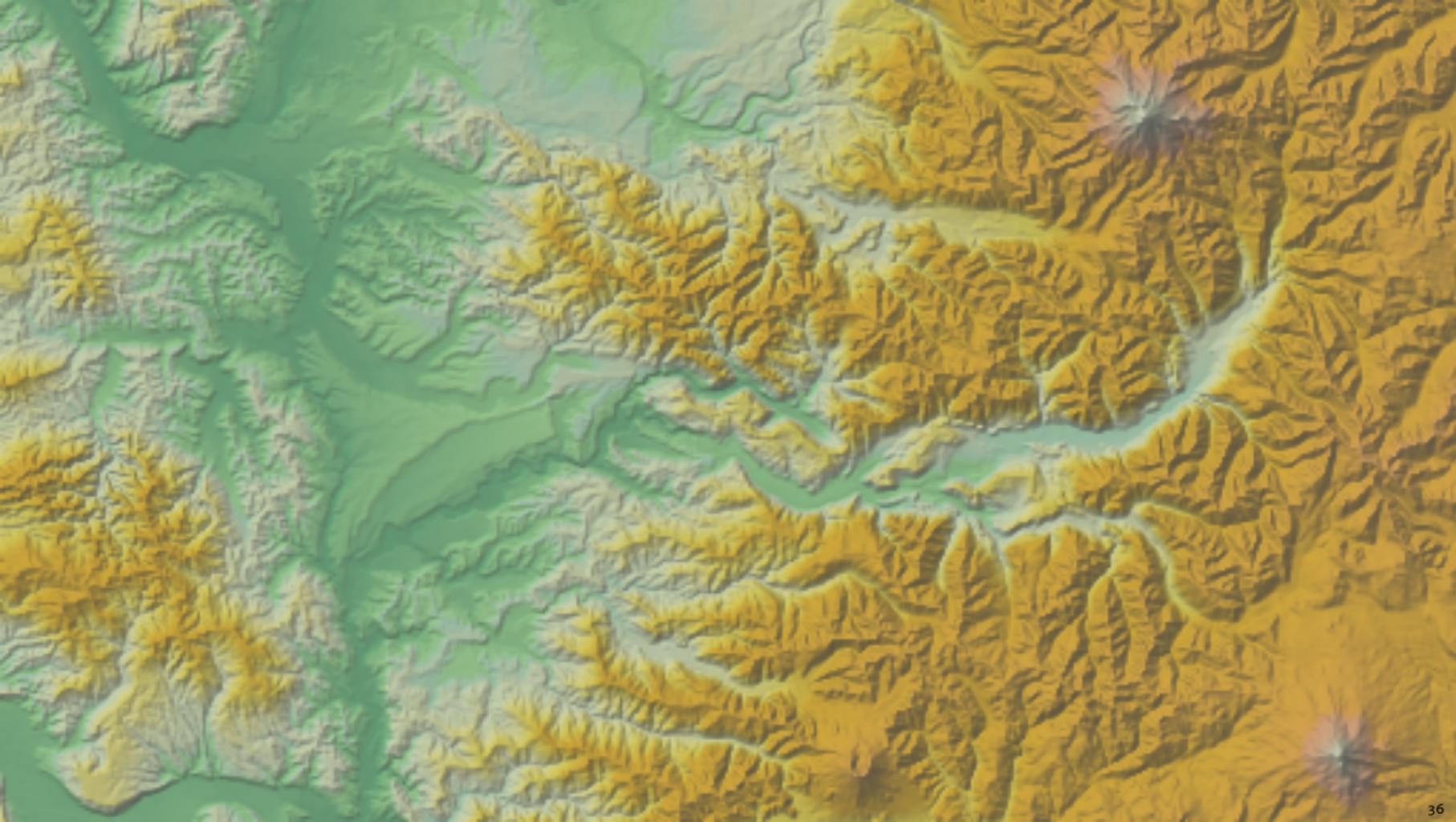
*This lower bound can be achieved for a function on a surface*

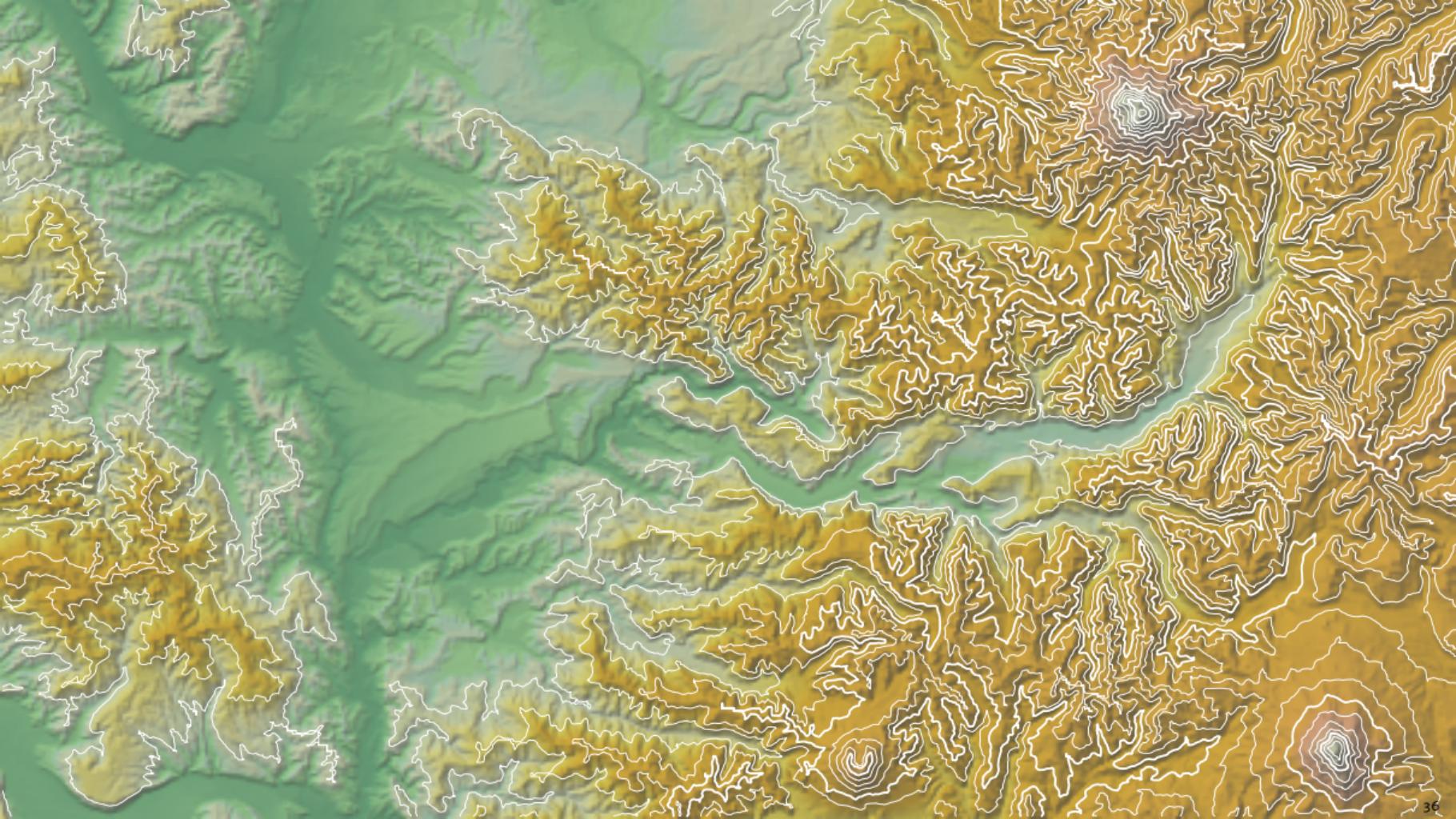
- *by canceling all critical points with persistence  $\leq 2\delta$ .*

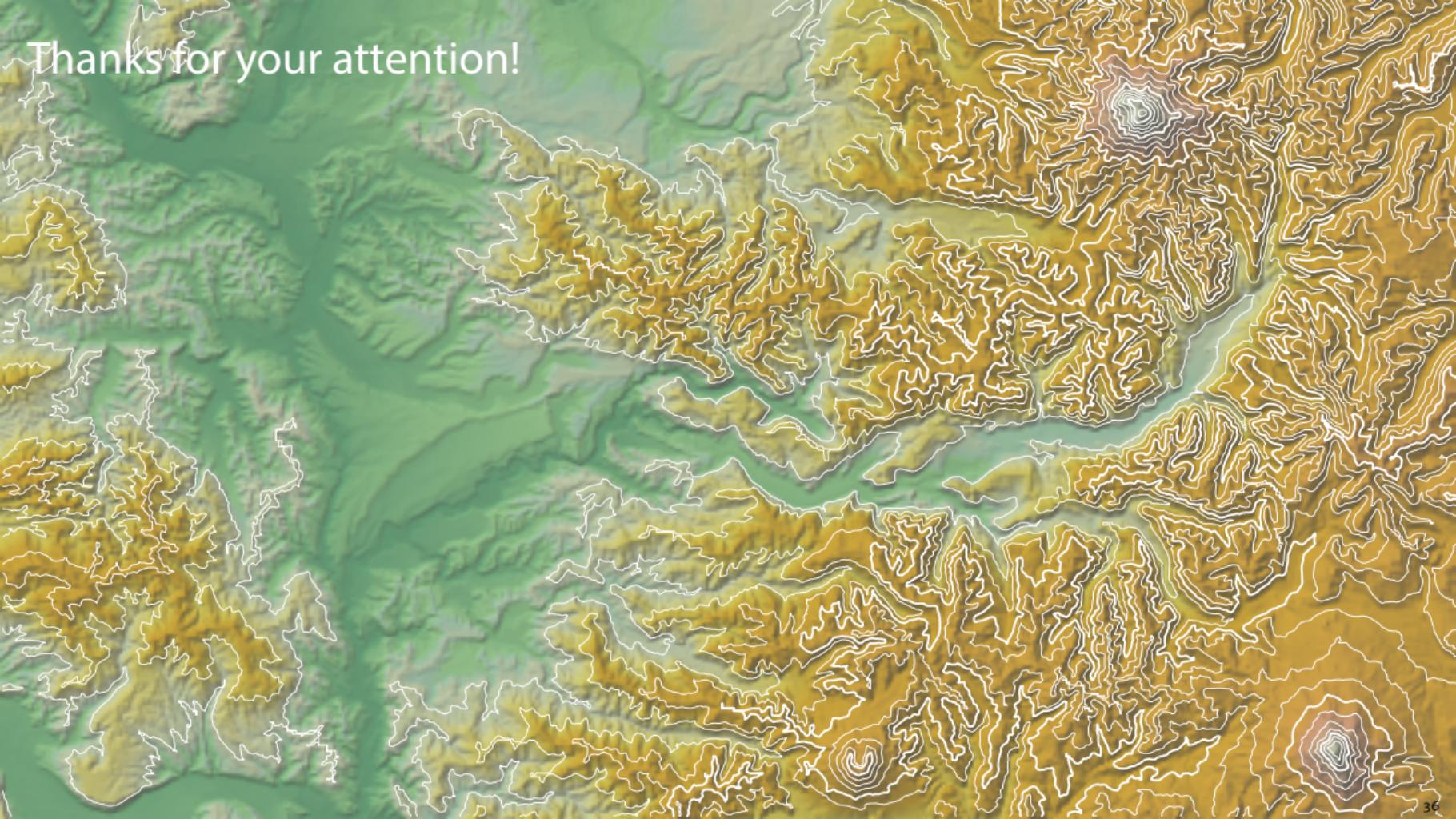












Thanks for your attention!