

Topological Data Analysis: An Introduction to Persistent Homology

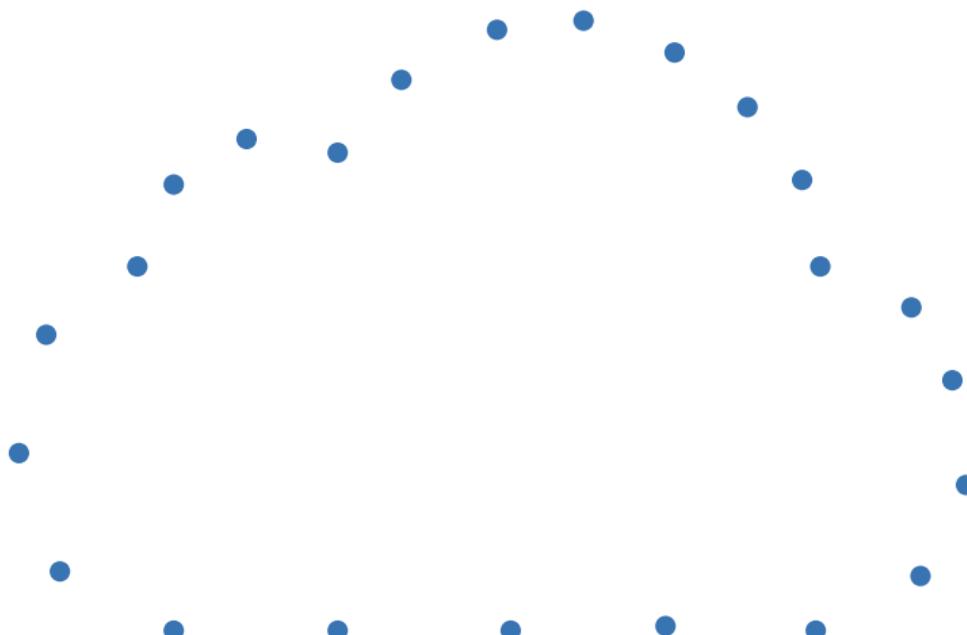
Part 2: complexes and computation

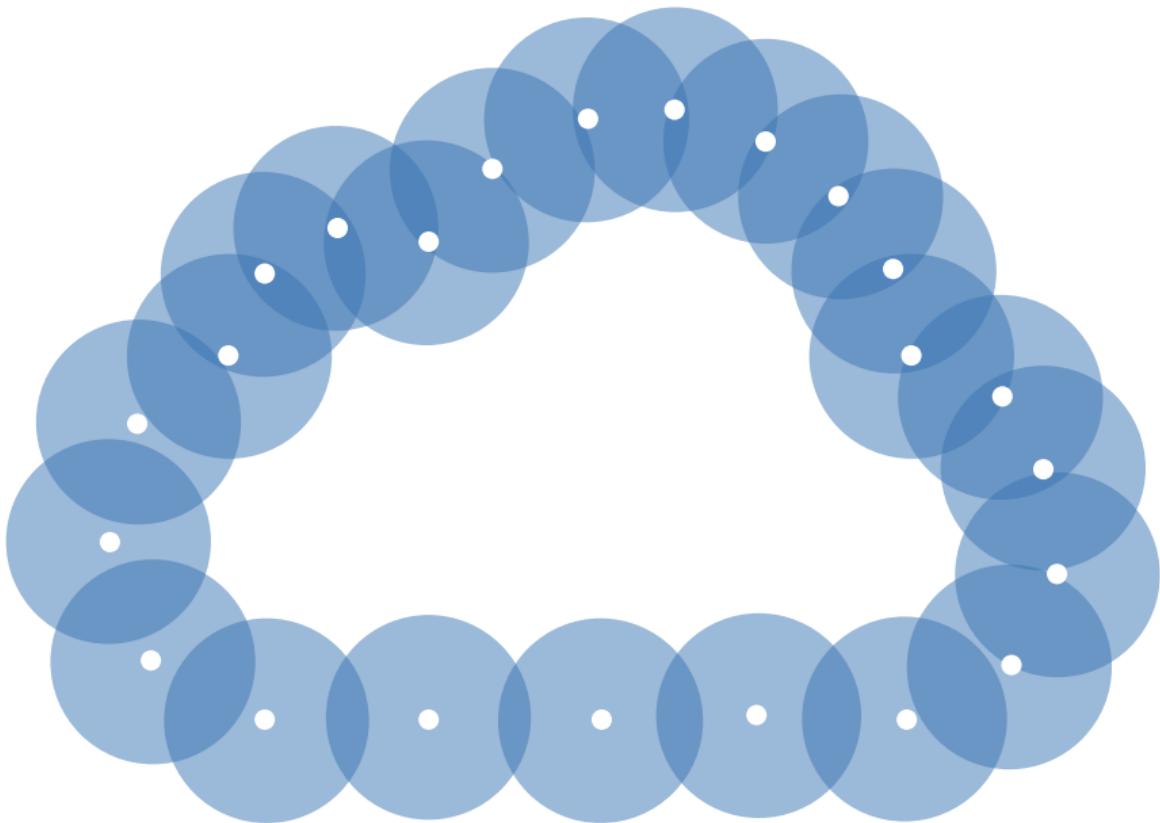
Ulrich Bauer

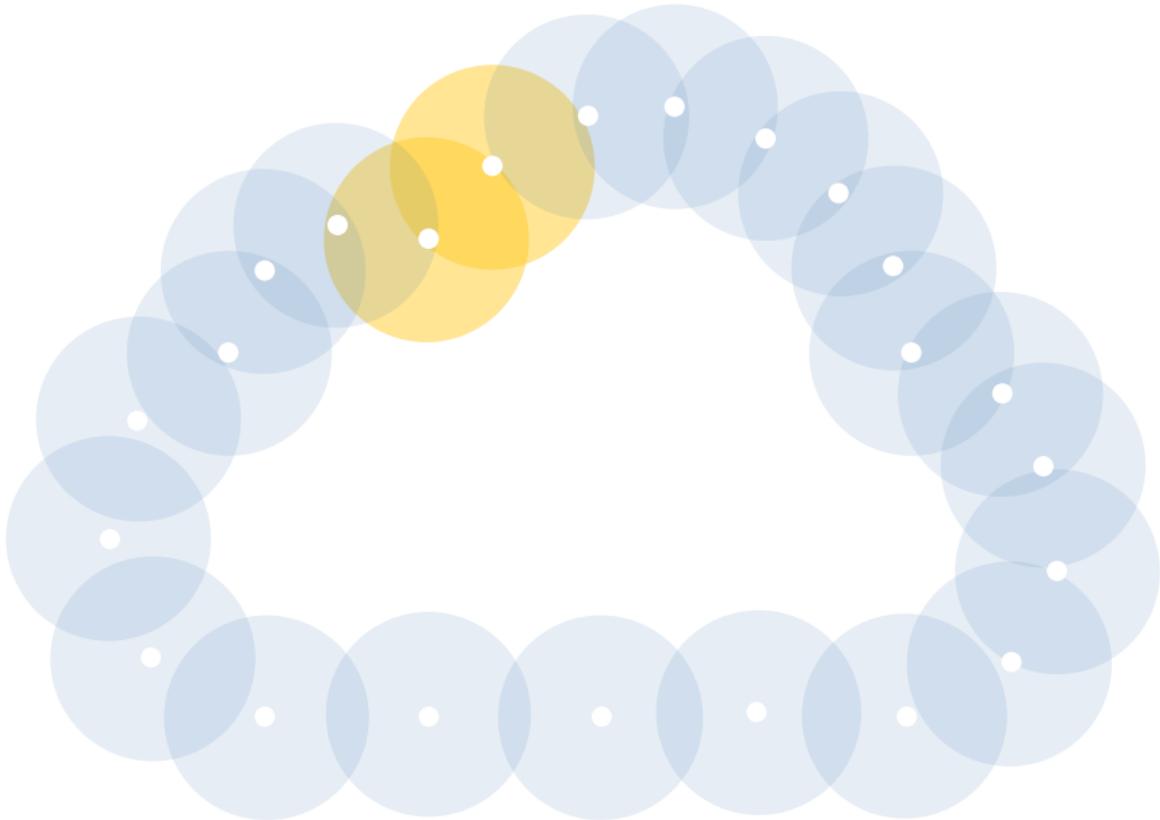


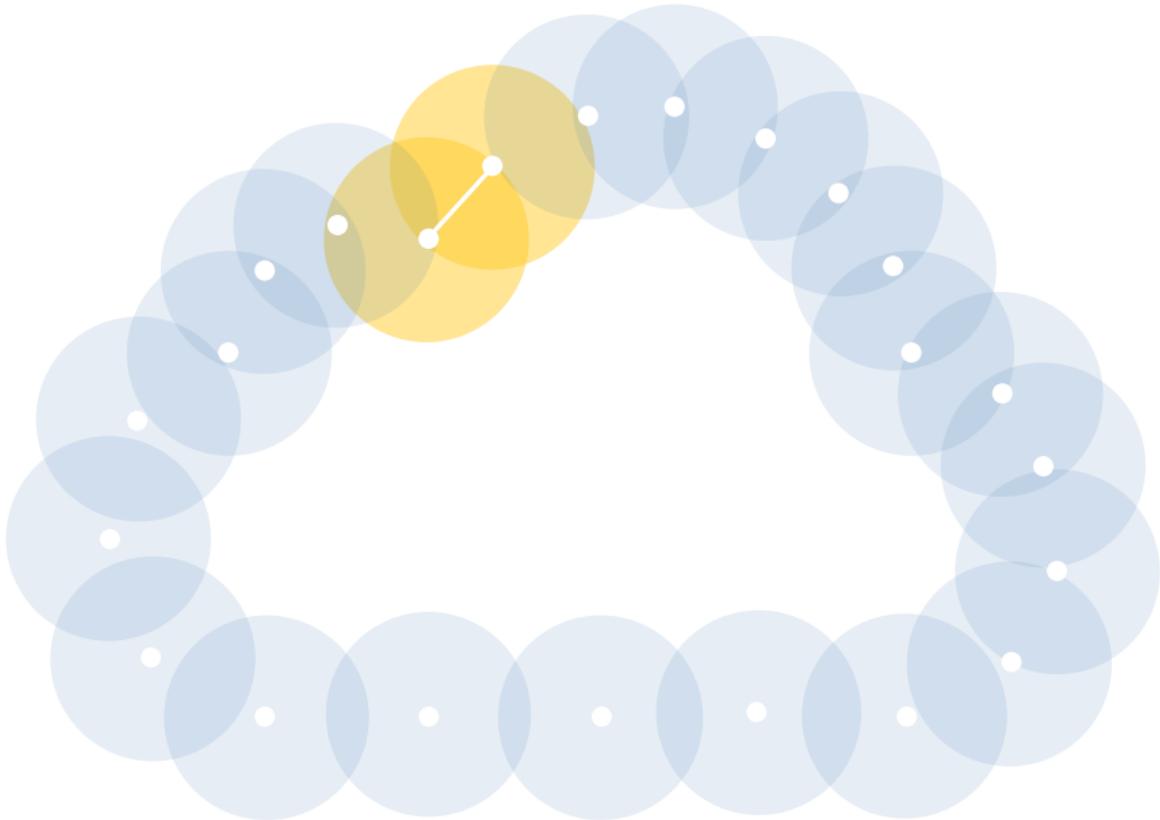
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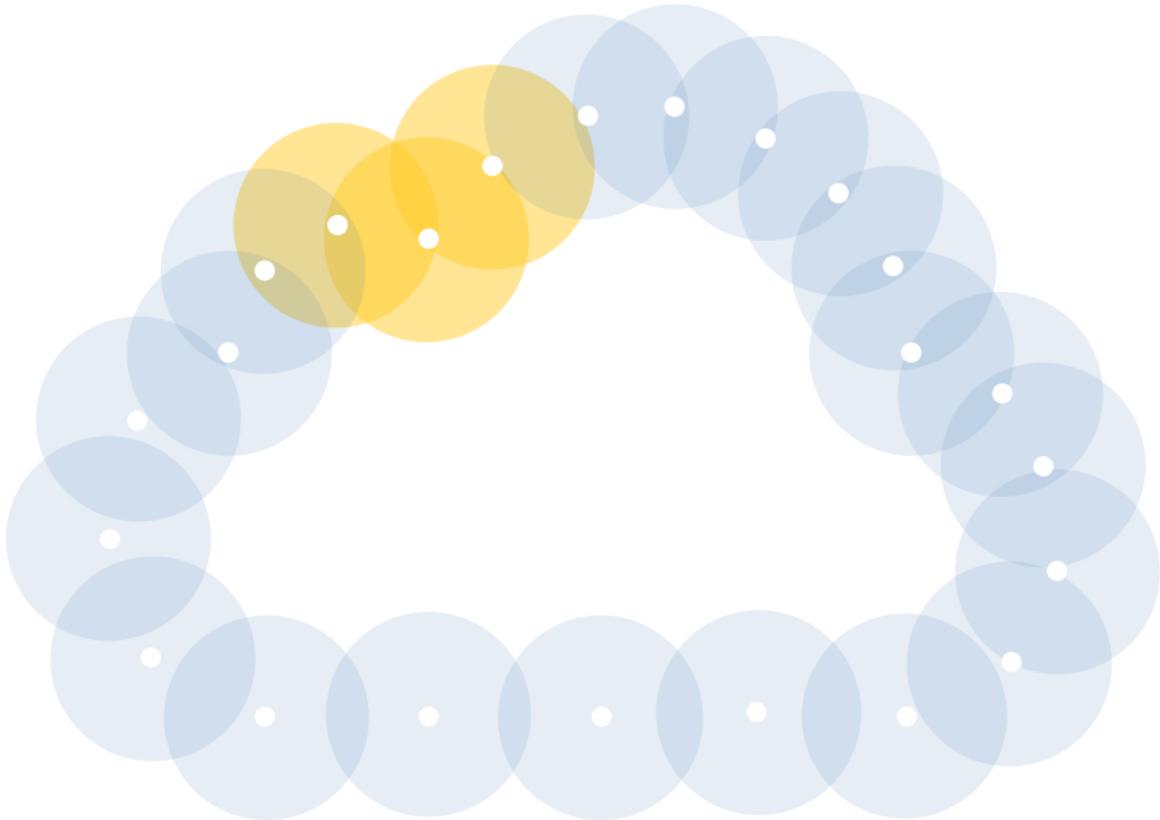
Machine learning summer school 2019
Skoltech, Moscow

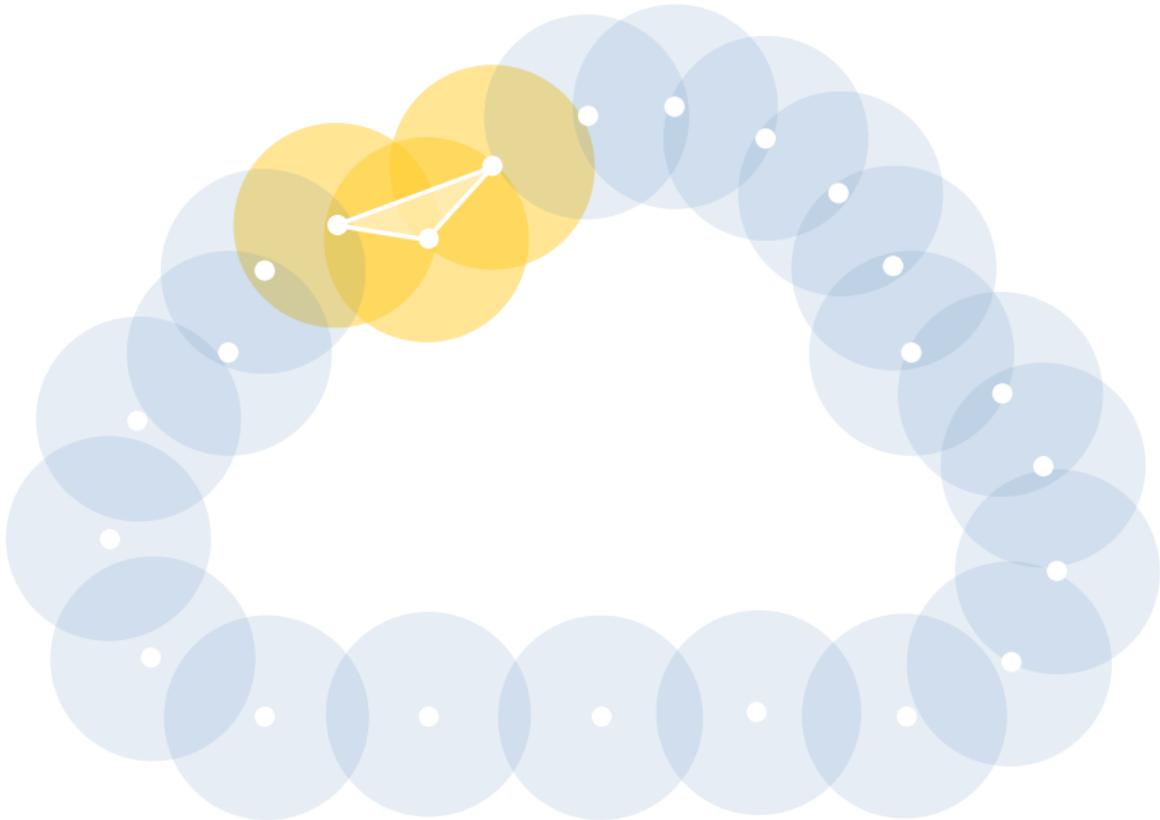


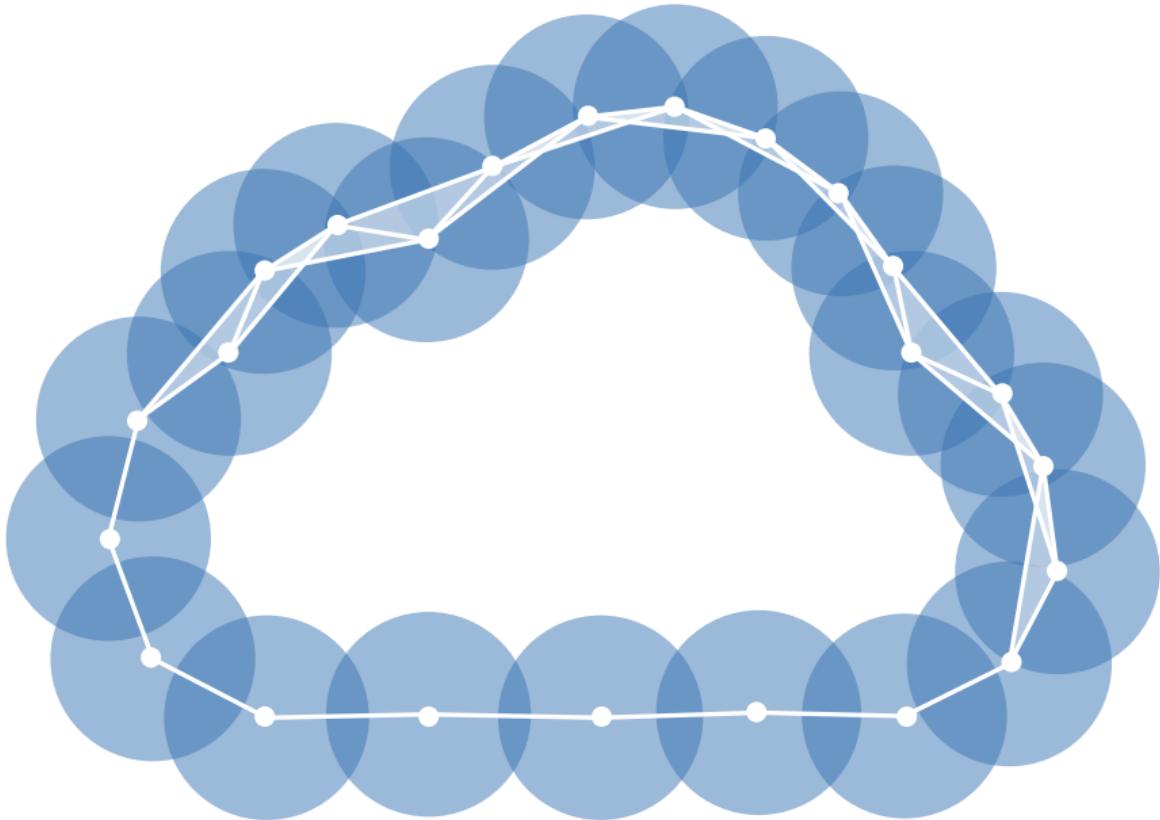


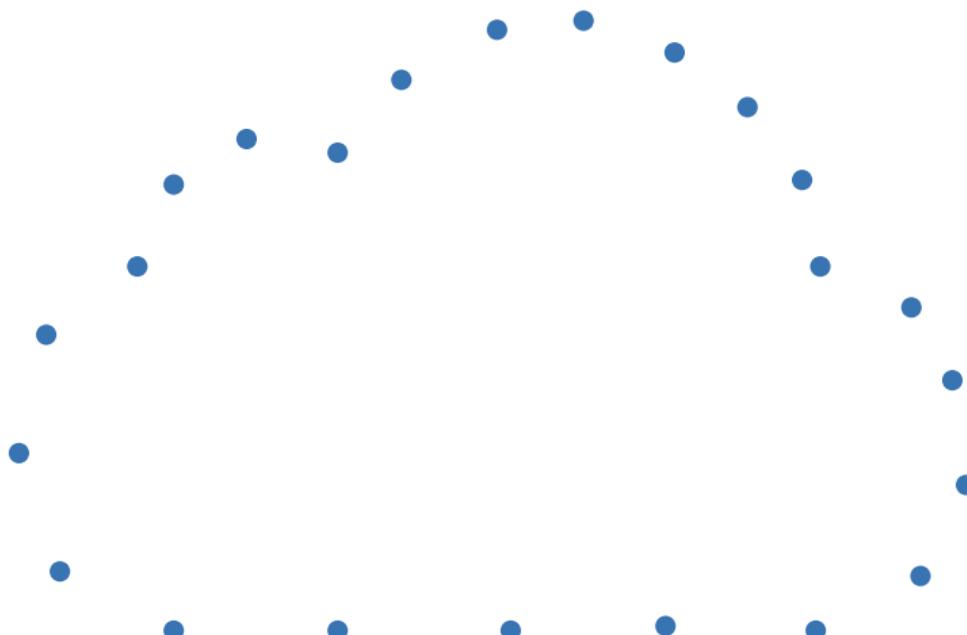


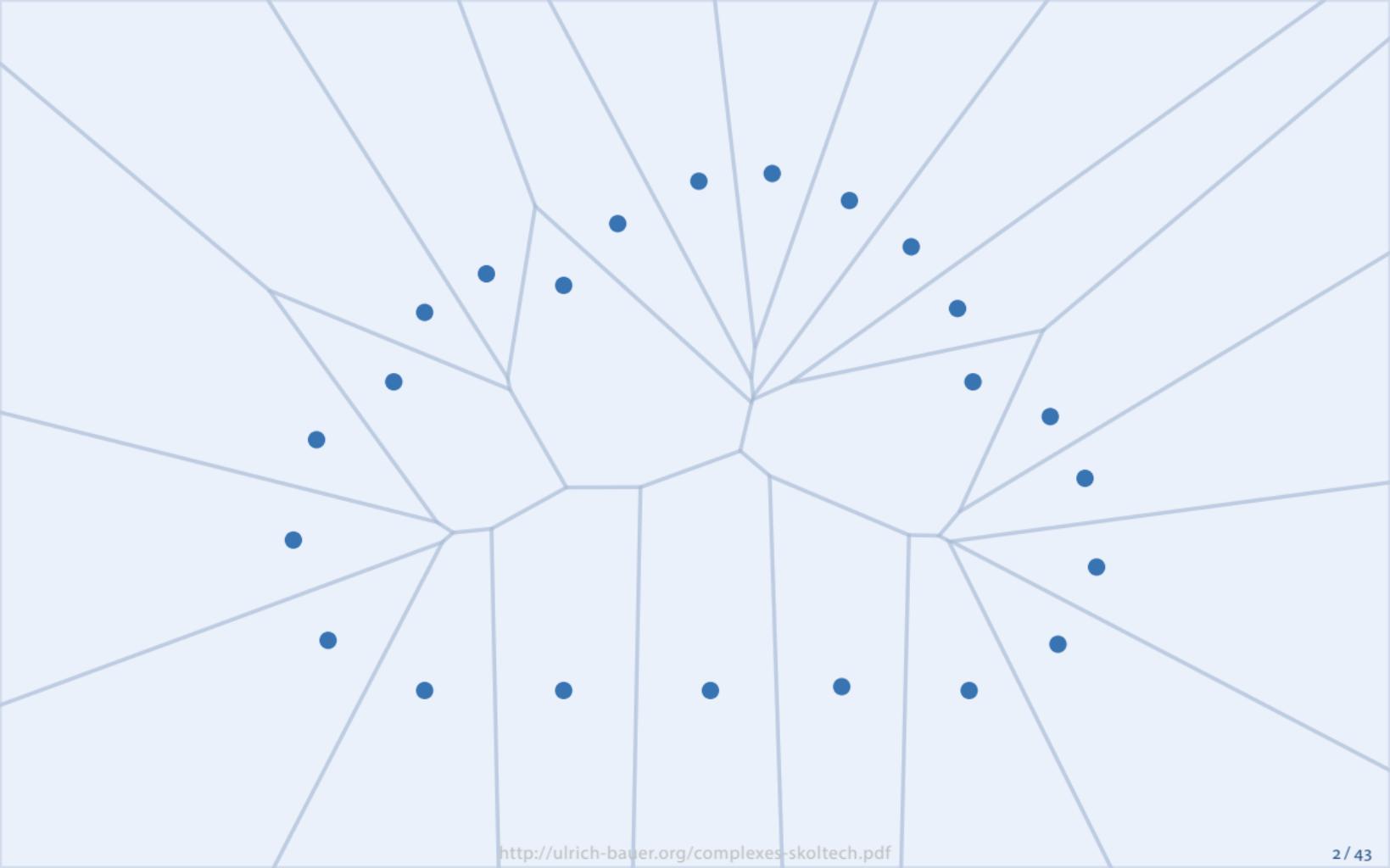


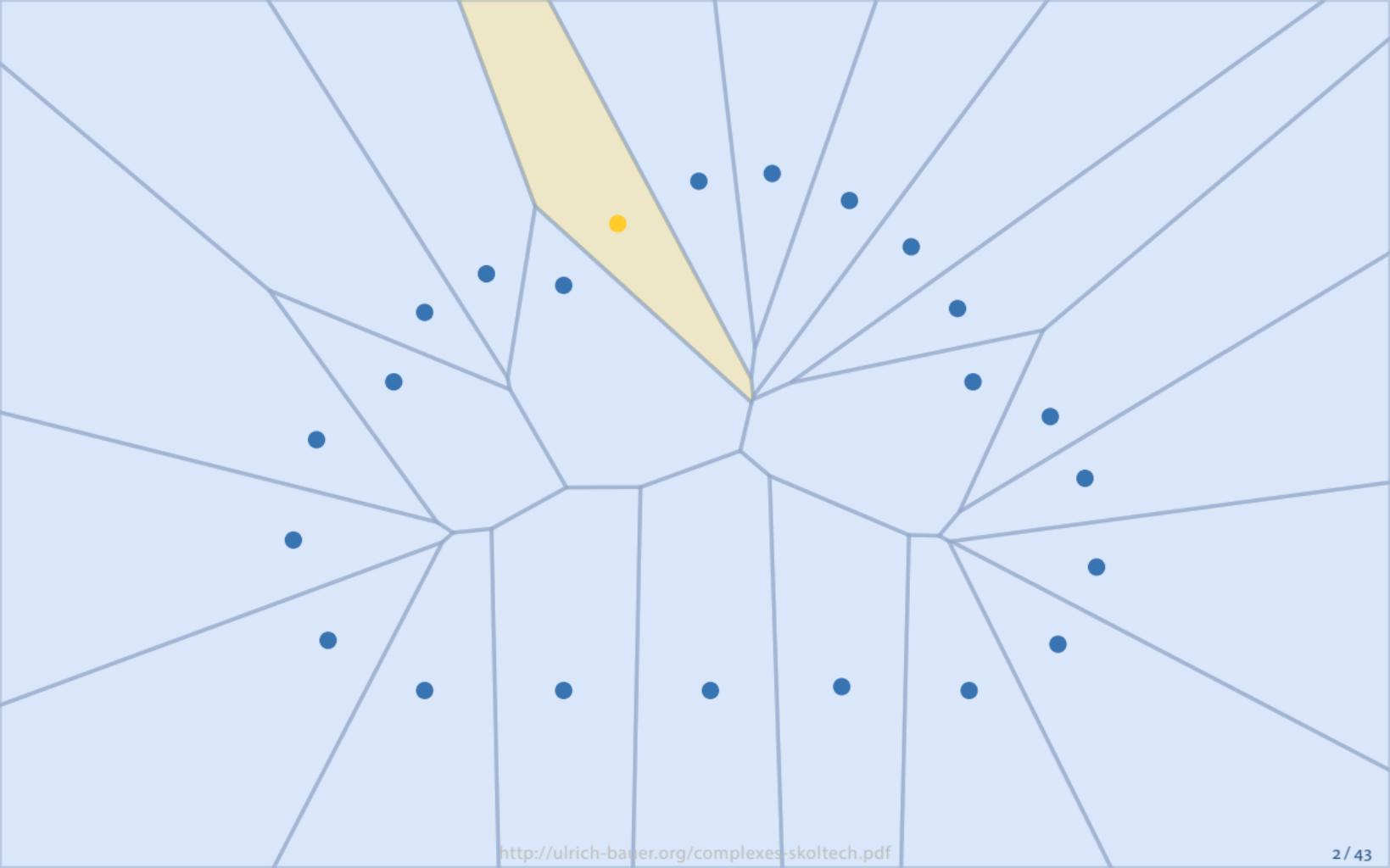


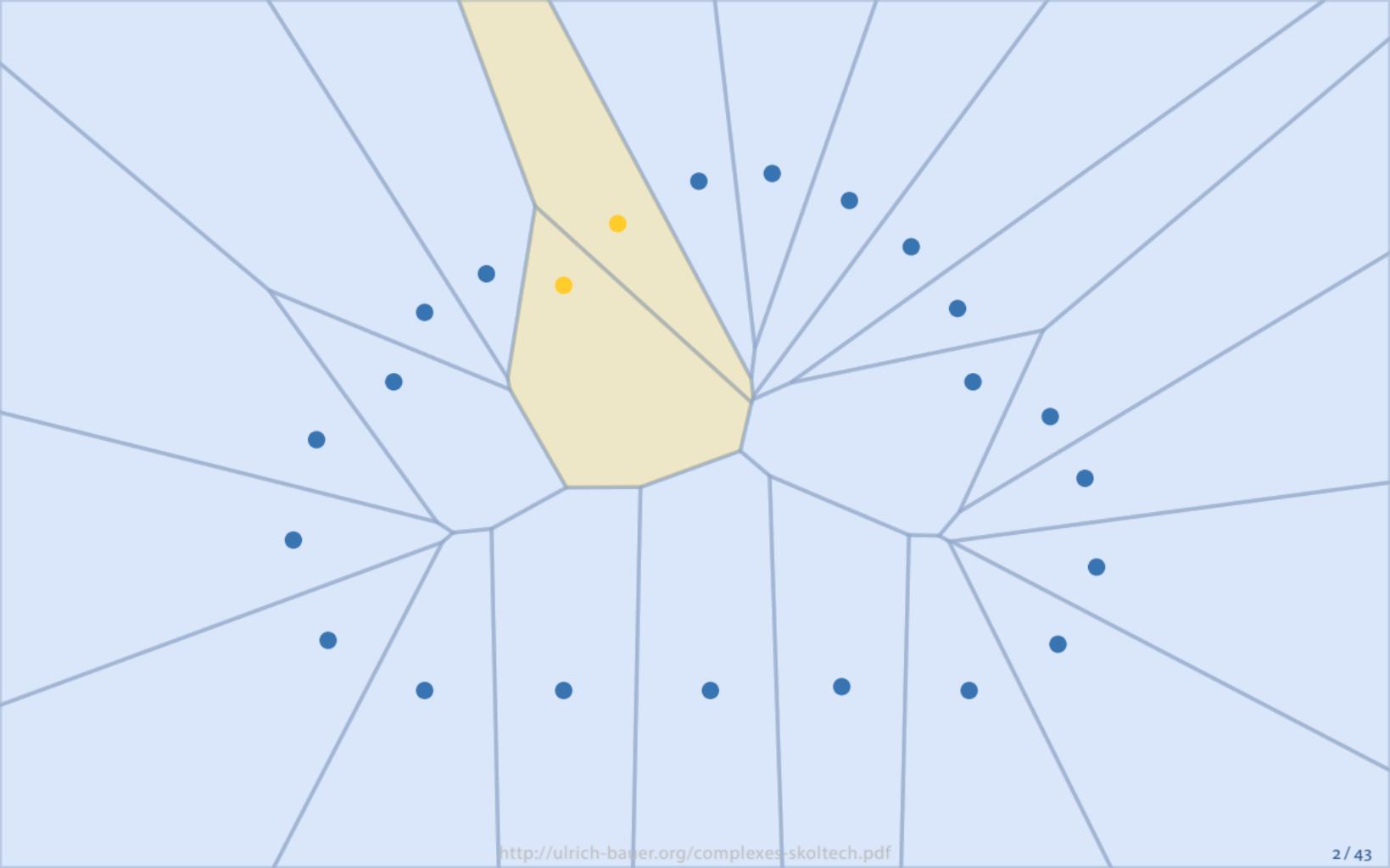


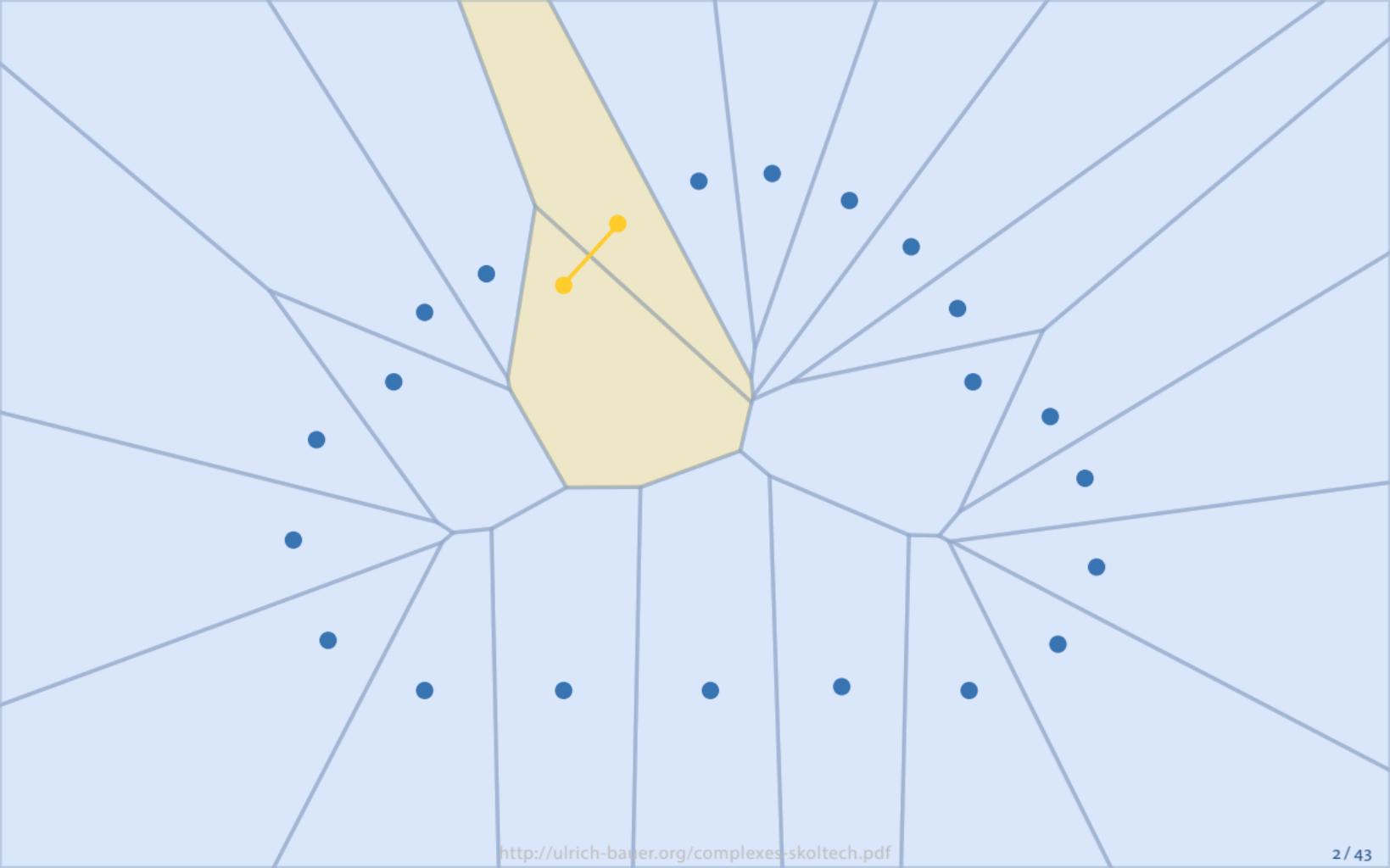


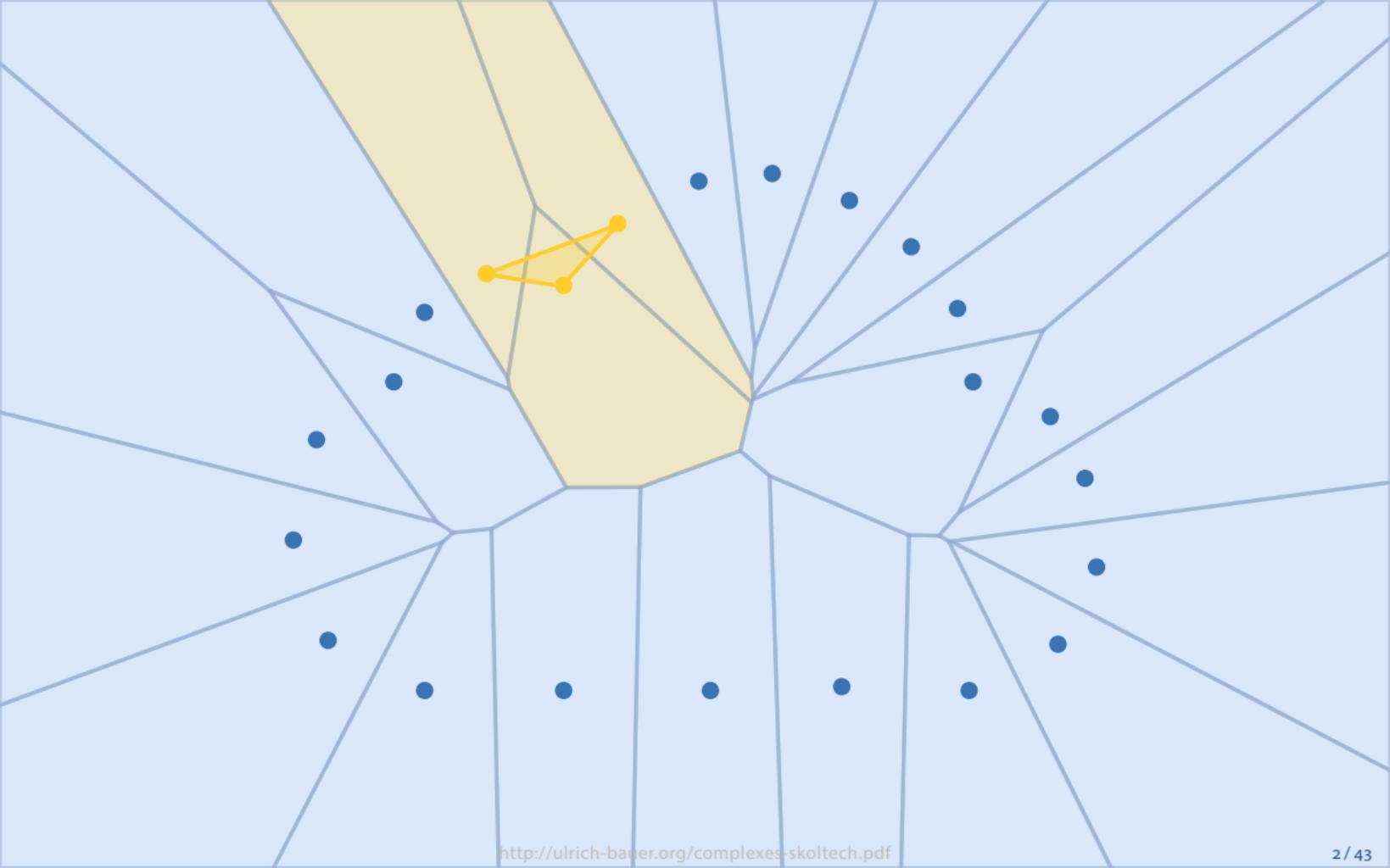


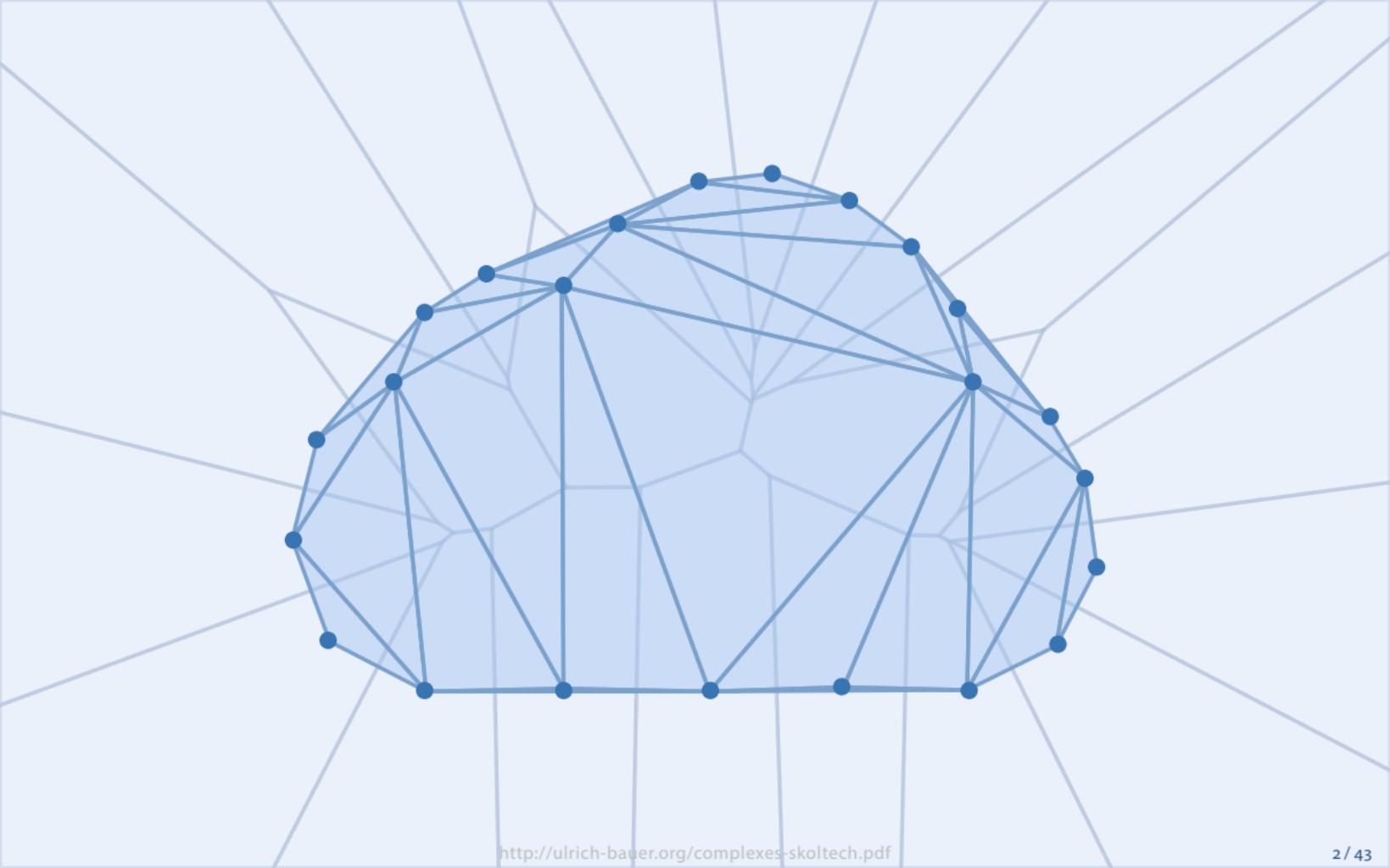


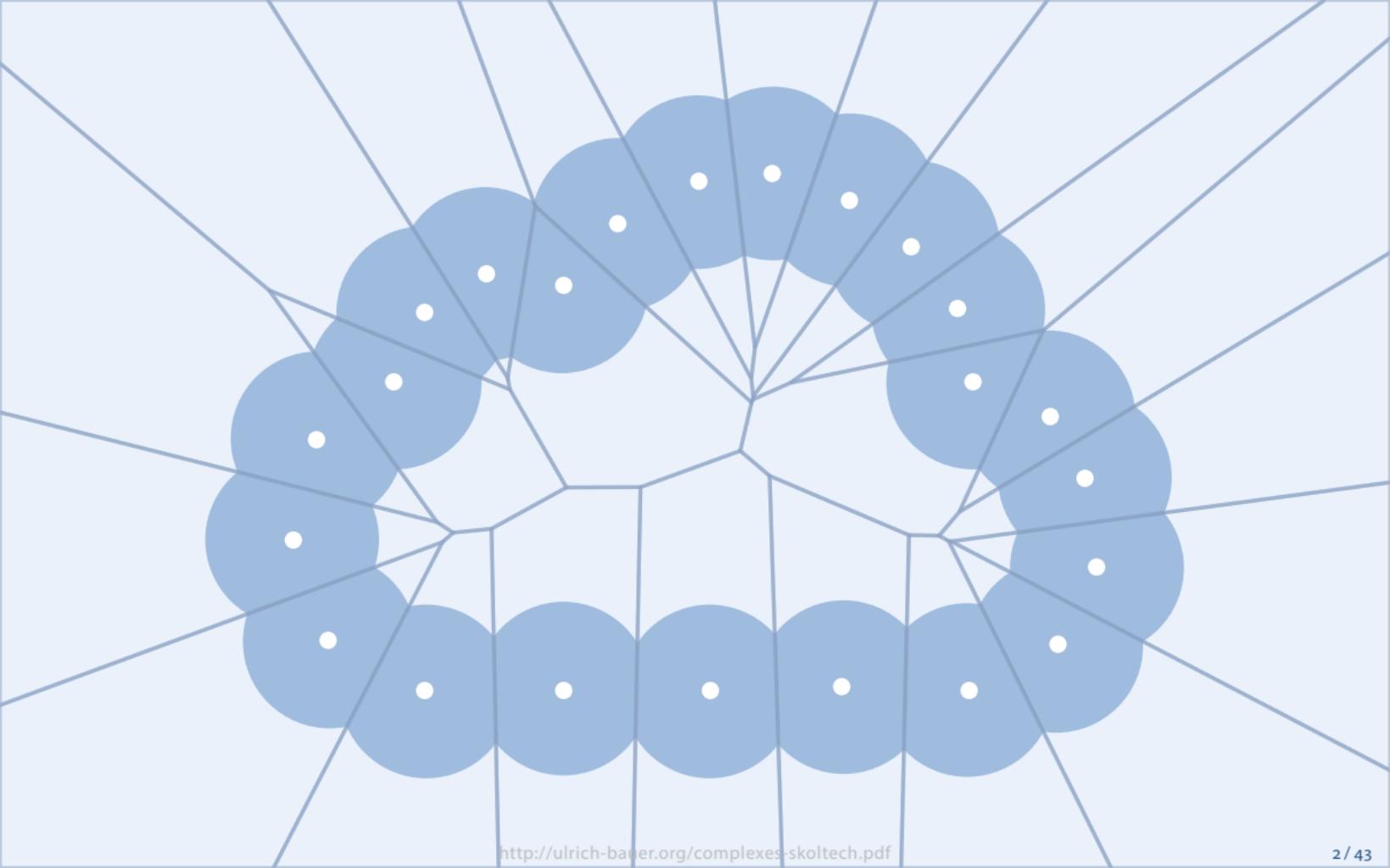


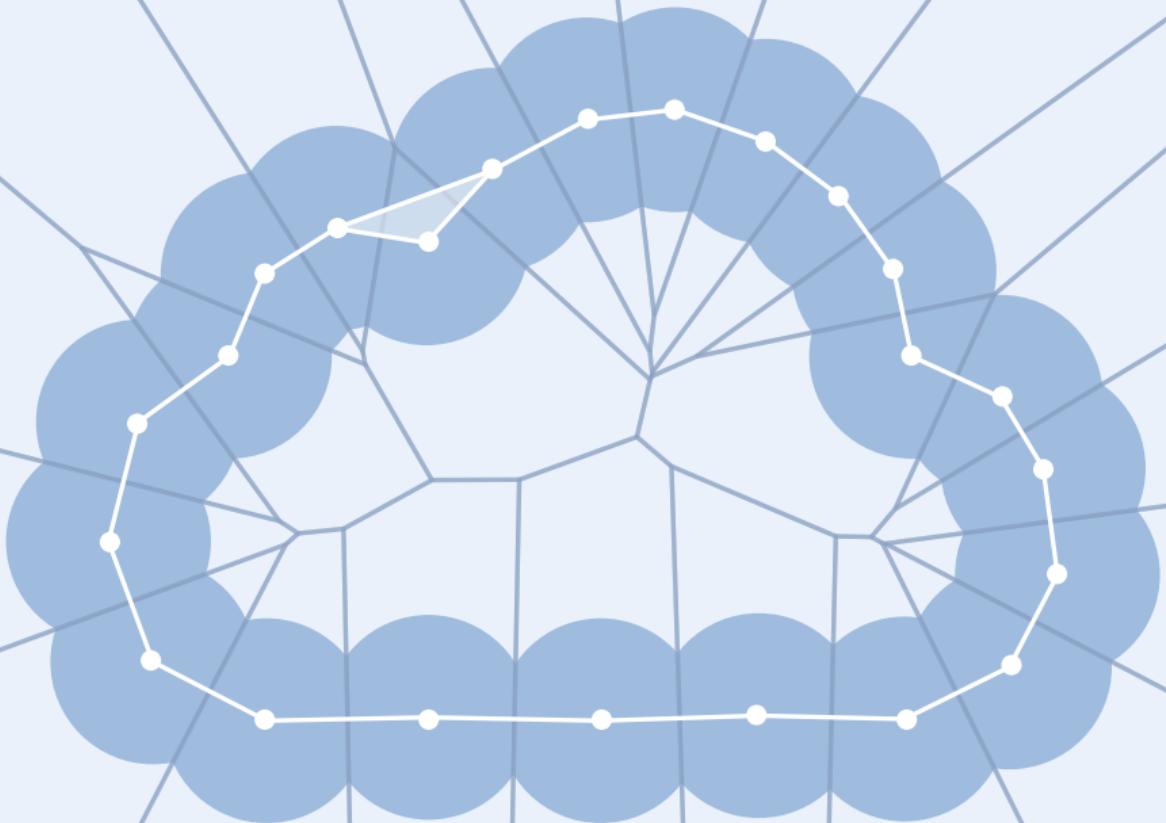


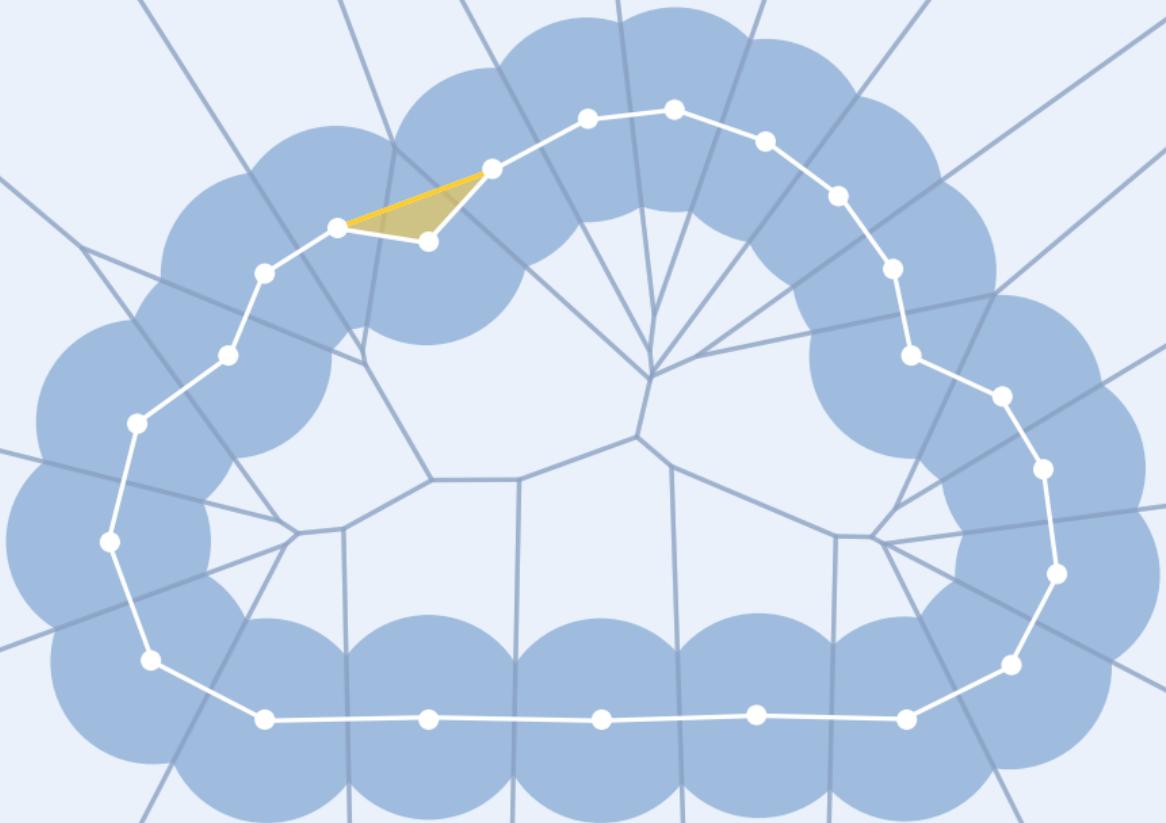


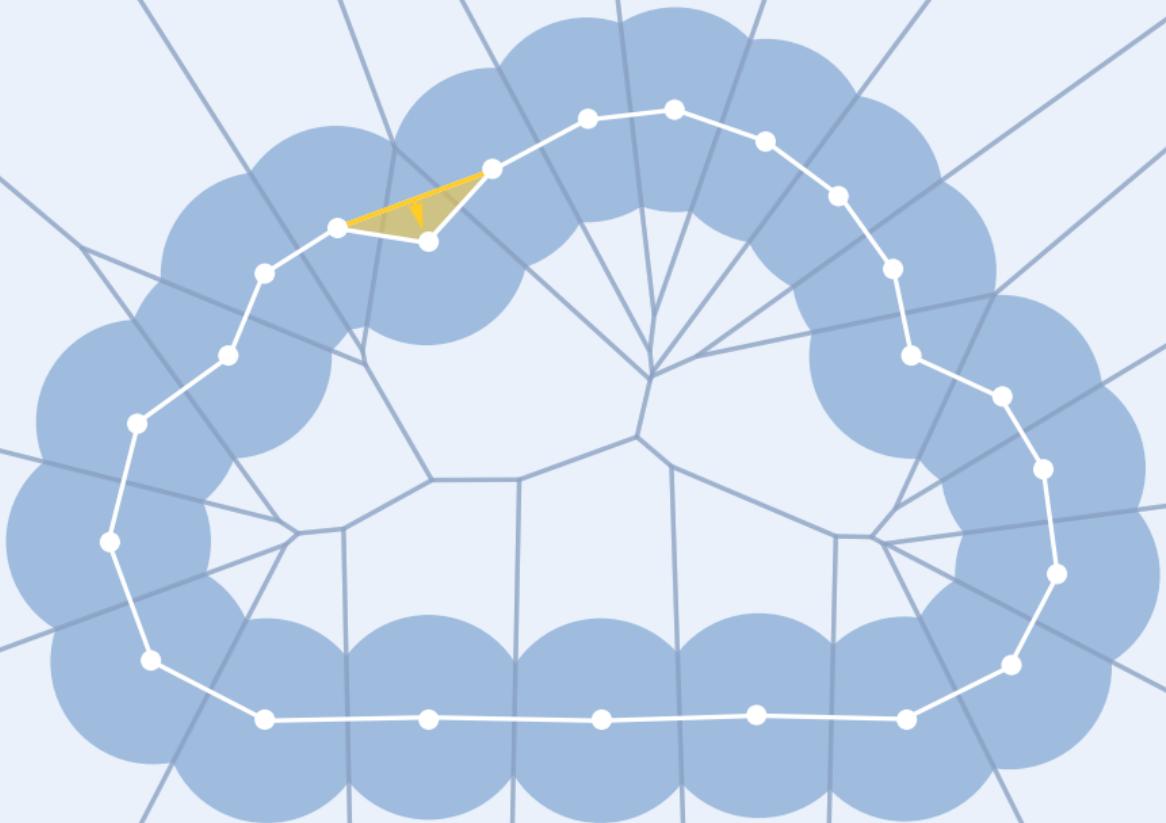


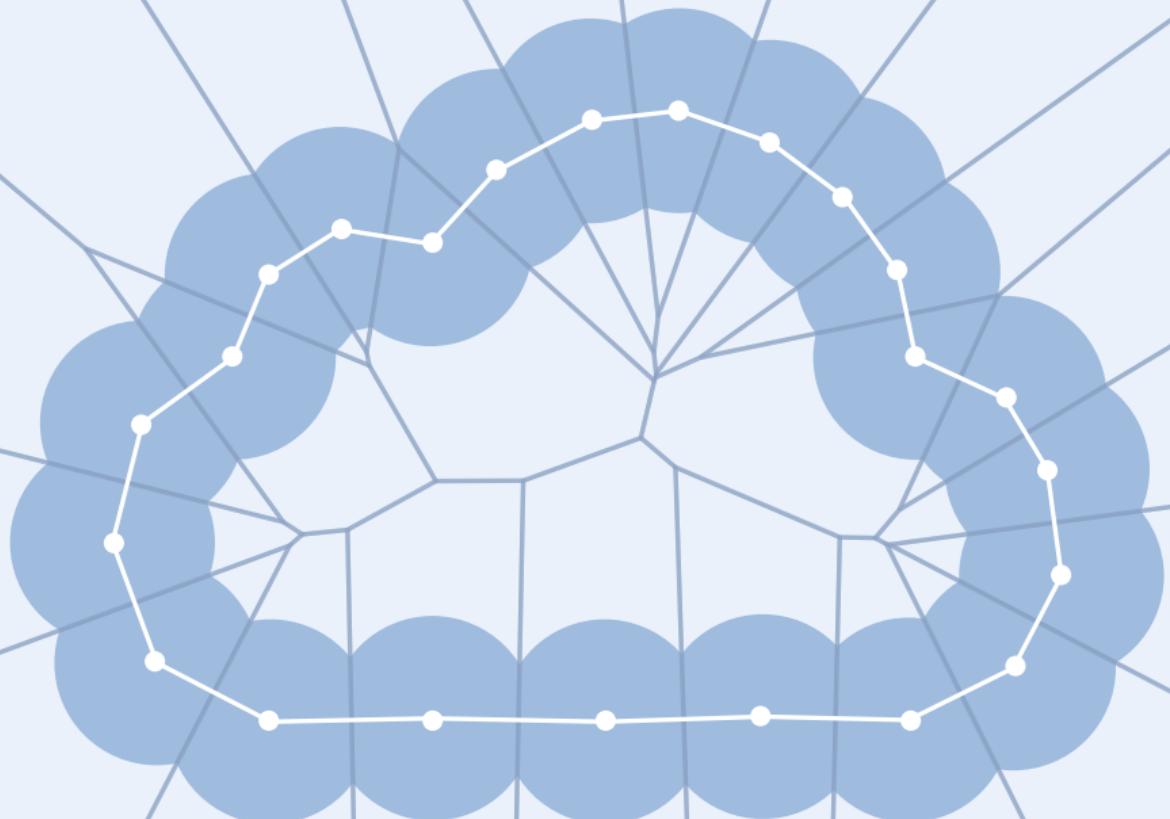


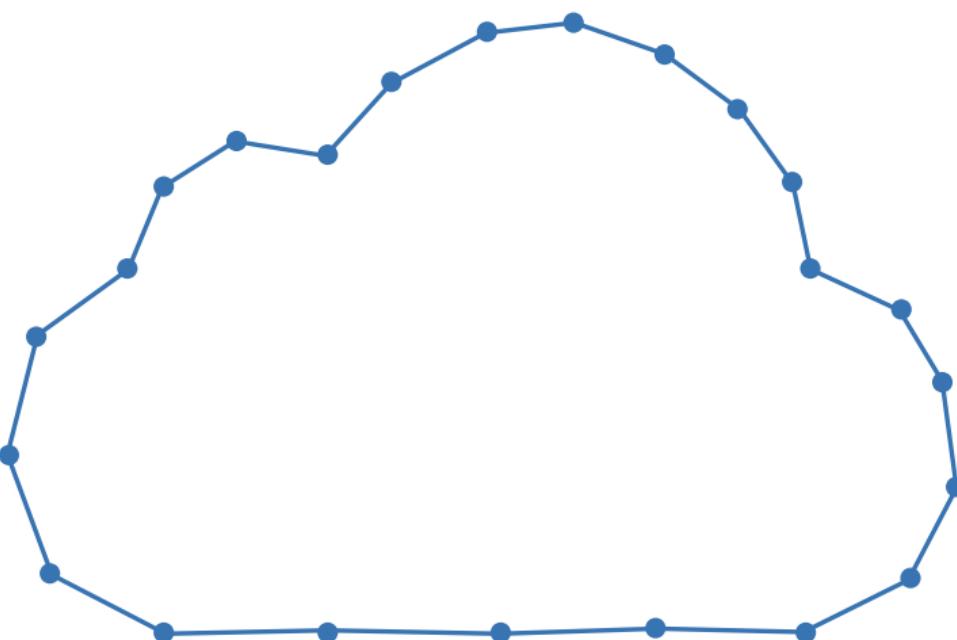












Connecting Čech and Delaunay complexes

By the *Nerve theorem* (Borsuk 1947):

$$\text{Del}_r(X) \simeq \text{Cech}_r(X) \simeq B_r(X).$$

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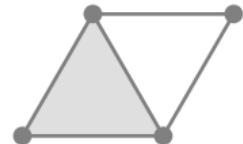
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- Are all three complexes homotopy equivalent?
- Are they related by a sequence of *simplicial collapses*?

Simplicial collapses

Definition (Whitehead 1938)

Let K be a simplicial complex.

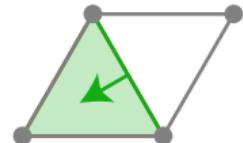


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If there is a sequence of such elementary collapses from K to M , we say that K *collapses* to M (written $K \searrow M$).

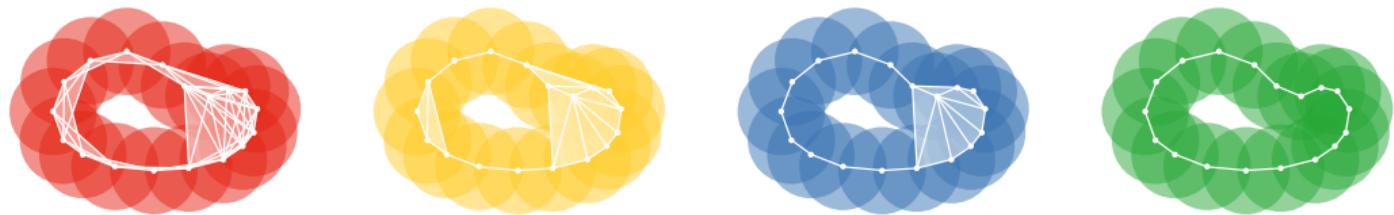


Main result: a sequence of collapses

Theorem (B, Edelsbrunner 2017)

Čech, Delaunay–Čech, Delaunay, and Wrap complexes are homotopy equivalent through a sequence of collapses

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

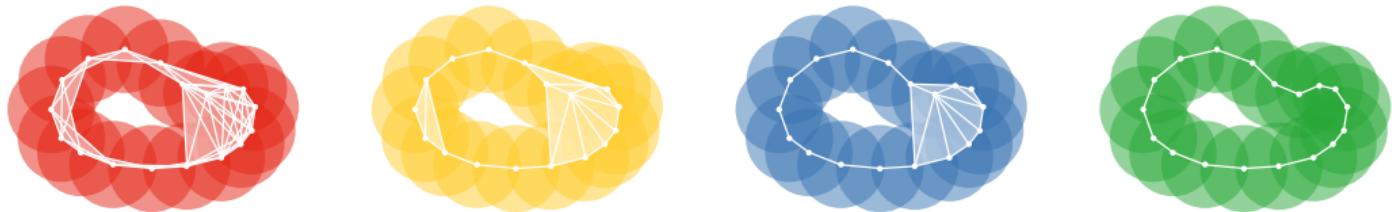


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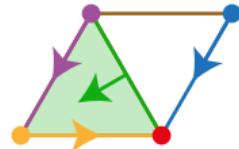
- Extends to weighted Delaunay triangulations
- All collapses are induced by a single *discrete gradient field*
- This yields explicit isomorphisms in persistent homology

Discrete Morse theory

Definition (Forman 1998)

A *discrete vector field* on a simplicial complex is a partition of the simplices into singletons and pairs $\{L, U\}$, with L a facet of U .

- indicated by an arrow from L to U

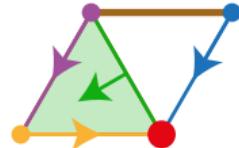


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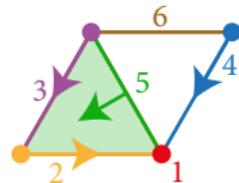
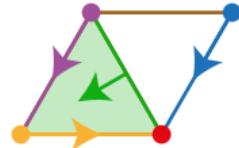
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A function $f : K \rightarrow \mathbb{R}$ on a simplicial complex is a *discrete Morse function* if for all $t \in \mathbb{R}$:

- sublevel sets $K_t = f^{-1}(-\infty, t]$ are subcomplexes



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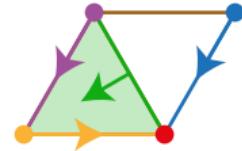
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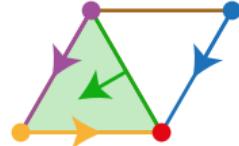
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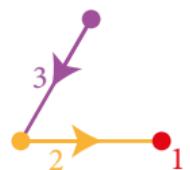
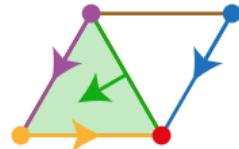
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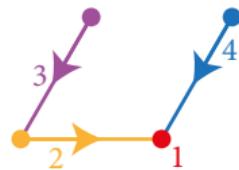
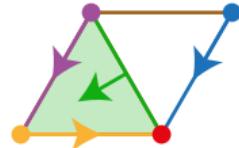
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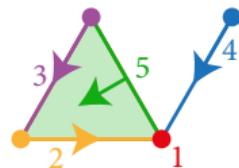
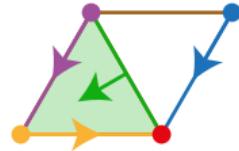
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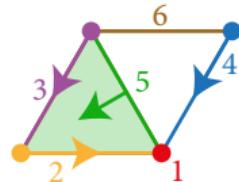
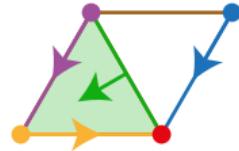
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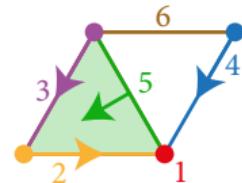
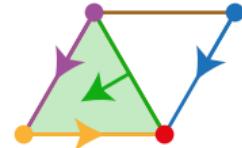
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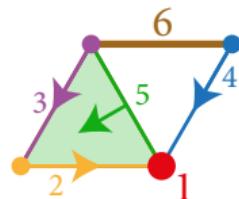
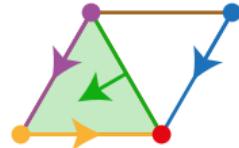
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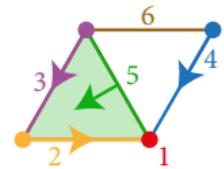
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If $f^{-1}(t) = \{Q\}$ then t is a *critical value*.



Collapses from Morse functions and gradients

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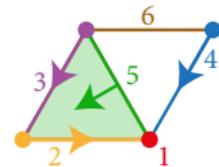


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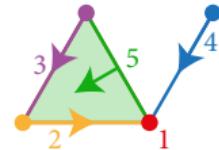


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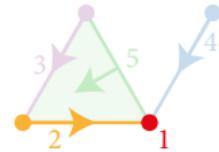


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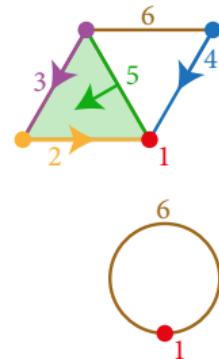
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K is homotopy-equivalent to a CW complex
with one d -cell for each critical d -simplex.



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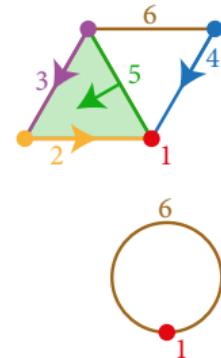
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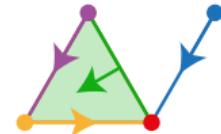


Let V be a discrete gradient field on a simplicial complex K , and let L be a subcomplex of K .

Corollary

If $K \setminus L$ is a union of pairs of V , then $K \searrow L$.

We say that V induces the collapse $K \searrow L$.



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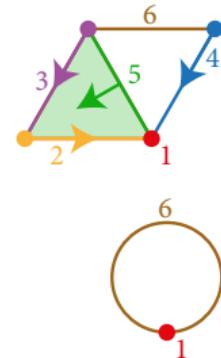
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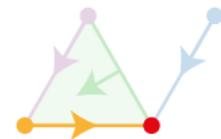


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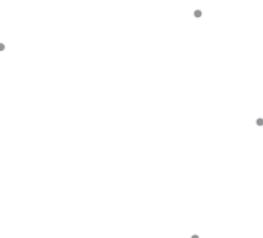
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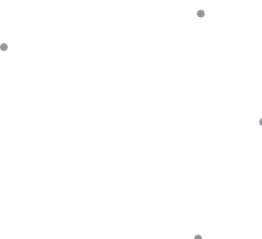
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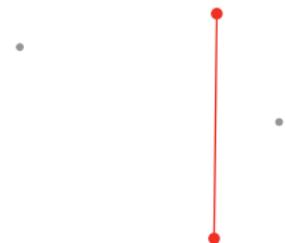
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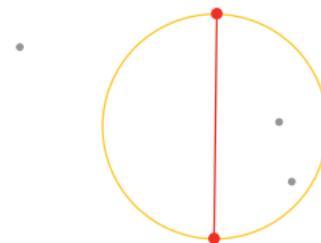
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Two radius functions:

- Čech radius function $f_{\text{Čech}}(Q)$:
radius of smallest enclosing sphere of Q



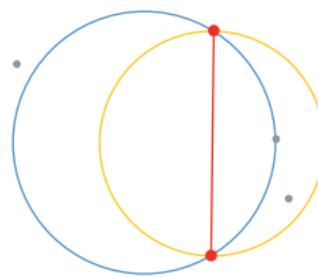
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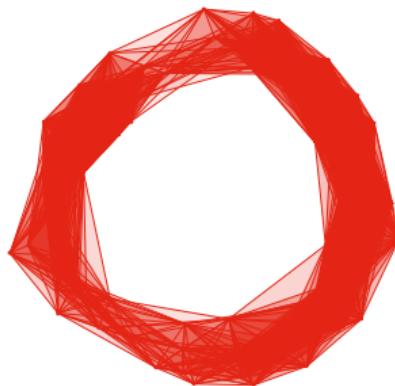
- *$\check{\text{C}}\text{ech radius function}$* $f_{\text{Cech}}(Q)$:
radius of *smallest enclosing sphere* of Q
- *$\text{Delaunay radius function}$* $f_{\text{Del}}(Q)$:
radius of *smallest empty circumsphere*
 - defined only on $\text{Del}(X)$



Čech and Delaunay complexes from functions

For any radius r :

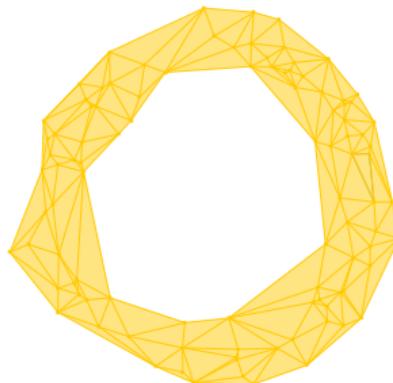
- $\text{Cech}_r(X) = f_{\text{Cech}}^{-1}(-\infty, r]$
 - simplices with smallest enclosing radius $\leq r$



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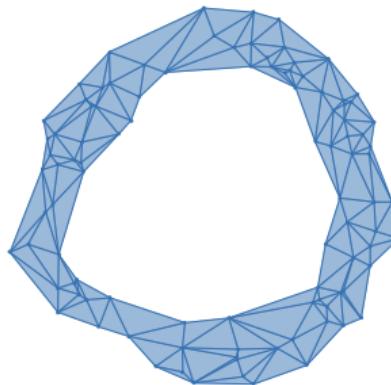
- $\text{Cech}_r(X) = f_{\text{Cech}}^{-1}(-\infty, r]$
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- $\text{DelCech}_r(X) = \text{Del}(X) \cap \text{Cech}_r(X)$
 - restriction of Čech complex to Delaunay simplices



Čech and Delaunay complexes from functions

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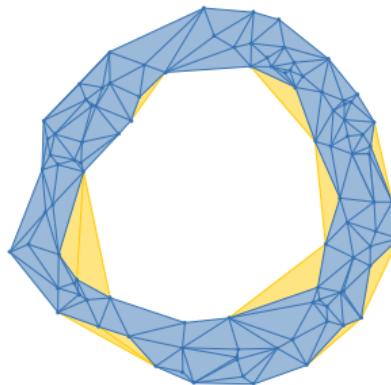
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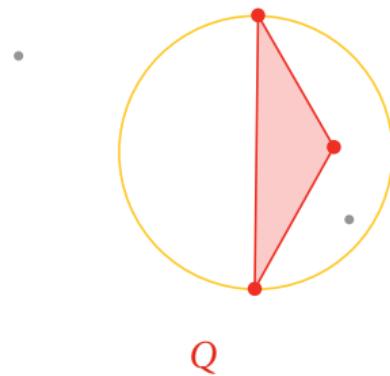
Unfortunately...

Neither the Čech nor the Delaunay functions
are discrete Morse functions!

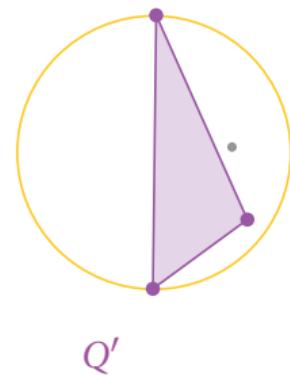
Unfortunately...

Neither the Čech nor the Delaunay functions
are discrete Morse functions!

- Example: two simplices Q, Q' with $f_{\text{Čech}}(Q) = f_{\text{Čech}}(Q')$
where neither is a face of the other:



Q



Q'

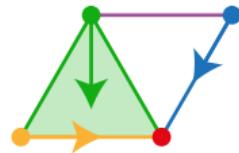
Generalized discrete Morse theory

Definition (Chari 2000, Freij 2009)

A *generalized discrete vector field* on a simplicial complex K is a partition of the simplices into *intervals* of the face poset:

$$[L, U] = \{Q : L \subseteq Q \subseteq U\}$$

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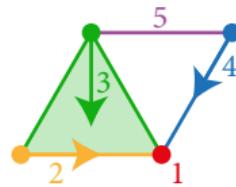
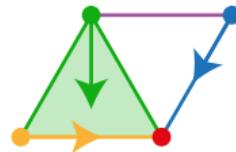
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A *generalized discrete Morse function* $f : K \rightarrow \mathbb{R}$ satisfies:

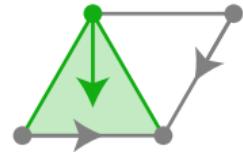
- the sublevel sets $K_t = f^{-1}(-\infty, t]$ are subcomplexes (for all $t \in \mathbb{R}$)
- the level sets $f^{-1}(t)$ form a generalized vector field (the *discrete gradient* of f)



Refining generalized vector fields

A generalized vector field V can be refined to a vector field.

For each non-critical face interval $[L, U] \in V$:

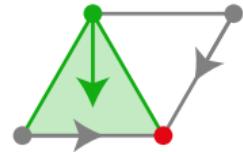


Refining generalized vector fields

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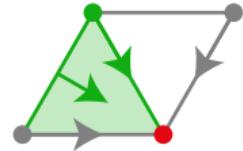


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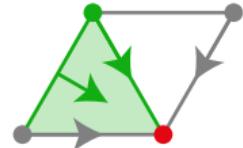


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Therefore the collapsing theorems also hold for generalized discrete Morse functions.

Morse theory of Čech and Delaunay complexes

Proposition

*The Čech function and the Delaunay function
are generalized discrete Morse functions.*

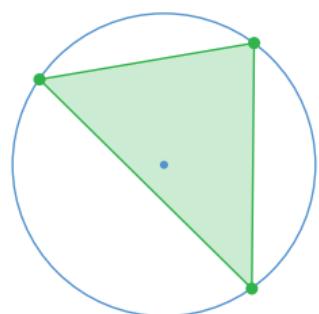
Morse theory of Čech and Delaunay complexes

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*The Čech function and the Delaunay function
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The following are equivalent:

- Q is a critical simplex of $f_{\text{Čech}}$
- Q is a critical simplex of f_{Del}
- $f_{\text{Čech}}(Q) = f_{\text{Del}}(Q)$
- Q is a centered Delaunay simplex
(containing the circumcenter in the interior)

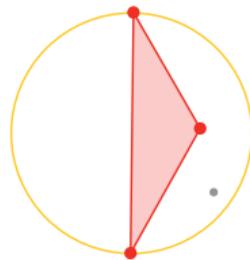


$\check{\text{C}}$ ech face intervals

Lemma

Let $Q \subseteq X$ be a simplex with smallest enclosing sphere S .

Then $R \subseteq X$ has the same smallest enclosing sphere S iff



Q

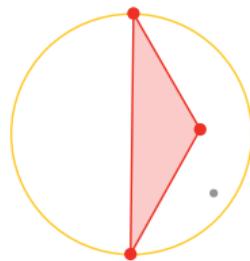
Čech face intervals

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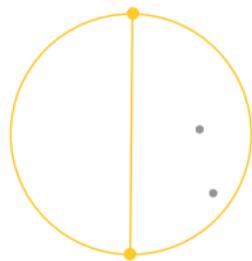
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On $S \subseteq R$



Q



On S

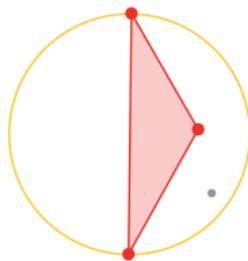
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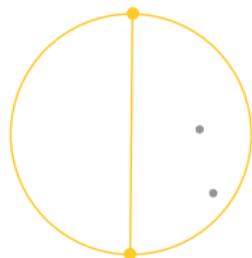
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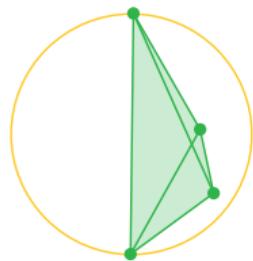
$$\text{On } S \subseteq R \subseteq \text{Encl } S.$$



Q



$\text{On } S$



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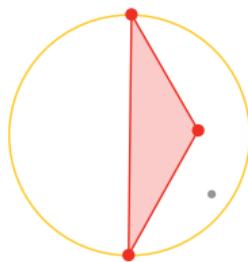
$\check{\text{C}}\text{ech}$ face intervals

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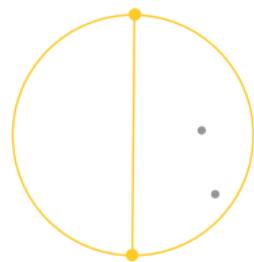
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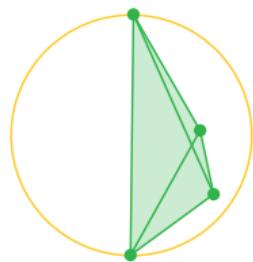
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$\text{On } S$



$\text{Encl } S$

The front and back faces of a simplex

Let S be the smallest circumsphere of a simplex $\text{On } S \subseteq X$.

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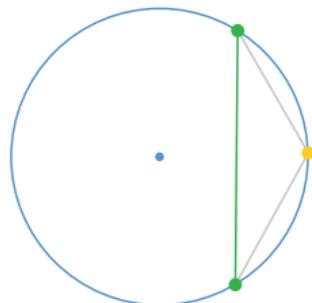
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$$\text{Front } S = \{x \in \text{On } S \mid \mu_x > 0\},$$

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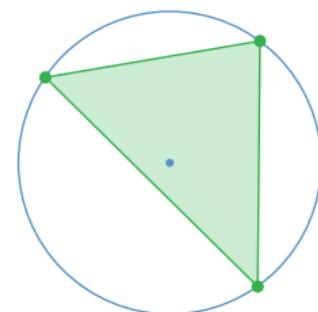
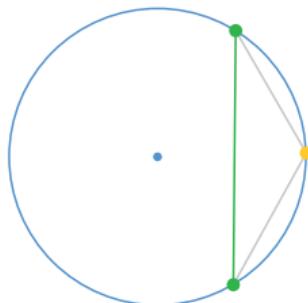
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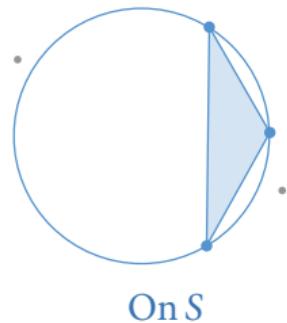
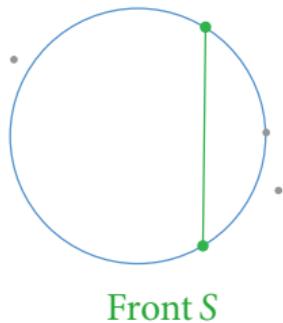
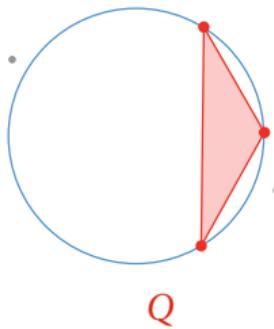


Delaunay face intervals

Lemma

Let $Q \subseteq X$ be a simplex with smallest empty circumsphere S .
Then $R \subseteq X$ has the same smallest empty circumsphere S iff

$$R \in [\text{Front } S, \text{On } S].$$



Selective Delaunay complexes

Sphere optimization problems

Both Čech and Delaunay functions are defined using the smallest sphere S satisfying certain constraints:

$$\begin{array}{ll} \text{minimize}_{r,z} & r \\ \text{subject to} & \|z - q\| \leq r, \quad q \in Q, \\ & \|z - e\| \geq r, \quad e \in E. \end{array}$$

Here r is the radius of the sphere S , and z is the center of S .

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$$\begin{array}{lll} \text{minimize}_{a,z} & \|z\|^2 - a & (r^2 = \|z\|^2 - a) \\ \text{subject to} & \|z - q\|^2 \leq \|z\|^2 - a, & q \in Q, \\ & \|z - e\|^2 \geq \|z\|^2 - a, & e \in E. \end{array}$$

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$$\begin{array}{ll} \text{minimize}_{a,z} & \|z\|^2 - a \\ \text{subject to} & \|z\|^2 - 2\langle z, q \rangle + \|q\|^2 \leq \|z\|^2 - a, \quad q \in Q, \\ & \|z\|^2 - 2\langle z, e \rangle + \|e\|^2 \geq \|z\|^2 - a, \quad e \in E. \end{array}$$

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Here r is the radius of the sphere S , and z is the center of S .

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The Karush–Kuhn–Tucker optimality conditions

Consider an optimization problem of the form

$$\begin{array}{ll} \underset{x}{\text{minimize}} & f(x) \\ \text{subject to} & g_j(x) \geq 0, \quad \forall j \in J, \\ & g_k(x) = 0, \quad \forall k \in K, \\ & g_l(x) \leq 0, \quad \forall l \in L. \end{array}$$

where the function f is convex and g_i are affine ($i \in I = J \cup K \cup L$).

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where the function f is convex and g_i are affine ($i \in I = J \cup K \cup L$).

Theorem (Karush 1939, Kuhn–Tucker 1951)

A feasible x is optimal iff there exist $(\lambda_i)_{i \in I}$ such that

$$\nabla f(x) + \sum_{i \in I} \lambda_i \nabla g_i(x) = 0, \quad (\text{stationarity})$$

$$\lambda_i g_i(x) = 0, \quad \forall i \in I, \quad (\text{complementary slackness})$$

$$\begin{aligned} \lambda_j &\leq 0, & \forall j \in J, \\ \lambda_l &\geq 0, & \forall l \in L. \end{aligned} \quad (\text{dual feasibility})$$

KKT conditions for the smallest sphere problem

The KKT conditions for our sphere optimization problem are:

Proposition

*A sphere S enclosing Q and excluding E is minimal iff
its center z can be written as an affine combination*

$$z = \sum_{x \in Q \cup E} \lambda_x x, \quad 1 = \sum_{x \in Q \cup E} \lambda_x$$

such that

- $\lambda_x = 0$ whenever x does not lie on S ,
- $\lambda_x \leq 0$ whenever $x \in E \setminus Q$, and
- $\lambda_x \geq 0$ whenever $x \in Q \setminus E$.

Čech and Delaunay face intervals from KKT

The Karush–Kuhn–Tucker optimality conditions yield:

Proposition (Geometric KKT conditions)

A sphere S enclosing Q and excluding E is minimal iff

- S is the smallest circumsphere of $\text{On } S$,
- $Q \in [\text{Front } S, \text{Encl } S]$ (i.e., $\text{Front } S \subseteq Q \subseteq \text{Encl } S$), and
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Corollary

- The Čech face intervals are of the form $[\text{On } S, \text{Encl } S]$.

$\check{\text{C}}\text{ech}$ and Delaunay face intervals from KKT

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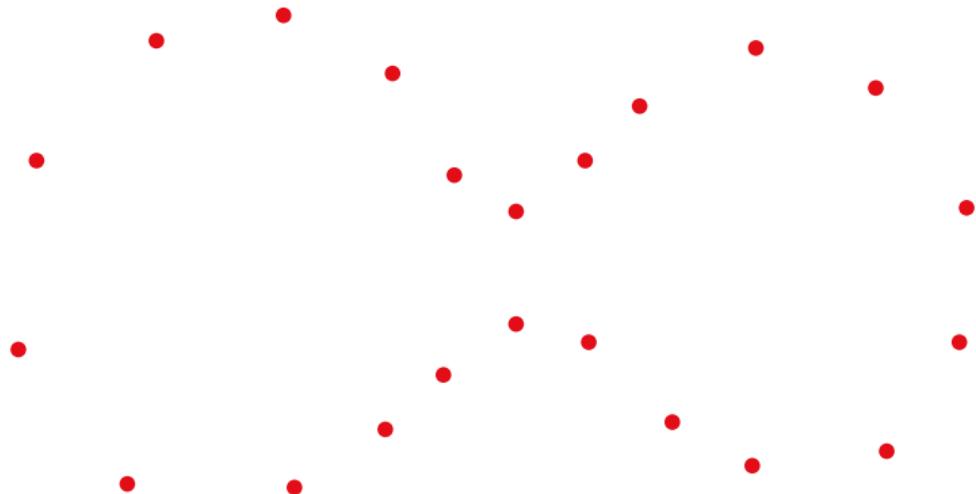
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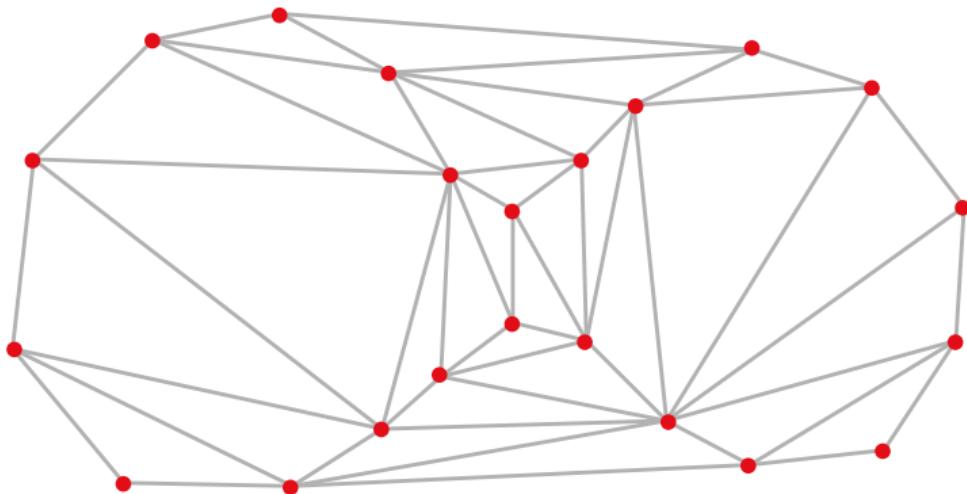
Corollary

- The $\check{\text{C}}\text{ech}$ face intervals are of the form $[\text{On } S, \text{Encl } S]$.
- The Delaunay face intervals are of the form $[\text{Front } S, \text{On } S]$.

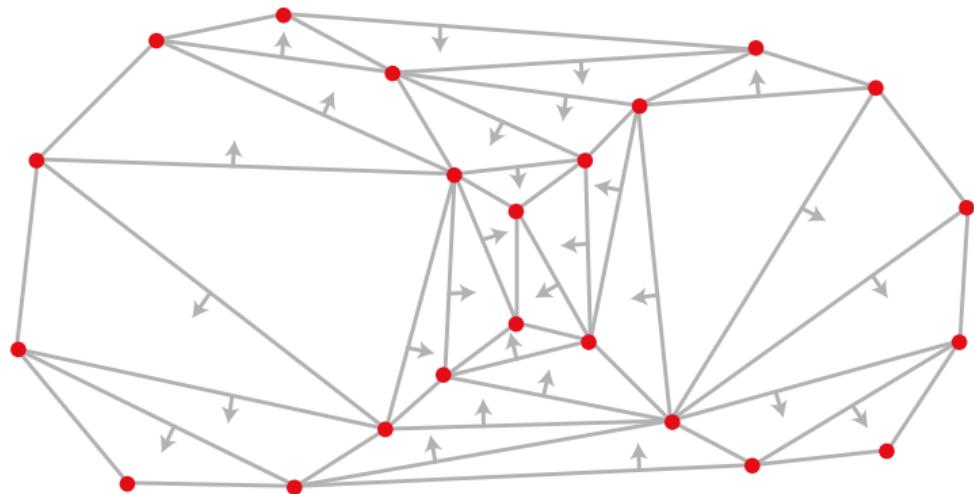
The Delaunay gradient



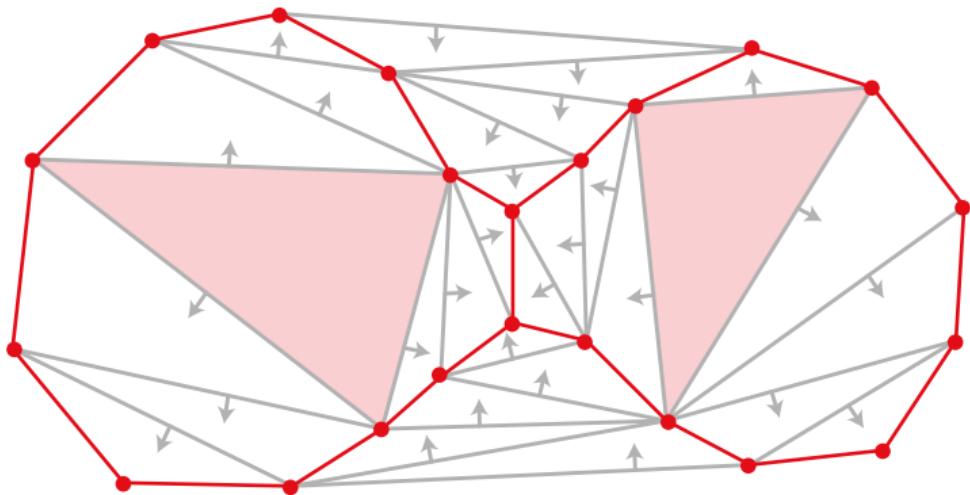
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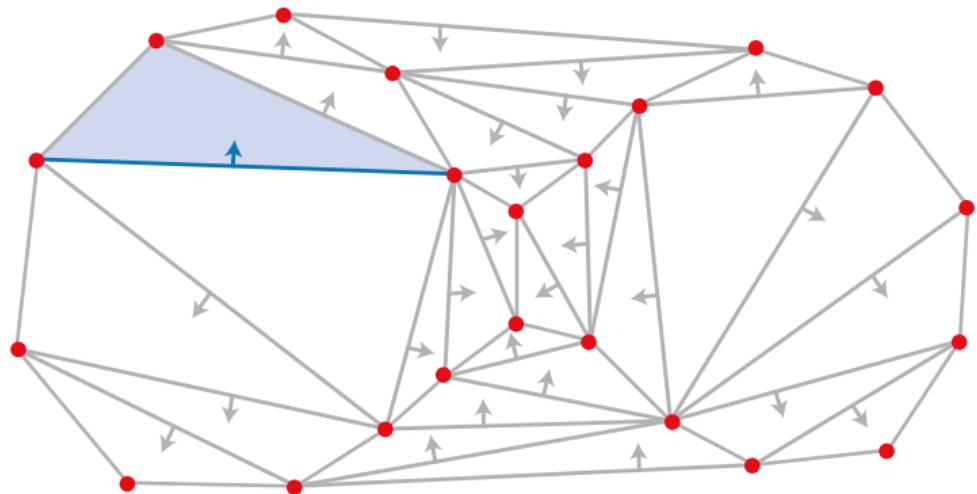
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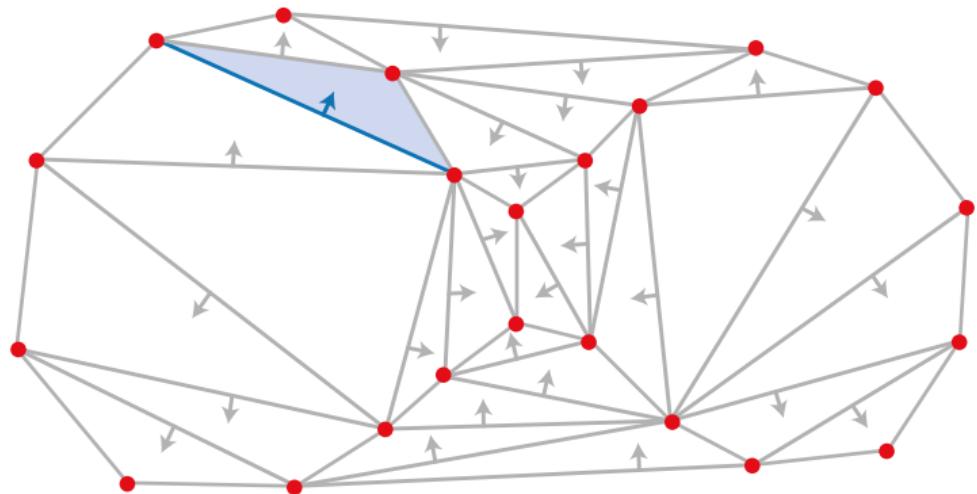
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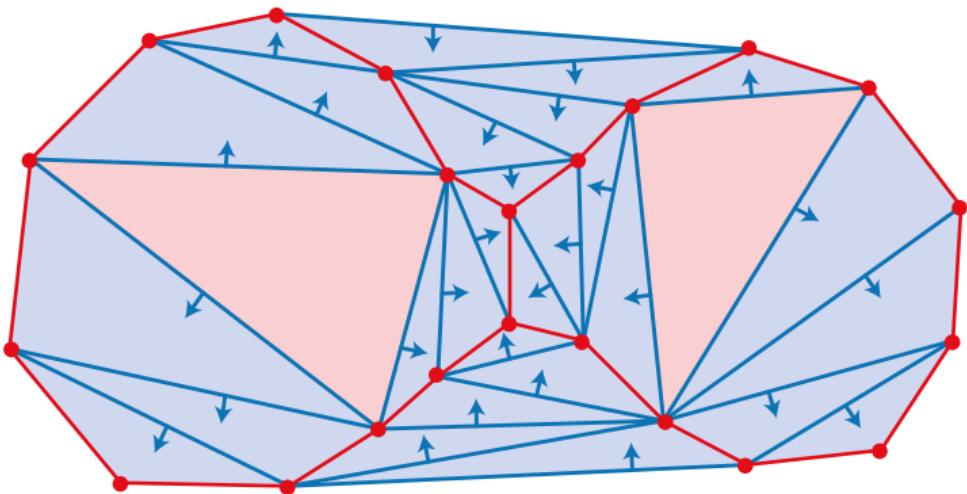
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Wrap complexes

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Generalize and simplify the surface reconstruction method *Wrap* (Edelsbrunner 1995)

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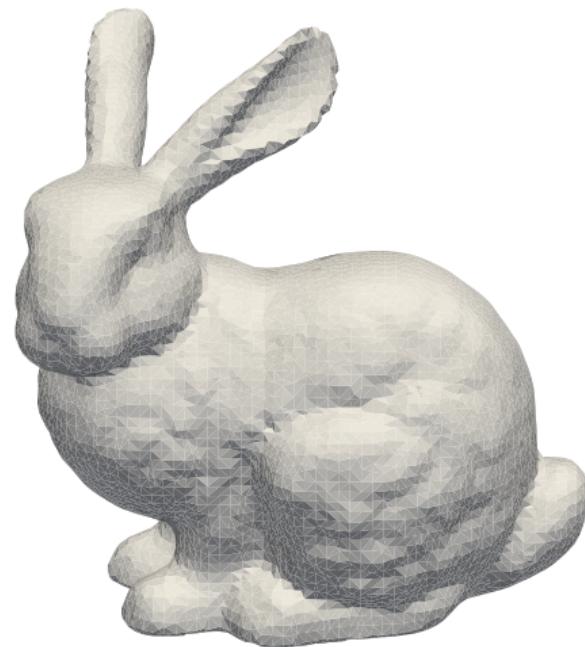
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Generalize and simplify the surface reconstruction method *Wrap* (Edelsbrunner 1995)



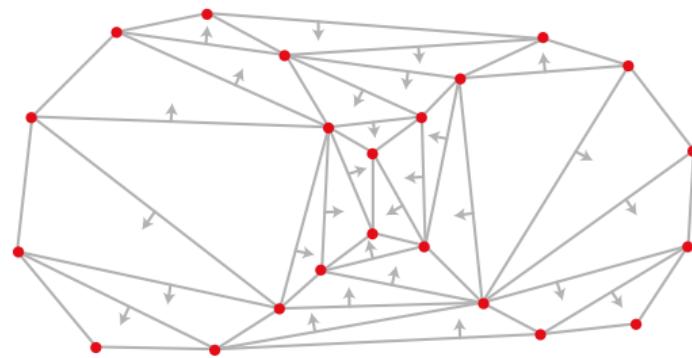
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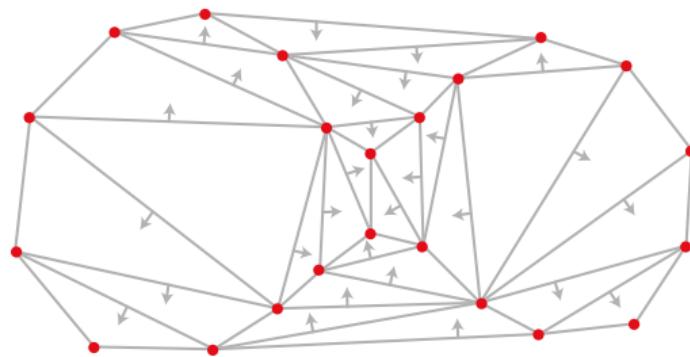
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Consider the Delaunay gradient V_D of $X \subset \mathbb{R}^D$.



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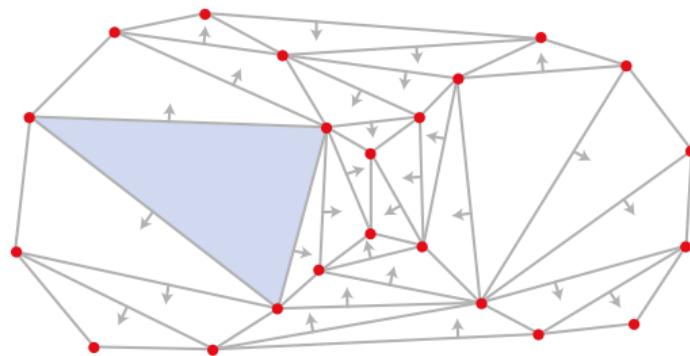


Define $\text{Wrap}_r(X)$ as the smallest subcomplex of $\text{Del } X$ that

- contains all critical simplices with circumradius $\leq r$ and
- is a union of face intervals of V_D .

Wrap complexes

Consider the Delaunay gradient V_D of $X \subset \mathbb{R}^D$.

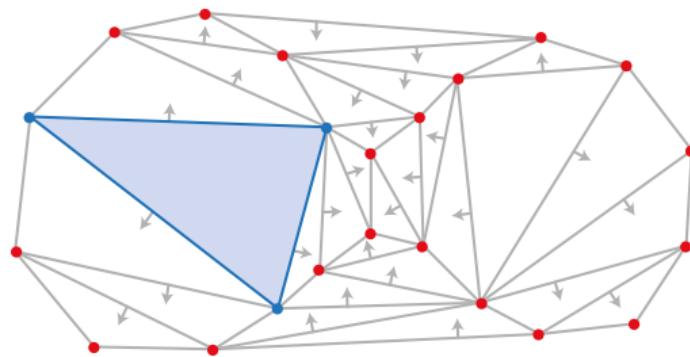


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Consider the Delaunay gradient V_D of $X \subset \mathbb{R}^D$.

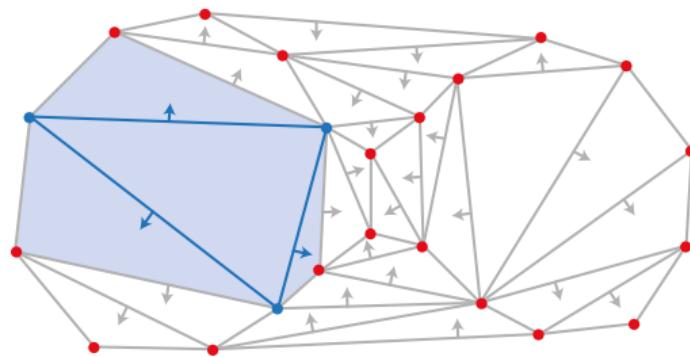


Define $\text{Wrap}_r(X)$ as the smallest subcomplex of $\text{Del } X$ that

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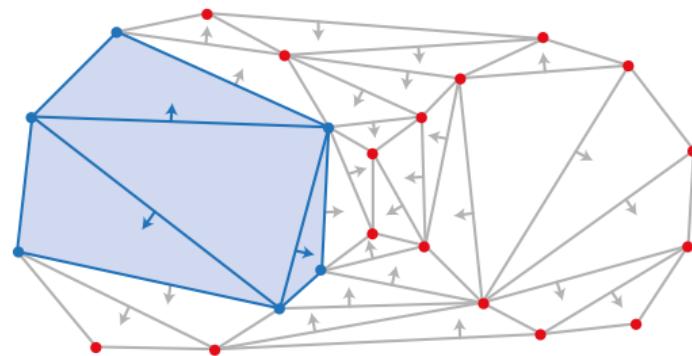


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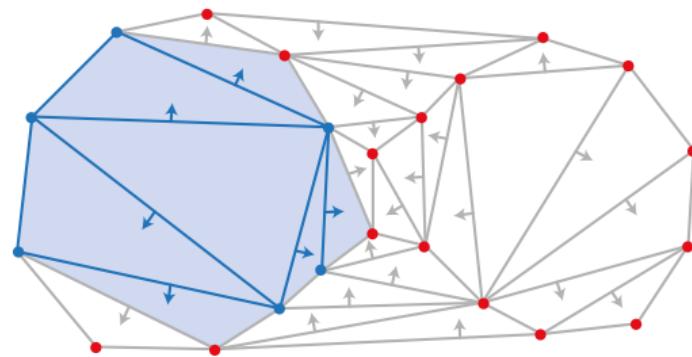


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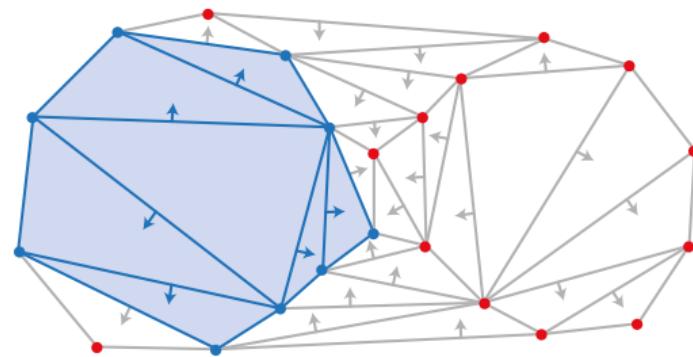


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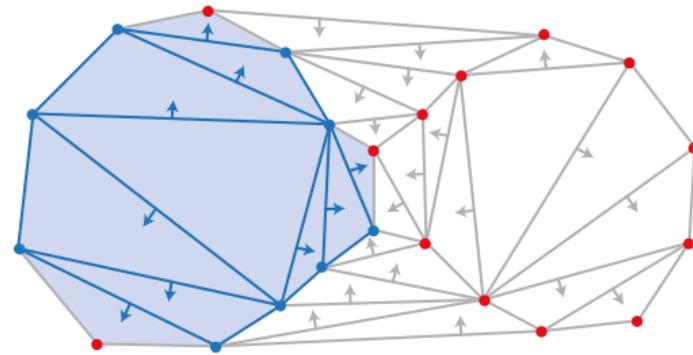


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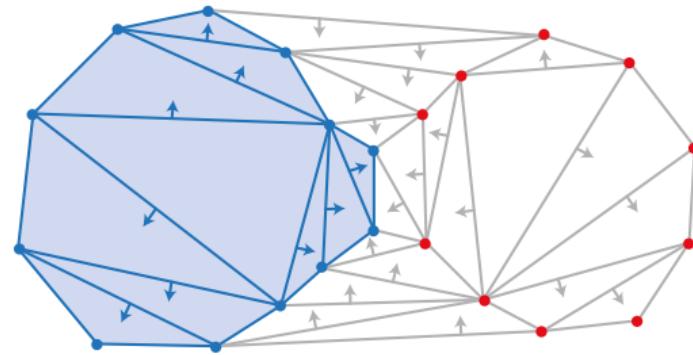


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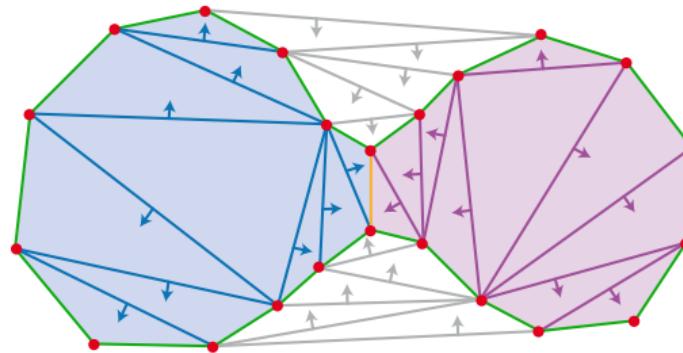


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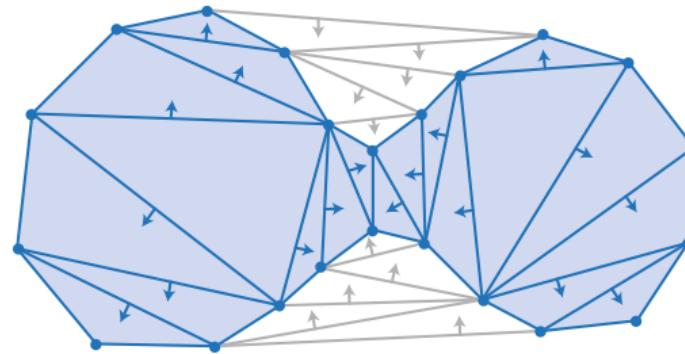


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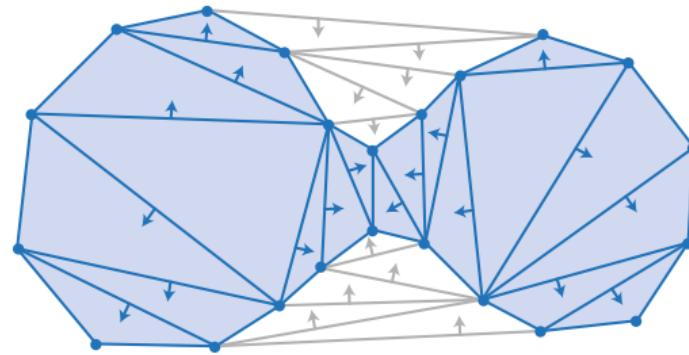


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Corollary

The Delaunay face intervals induce a collapse $\text{Del}_r \searrow \text{Wrap}_r$.

Vietoris–Rips complexes

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Consider a finite metric space (X, d) .

The *Vietoris–Rips complex* is the simplicial complex

$$\text{Rips}_t(X) = \{S \subseteq X \mid \text{diam } S \leq t\}$$

- all edges with pairwise distance $\leq t$
- all possible higher simplices

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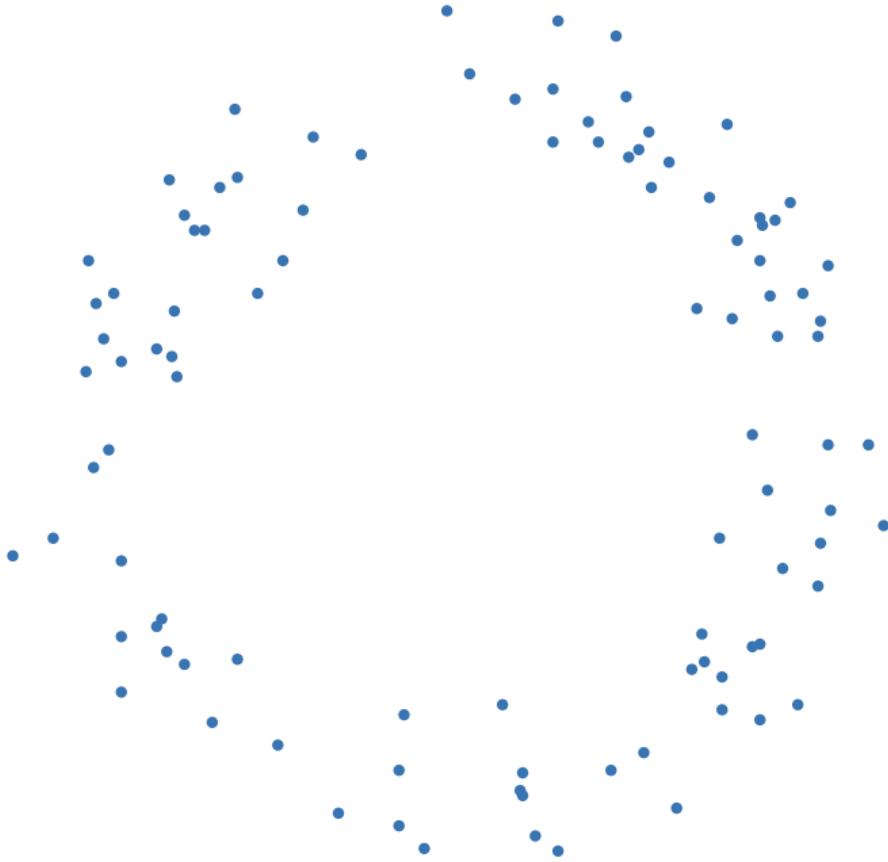
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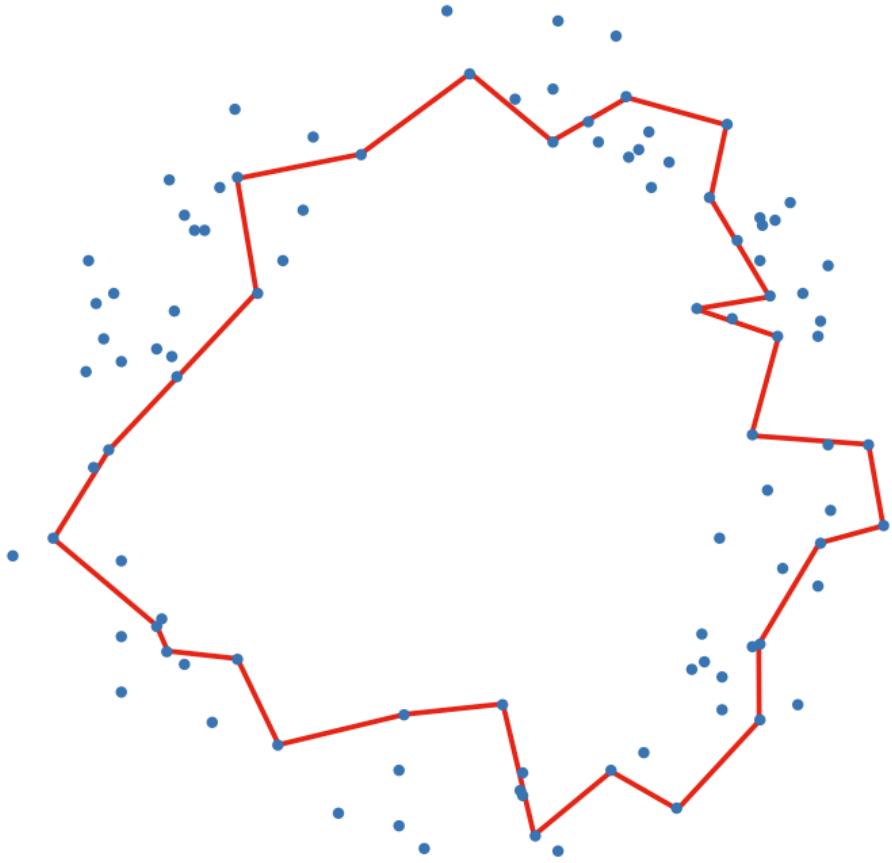
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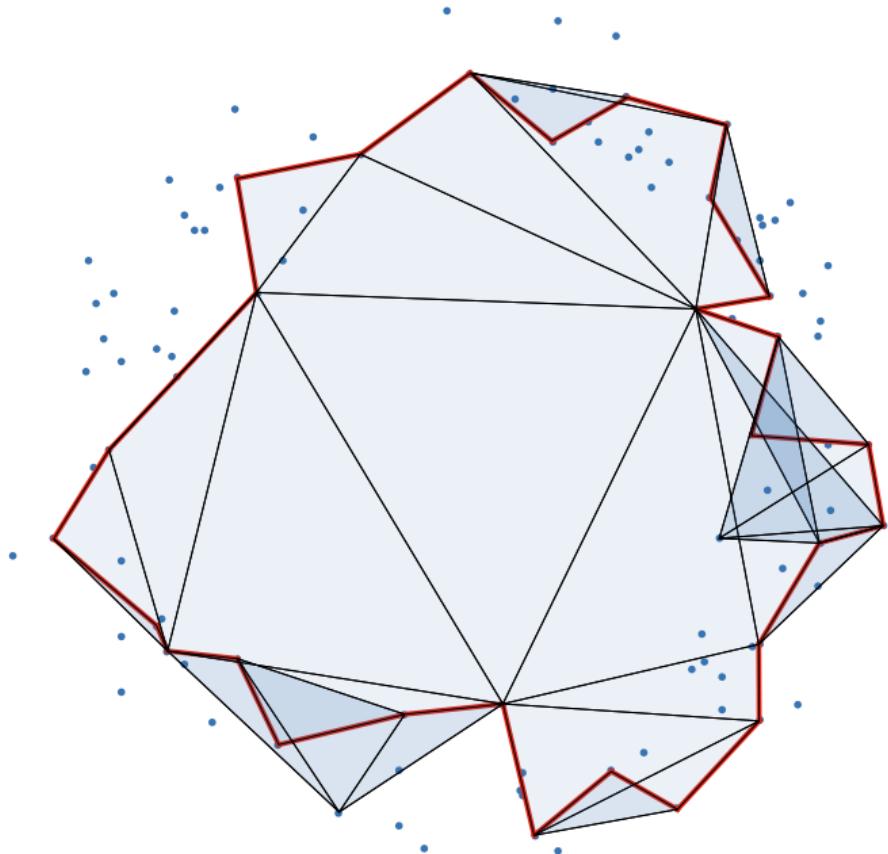
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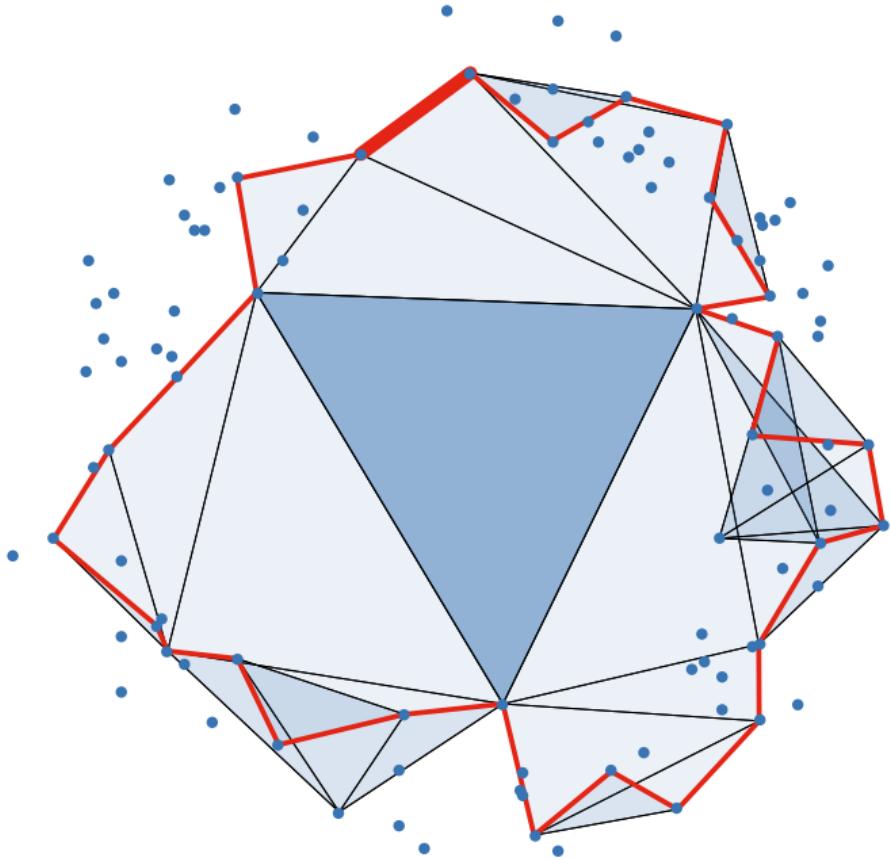
For large t , $\text{Rips}_t(X)$ is the full simplex with vertices X

- Number of d -simplices is $\binom{|X|}{d+1}$
- Computation is one of the most important challenges in applied topology!









A data set with interesting topology



(Columbia Object Image Library)

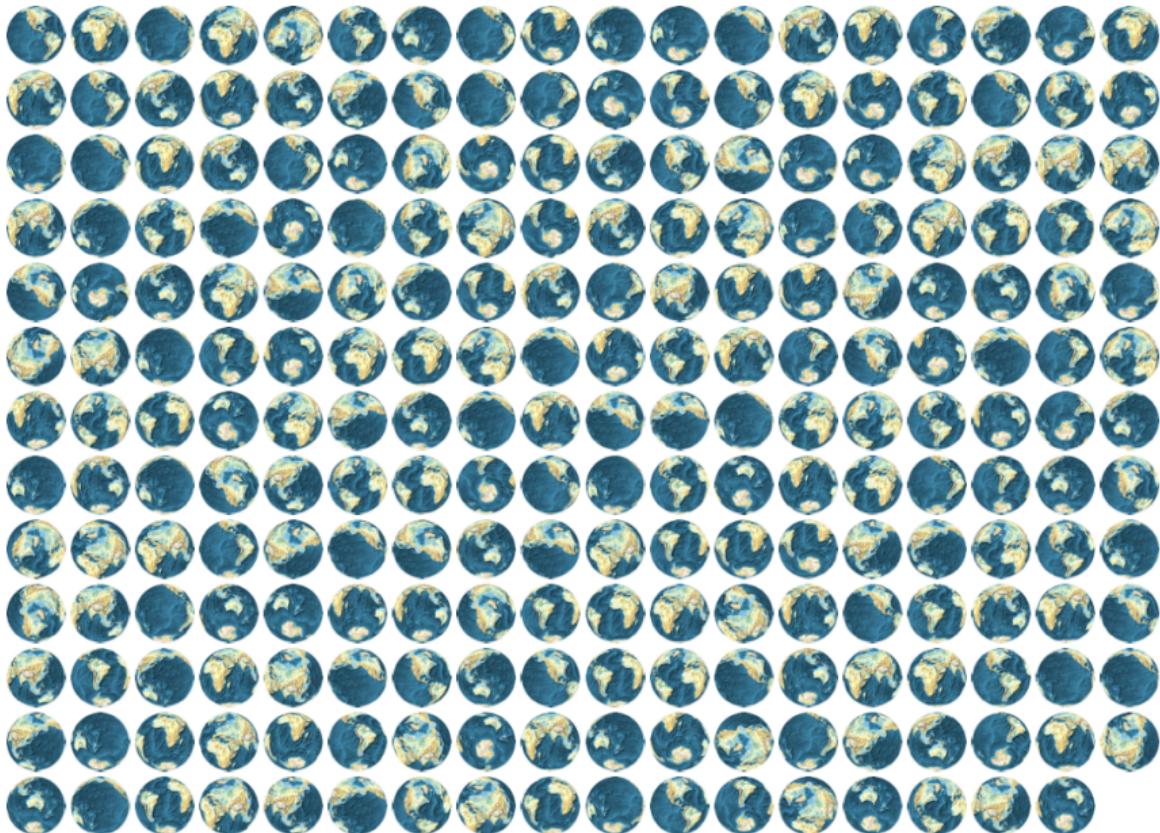
The earth is not a disk



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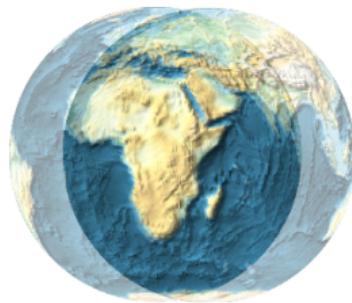
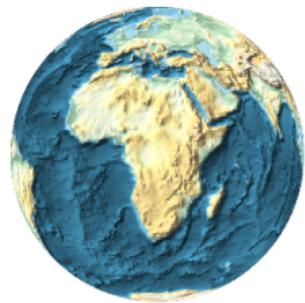
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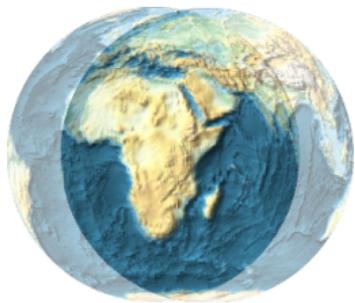
The earth is not a disk



The earth is not a disk



The earth is not a disk



A software for computing Vietoris–Rips persistence barcodes

- around 1000 lines of C++ code, no external dependencies
- support for
 - coefficients in a prime field $\mathbb{Z}/p\mathbb{Z}$
 - sparse distance matrices (for distance threshold)
- open source (<http://ripser.org>)
- online version (<http://live.ripser.org>)
- 2016 ATMCS Best New Software Award (joint with RIVET by M. Lesnick and M. Wright)

The four special ingredients

Main improvements to the standard algorithm:

- Clearing inessential columns [Chen, Kerber 2011]
- Computing cohomology [de Silva et al. 2011]
- Implicit matrix reduction
- Apparent and emergent pairs

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Lessons from previous work:

- Clearing and cohomology yield considerable speedup,
- but only when *both* are used in conjunction!

Matrix reduction

Computing homology

Computing homology $H_* = Z_*/B_*$:

- compute basis for boundaries $B_* = \text{im } \partial_*$
- extend to basis for cycles $Z_* = \ker \partial_*$
- new (non-boundary) basis cycles generate quotient Z_*/B_*

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Computing *persistent* homology $H_* = Z_*/B_*$ (for a simplexwise filtration $K_i \subseteq K$):

- compute *filtered* basis for boundaries $B_* = \text{im } \partial_*$
- extend to basis for cycles $Z_* = \ker \partial_*$
- all basis cycles generate *persistent* homology

Persistence by matrix reduction

Given:

- D : boundary matrix for a simplexwise filtration $(K_i)_i$

Wanted:

- persistent homology barcodes in dimensions $d = 0, \dots, k$

Notation:

- M_j : column j of M ; m_{ij} : entry in row i and column j
- PivotIndex $M_j = \min\{i : m_{kj} = 0 \text{ for all } k > i\}$.

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Computation: barcode is obtained by *matrix reduction* of D

- $R = D \cdot V$ reduced (non-zero columns have distinct pivots)
- V is regular upper triangular

Compatible basis cycles

For a reduced boundary matrix $R = D \cdot V$, call

$$I_b = \{i : R_i = 0\}$$

birth indices,

$$I_d = \{j : R_j \neq 0\}$$

death indices,

$$I_e = I_b \setminus \text{PivotIndices } R$$

essential indices.

(note: all pivot indices are birth indices).

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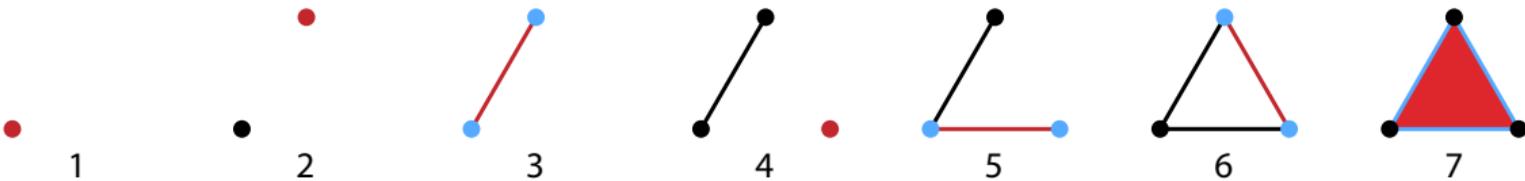
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Matrix reduction



	1	2	3	4	5	6	7
1			1	1			
2			1		1		
3							1
4				1	1		
5						1	
6						1	
7							1

$\underbrace{\hspace{10em}}_R$

= $D \cdot$

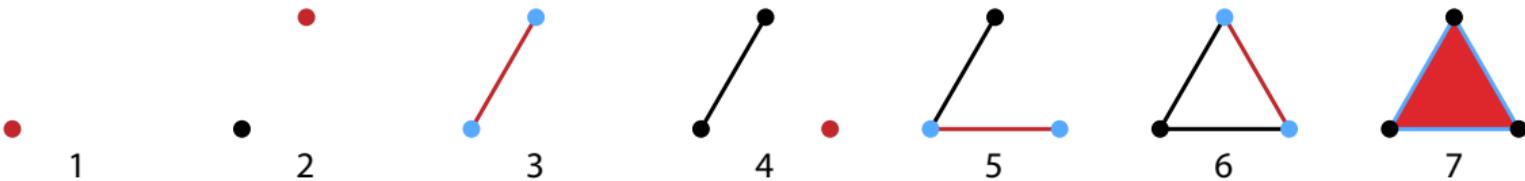
	1	2	3	4	5	6	7
1	1						
2		1					
3			1				
4				1			
5					1		
6						1	
7							1

$\underbrace{\hspace{10em}}_V$

Algorithm (over $\mathbb{Z}/2\mathbb{Z}$):

- while $\exists k < j$ with PivotIndex $R_k = \text{PivotIndex } R_j$
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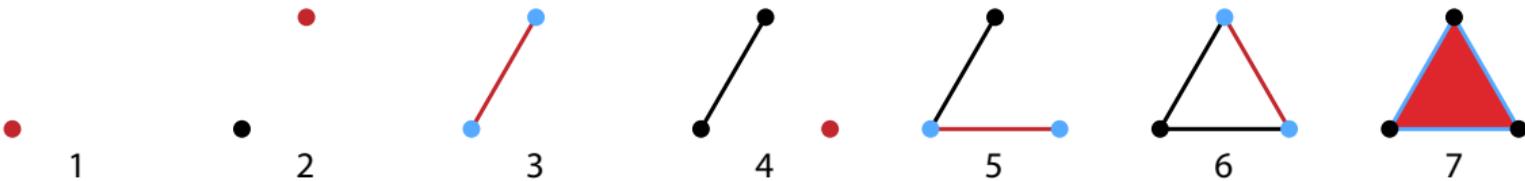


$$\begin{array}{c} \begin{array}{|c|c|c|c|c|c|c|c|} \hline & 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ \hline 1 & & & 1 & & 1 & & \\ \hline 2 & & & & & & 1 & \\ \hline 3 & & & & & & & 1 \\ \hline 4 & & & & & 1 & 1 & \\ \hline 5 & & & & & & & 1 \\ \hline 6 & & & & & & & 1 \\ \hline 7 & & & & & & & \\ \hline \end{array} \\ \underbrace{\hspace{10em}}_R \end{array} = D \cdot \begin{array}{c} \begin{array}{|c|c|c|c|c|c|c|c|} \hline & 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ \hline 1 & 1 & & & & & & \\ \hline 2 & & 1 & & & & & \\ \hline 3 & & & 1 & & & & \\ \hline 4 & & & & 1 & & & \\ \hline 5 & & & & & 1 & & \\ \hline 6 & & & & & & 1 & \\ \hline 7 & & & & & & & 1 \\ \hline \end{array} \\ \underbrace{\hspace{10em}}_V \end{array}$$

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1			1		1		
2			1			1	
3							1
4				1	1		
5						1	
6						1	
7							

$\underbrace{\hspace{10em}}$ _R

$= D \cdot$

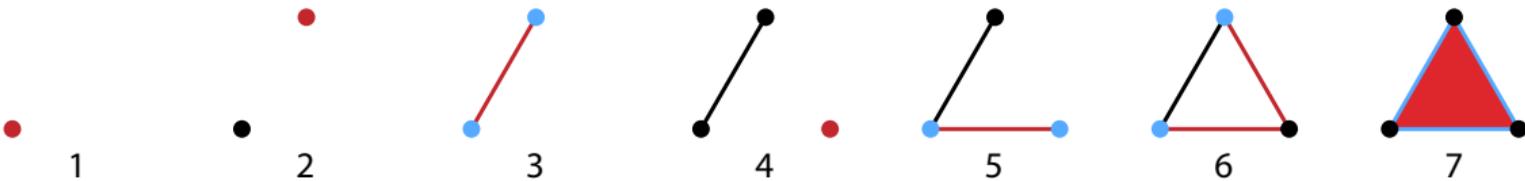
	1	2	3	4	5	6	7
1	1						
2		1					
3			1				
4				1			
5					1		
6						1	
7							1

$\underbrace{\hspace{10em}}$ _V

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	1	2	3	4	5	6	7
1			1	1	1	1	1
2			1		1		
3							1
4				1	0		
5						1	
6						1	
7							

$\underbrace{\hspace{10em}}_R$

= $D \cdot$

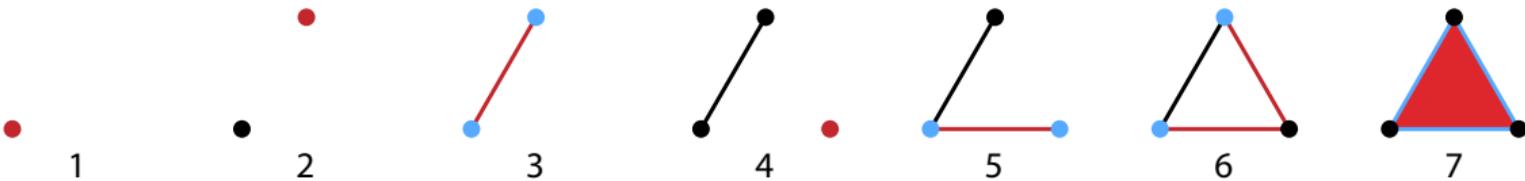
	1	2	3	4	5	6	7
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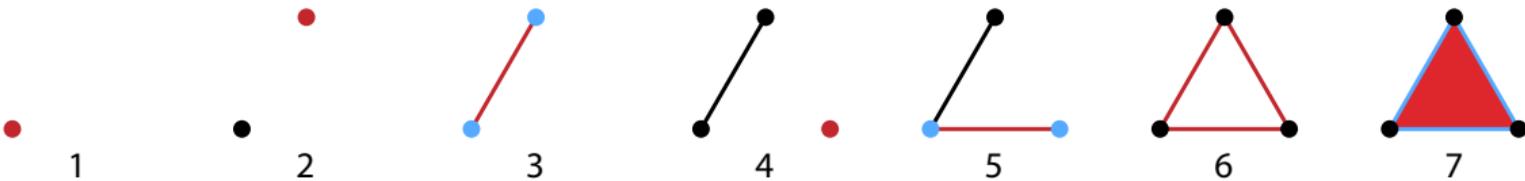
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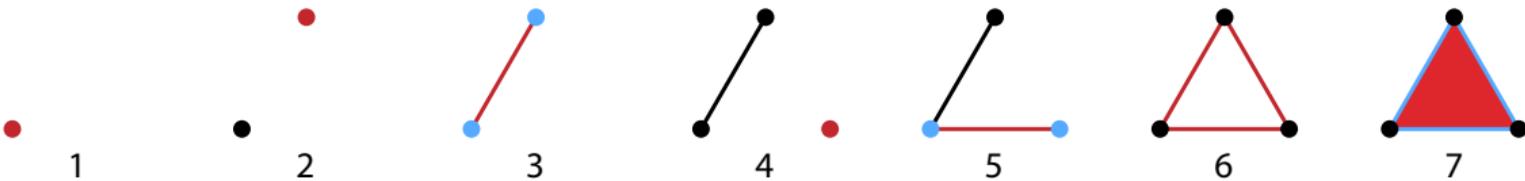
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The matrix is labeled R under the first column and V under the last column.

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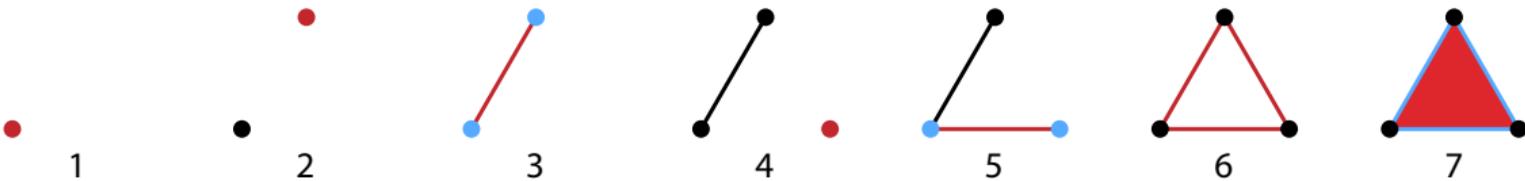
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3							1
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7							

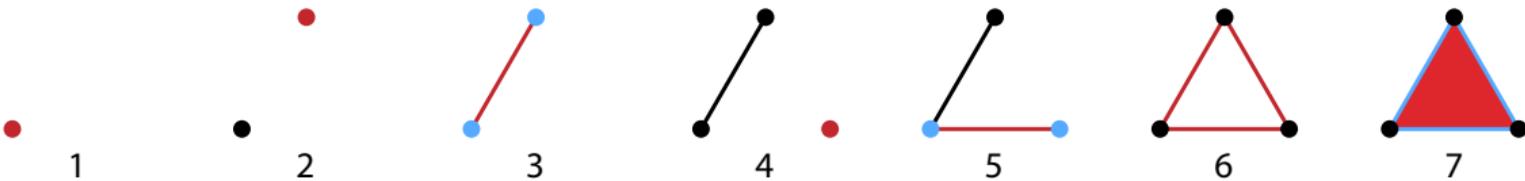
$\underbrace{\hspace{10em}}$ _R

$$= D \cdot \underbrace{\begin{array}{|c|c|c|c|c|c|c|} \hline & 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ \hline 1 & 1 & & & & & & \\ \hline 2 & & 1 & & & & & \\ \hline 3 & & & 1 & & & 1 & \\ \hline 4 & & & & 1 & & & \\ \hline 5 & & & & & 1 & 1 & \\ \hline 6 & & & & & & 1 & \\ \hline 7 & & & & & & & 1 \\ \hline \end{array}}_{V}$$

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1			1		1		
2			1				
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7							

$\underbrace{\hspace{10em}}_R$

= $D \cdot$

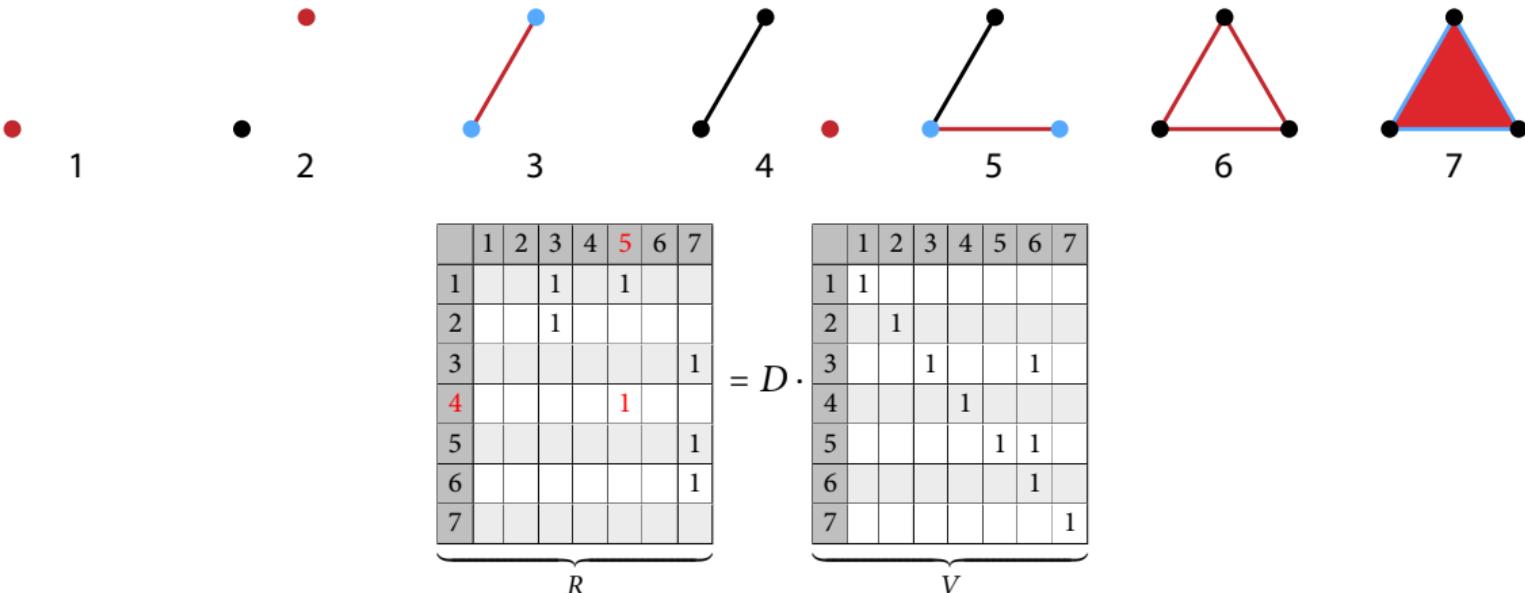
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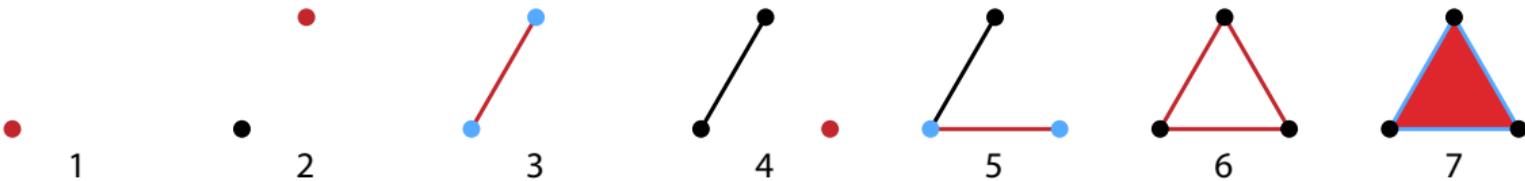
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Clearing

Clearing non-essential positive columns

Recall:

- Columns with indices PivotIndices R (non-essential birth indices) not used at all

Idea [Chen, Kerber 2011]:

- Don't reduce those columns
- Instead, *clear* them to 0
 - Use the fact that every pivot index is a birth index: $i = \text{PivotIndex } R_j$ implies $R_i = 0$
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Note:

- reducing *birth* columns typically harder than death columns:
 - $O(j^2)$ (birth) vs. $O((j - i)^2)$ (death)
- with clearing: need only reduce *essential* columns

Counting homology column reductions

Consider $k + 1$ -skeleton of $n - 1$ -simplex (Rips filtration)

Number of columns in boundary matrix:

$$\sum_{d=1}^{k+1} \underbrace{\binom{n}{d+1}}_{\text{total}} = \sum_{d=1}^{k+1} \underbrace{\binom{n-1}{d}}_{\text{death}} + \sum_{d=1}^{k+1} \underbrace{\binom{n-1}{d+1}}_{\text{birth}}$$

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$$k = 2, n = 192: \quad 56\,050\,096 = 1161\,471 + \cancel{53\,727\,345} + \textcolor{green}{1161\,280}$$

- Clearing didn't help much!

Cohomology

Cohomology and clearing

The persistence barcode can also be computed using *cohomology* (the vector space dual of homology)

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- Persistent homology and persistent cohomology have the same barcode.
- Persistent cohomology can be computed by reducing the transposed boundary matrix.
- Cohomology allows for clearing starting from dimension 0
- Persistence in dimension 0 has special algorithms
 - Kruskal's algorithm for minimum spanning tree
 - union-find data structure

Counting cohomology column reductions

Consider K : $k + 1$ -skeleton of $n - 1$ -simplex, Rips filtration

- Number of columns in coboundary matrix:

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- $k = 2, n = 192: 1179\,808 = 1161\,471 + 1 + 18\,336$

Observations

For a typical input:

- V has very few off-diagonal entries
- most death columns of D are already reduced

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Previous example ($k = 2, n = 192$):

- Only $79 + 42 + 1 = 122$ out of $192 + 18\,145 + 1\,143\,135 = 1161\,471$ columns are actually modified in matrix reduction

Implicit matrix reduction

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- Boundary matrix D for filtration-ordered basis
 - Explicitly generated and stored in memory

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Approach for Ripser:

- Boundary matrix D for lexicographically ordered basis
 - Columns recomputed on the fly
- Matrix reduction: store only coefficient matrix V
 - Columns of $R_j = D \cdot V_j$ recomputed on the fly
 - Typically, V is much sparser and smaller than R

Apparent pairs

Simplexwise filtrations

Call a filtration $K_\bullet = (K_i)_i$ of simplicial complexes *simplexwise* if in the filtration, the simplices enter one at a time.

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Note:

- This is required for computation.
- The *Vietoris–Rips filtration* (indexed by \mathbb{R}) is not simplexwise: several simplices appear simultaneously.
- To compute Vietoris–Rips persistence, we have to break ties.
- This creates (many) persistence pairs with persistence 0 (as an artifact of tie-breaking).

Apparent pairs

Definition

In a simplexwise filtration, a pair of simplices (σ, τ) is an *apparent* pair if

- σ is the youngest facet of τ , and
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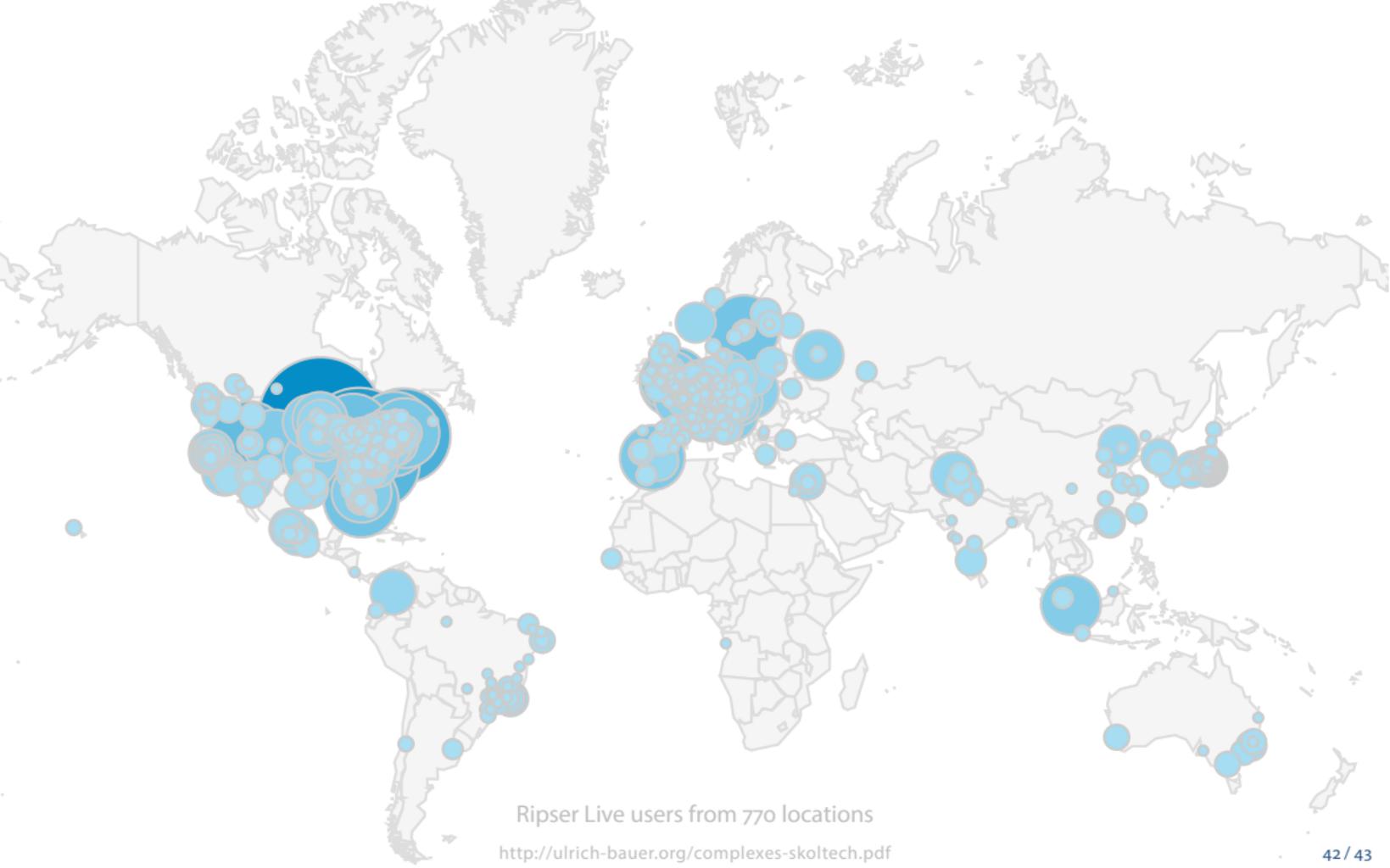
- σ is the youngest facet of τ , and
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Proposition

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Theorem

For the Vietoris–Rips filtration, in dimension 1, the 0-persistence pairs are the apparent pairs.



Ripser Live users from 770 locations

<http://ulrich-bauer.org/complexes-skoltech.pdf>



Ulrich Bauer.

Ripser: efficient computation of Vietoris–Rips persistence barcodes.

Submitted, Aug. 2019. arXiv:1908.02518

Software available at <http://ripser.org>.



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