Topological Data Analysis: An Introduction to Persistent Homology

Part 2: complexes and computation

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TUM

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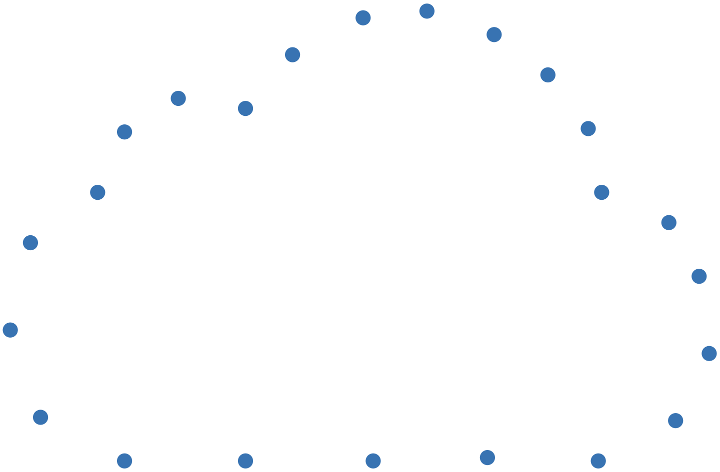
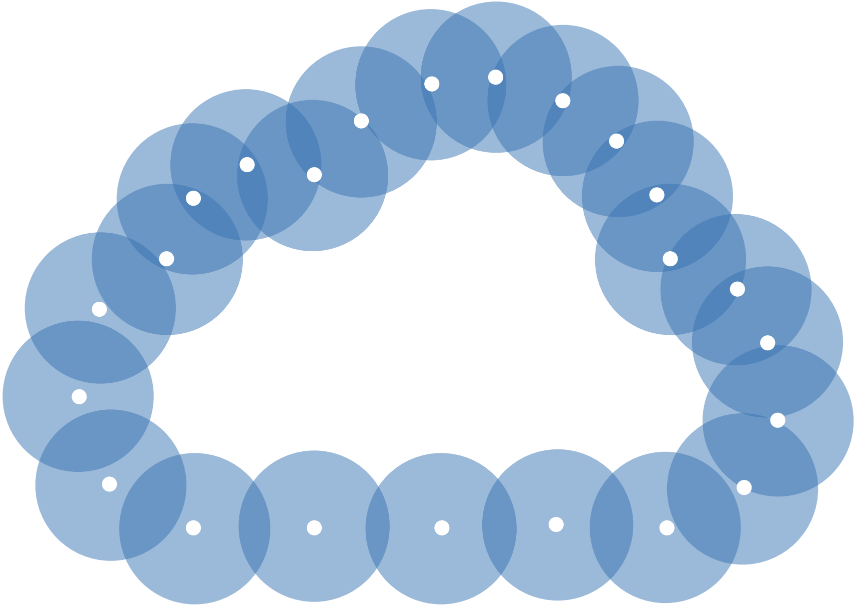
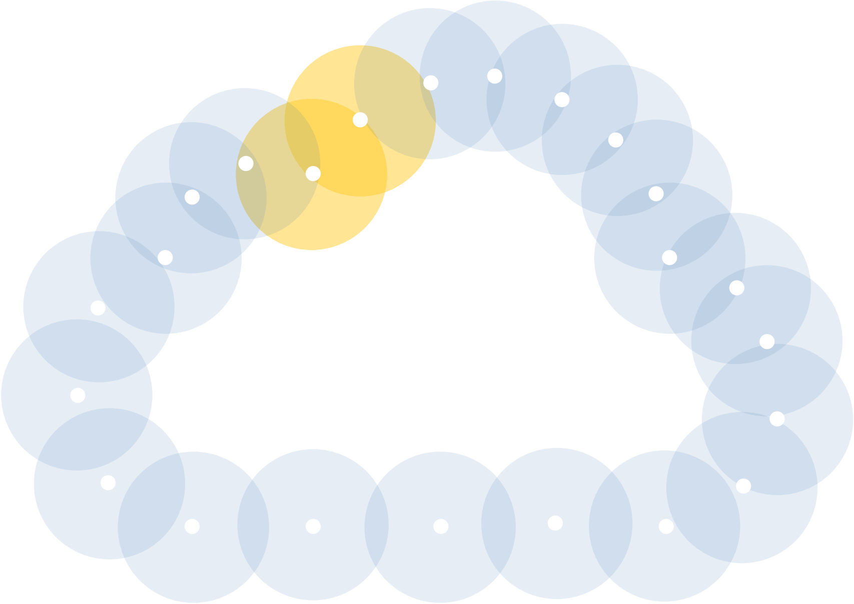
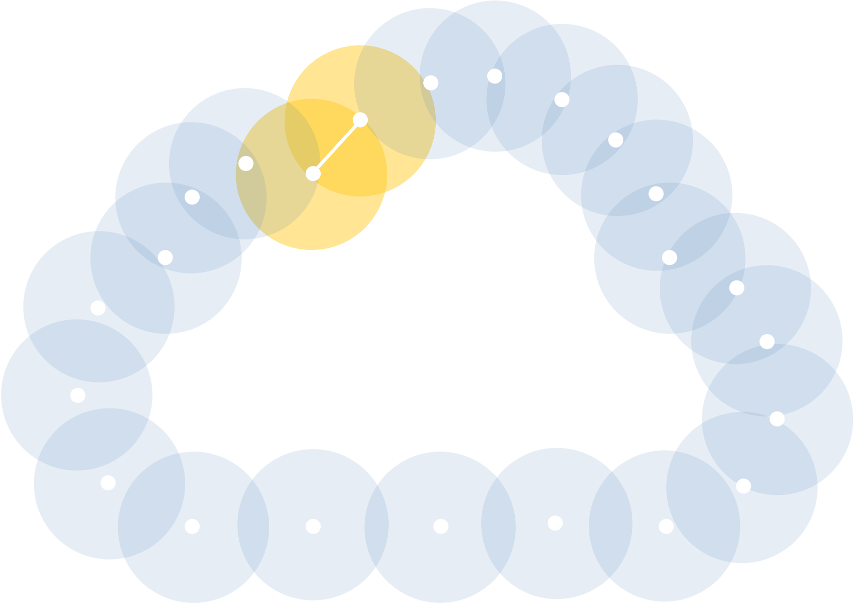
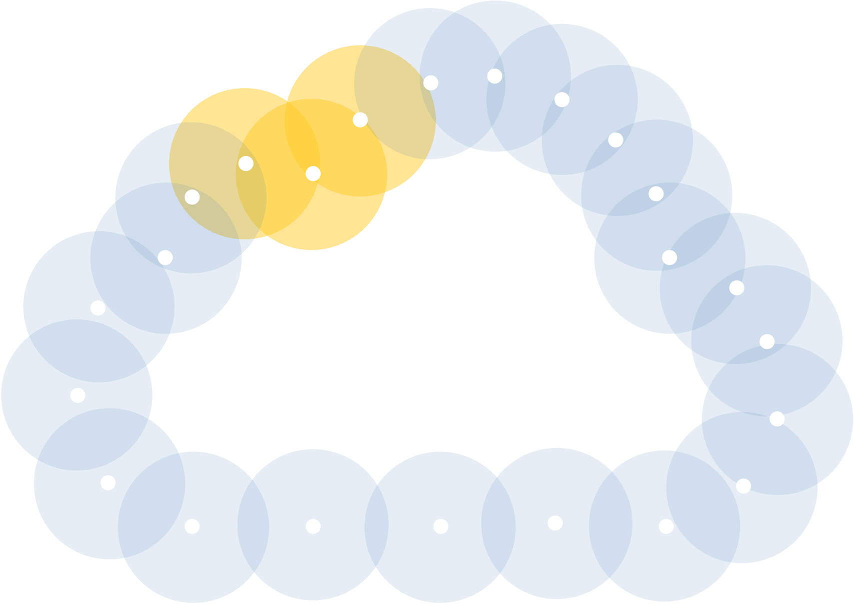
Machine learning summer school 2019
Skoltech, Moscow

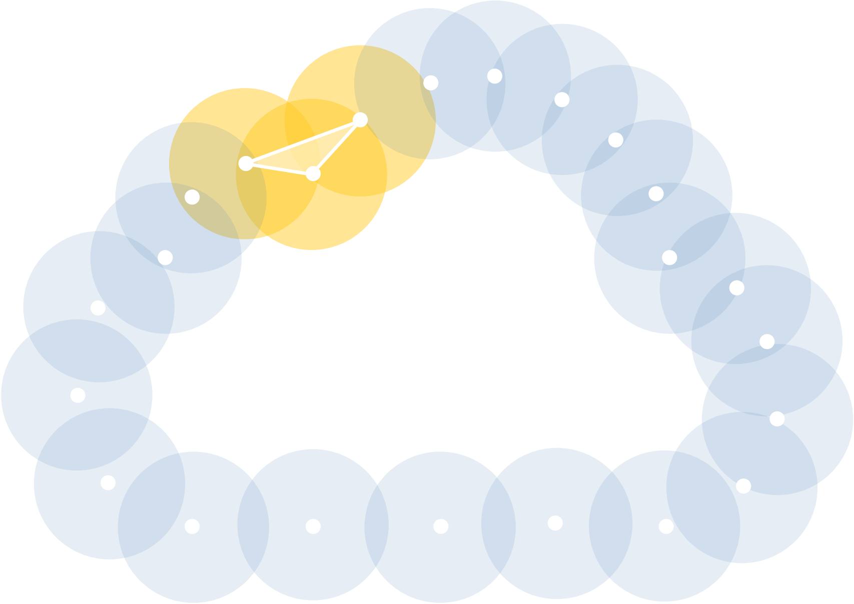


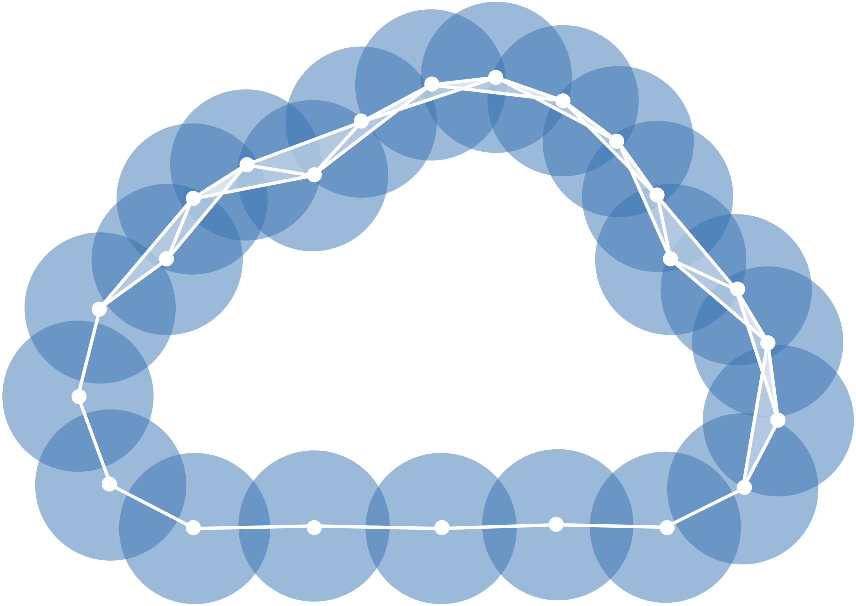


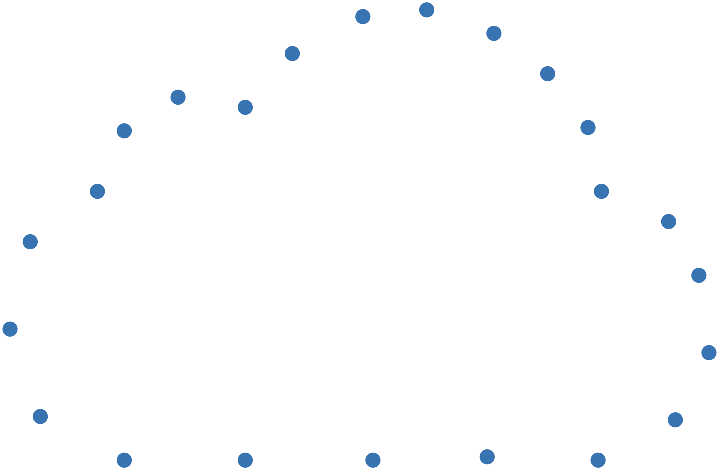


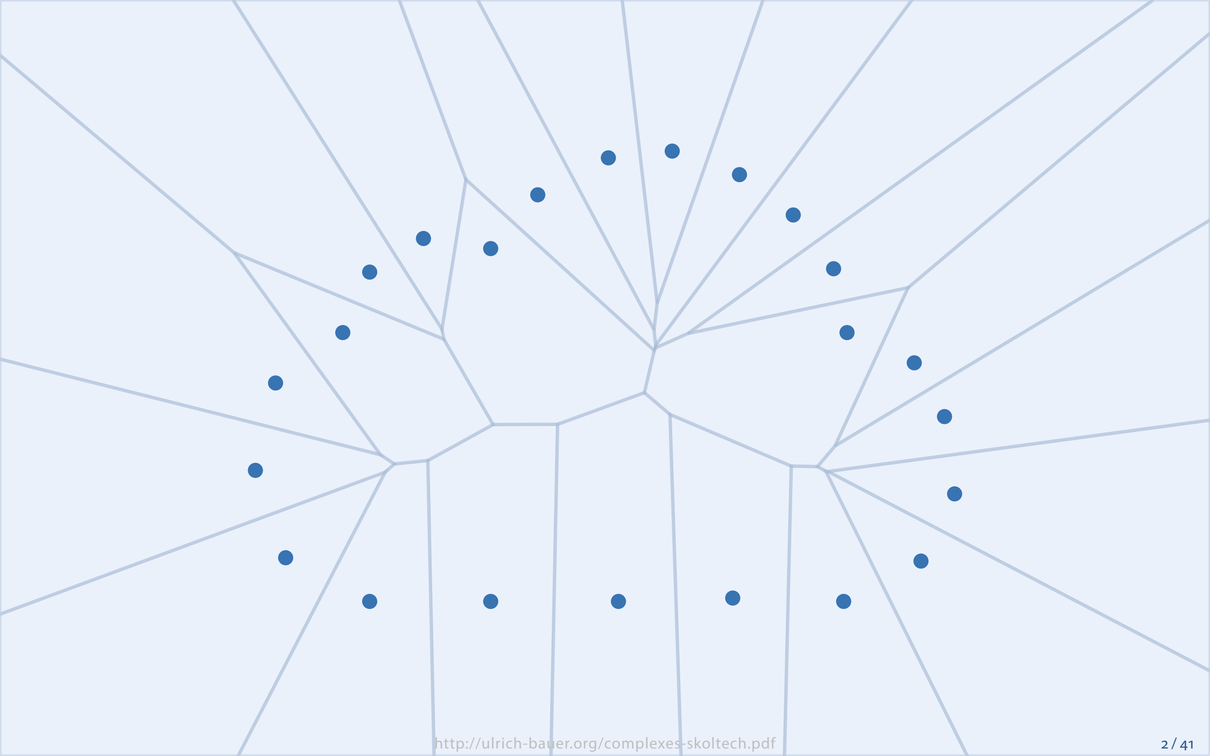


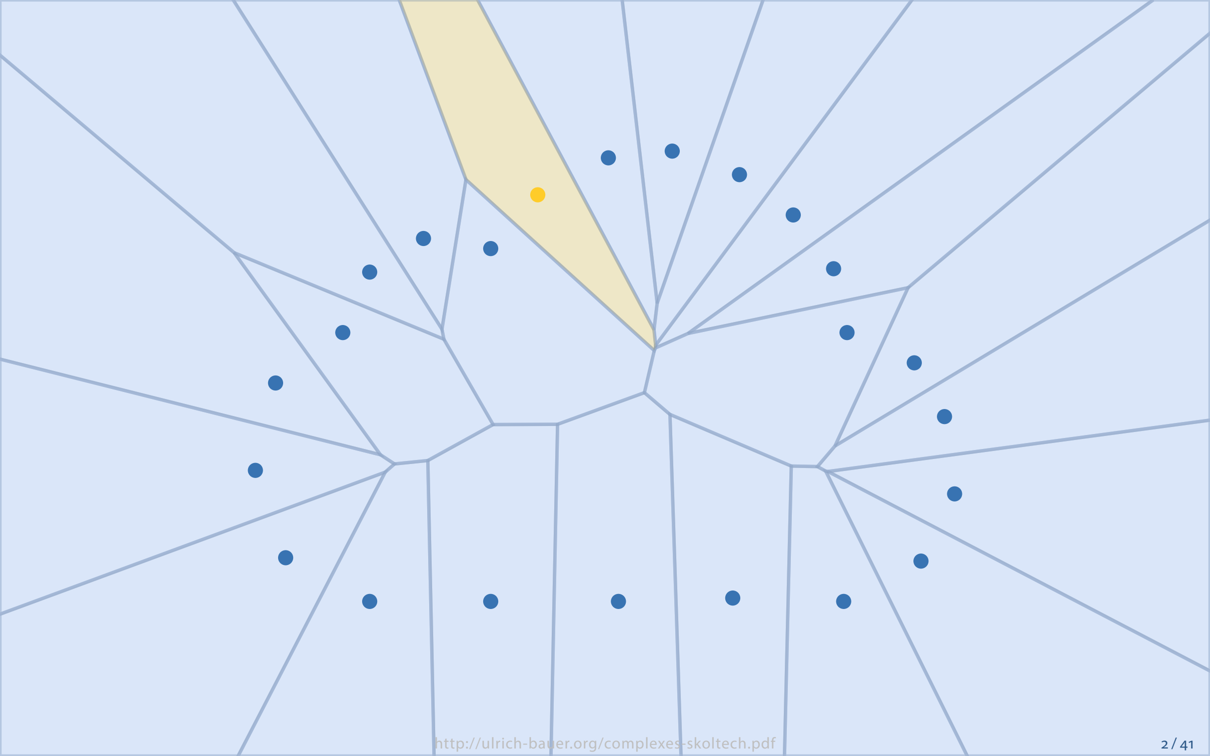


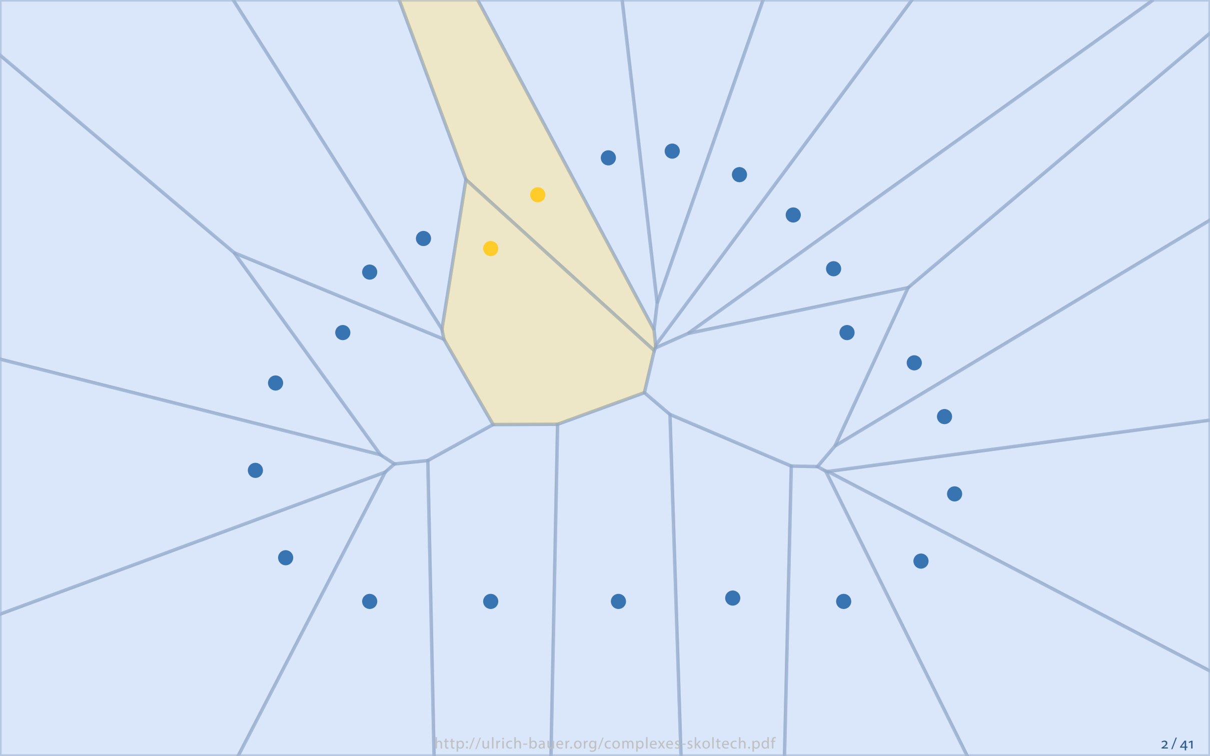


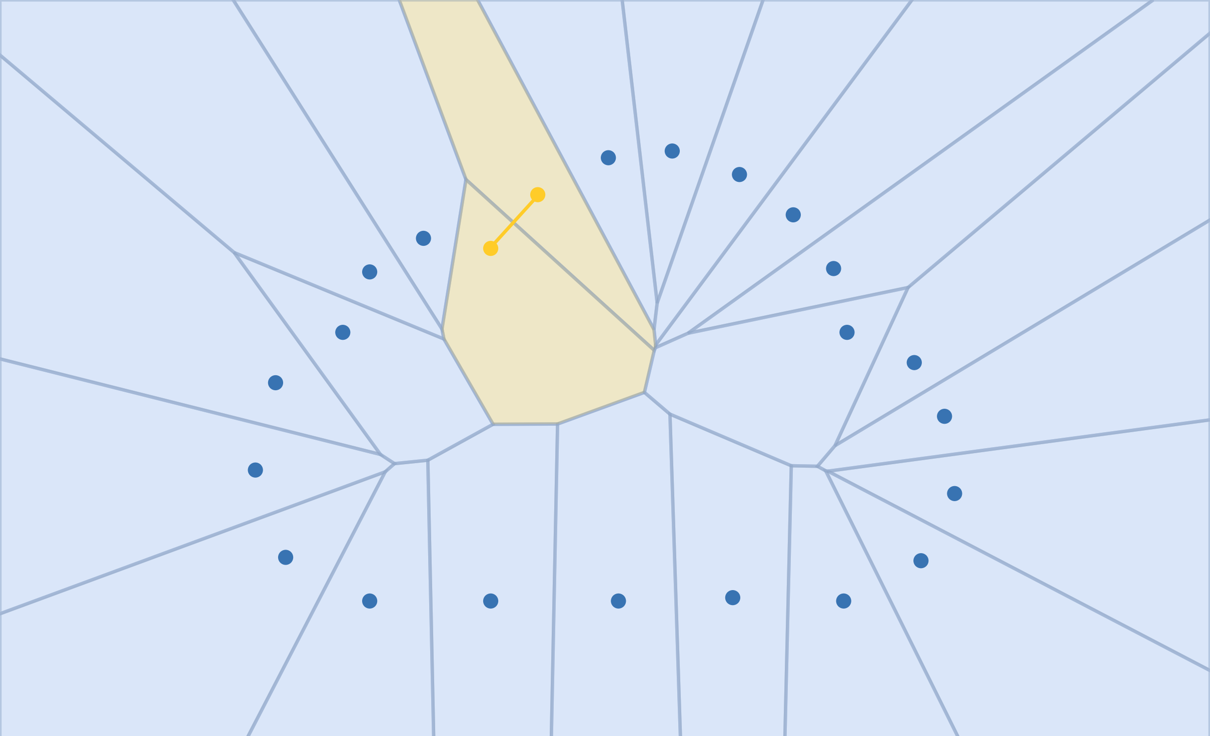


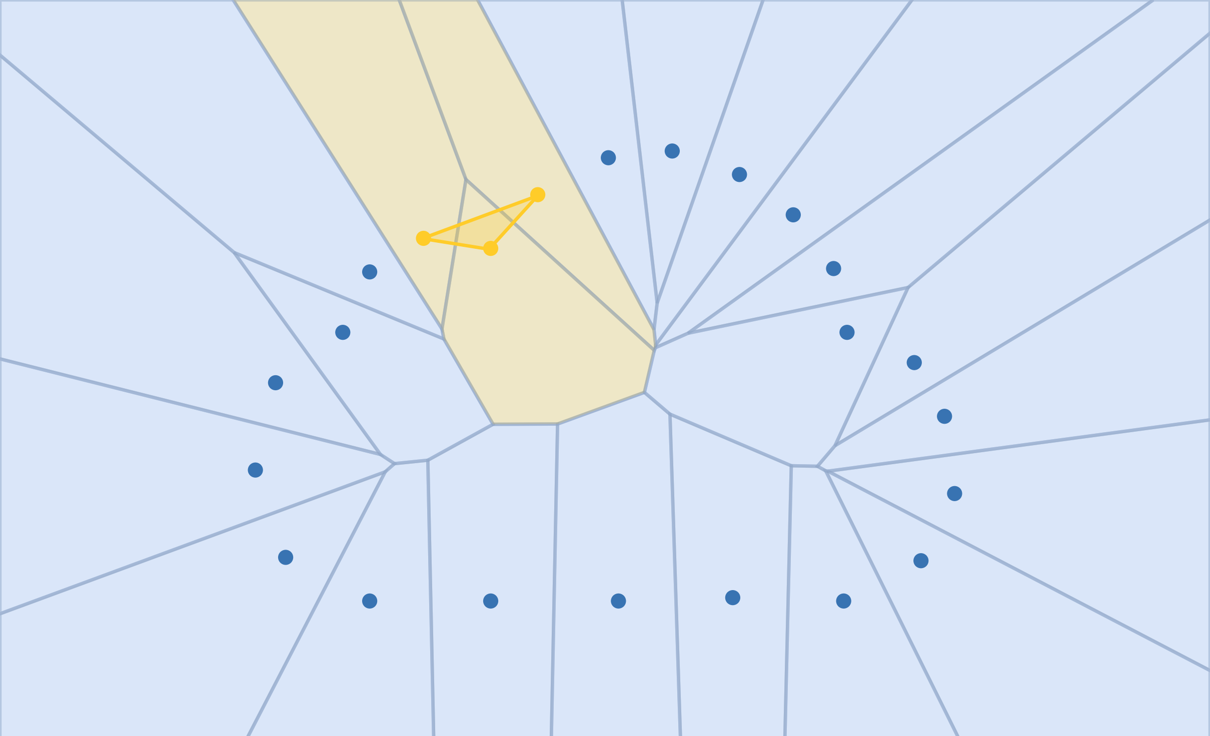


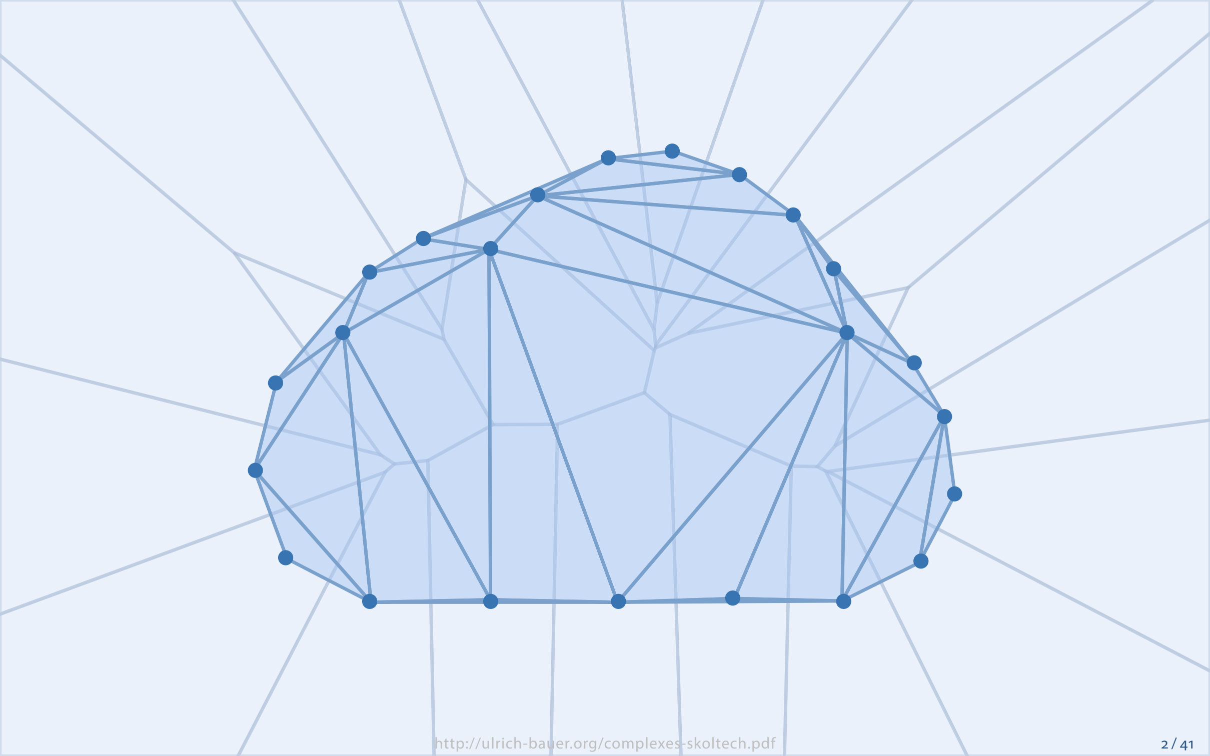


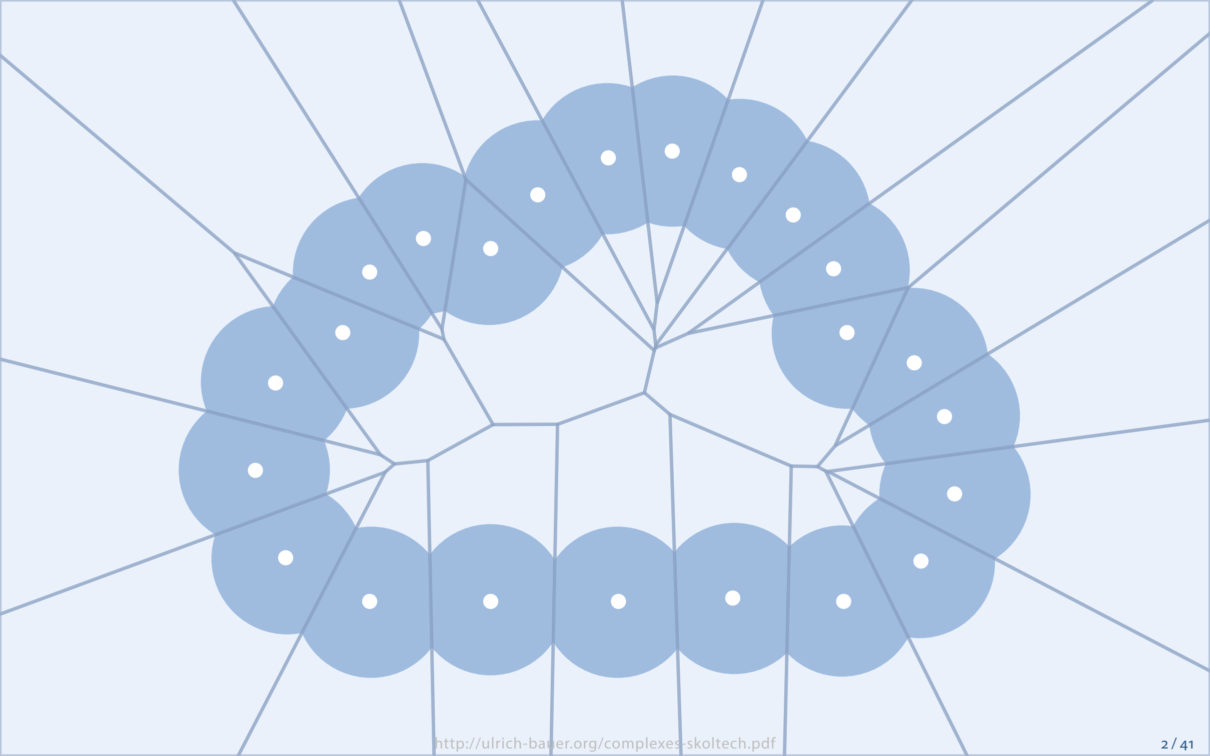


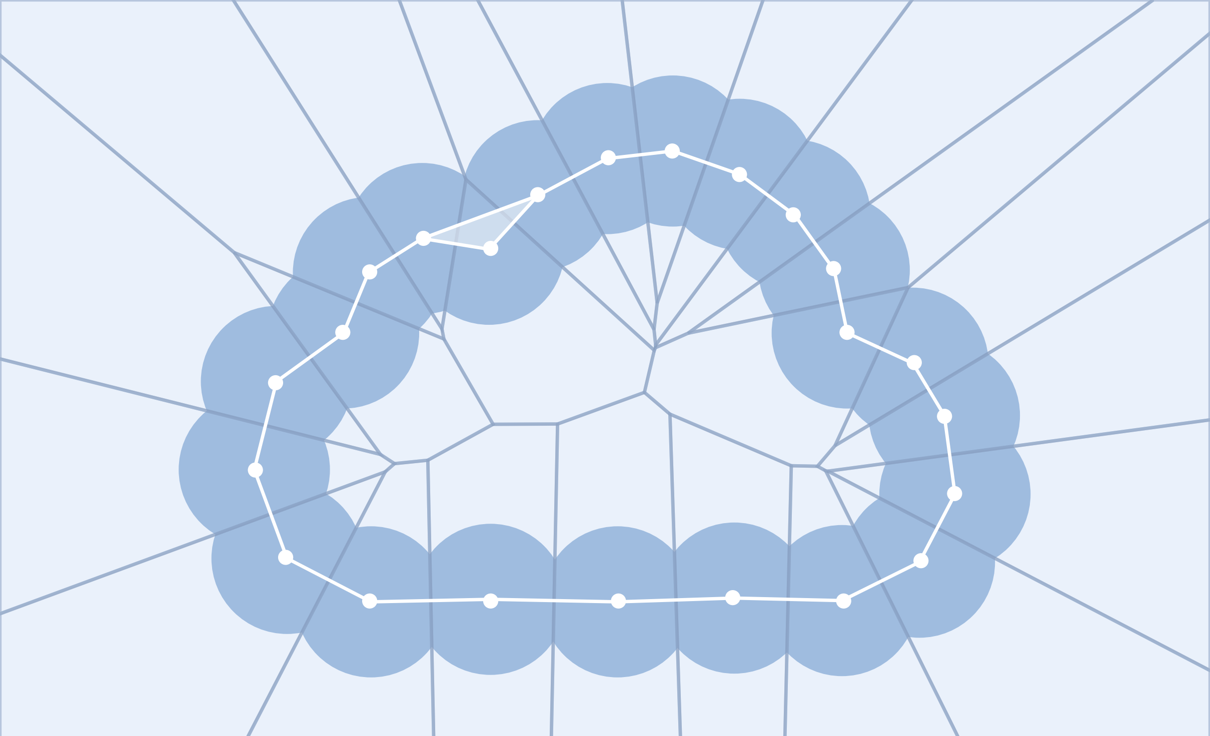


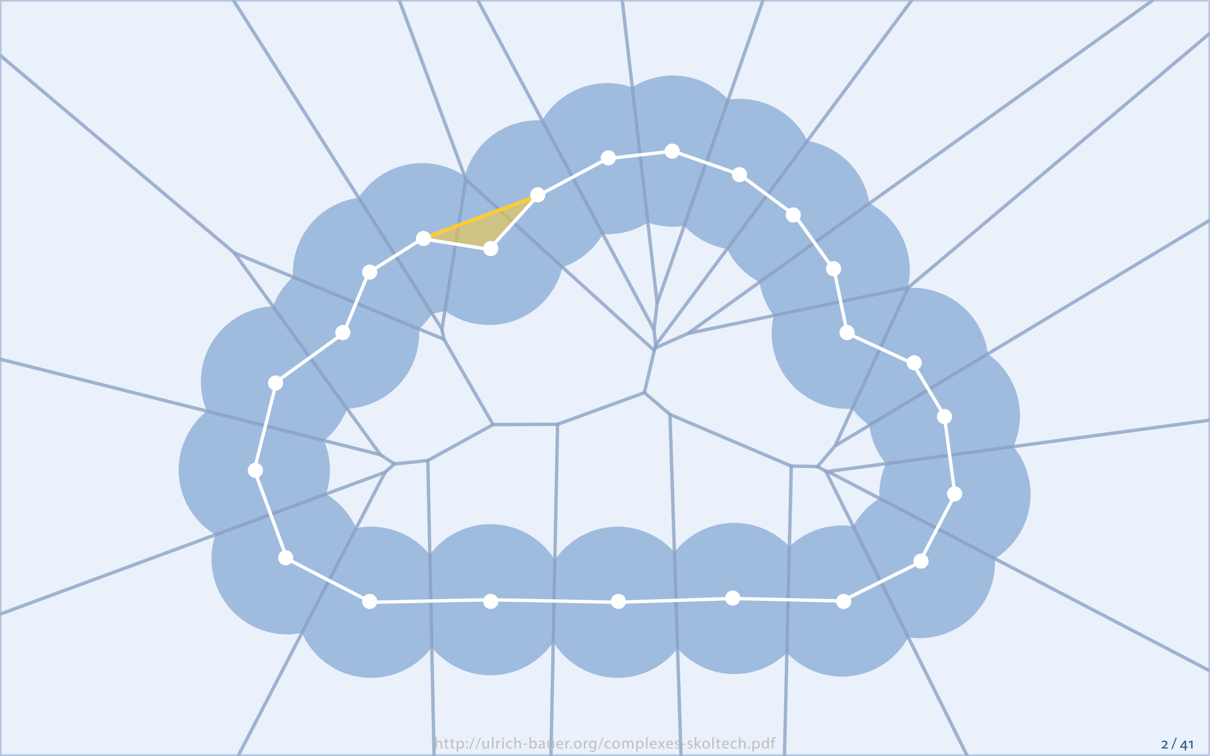


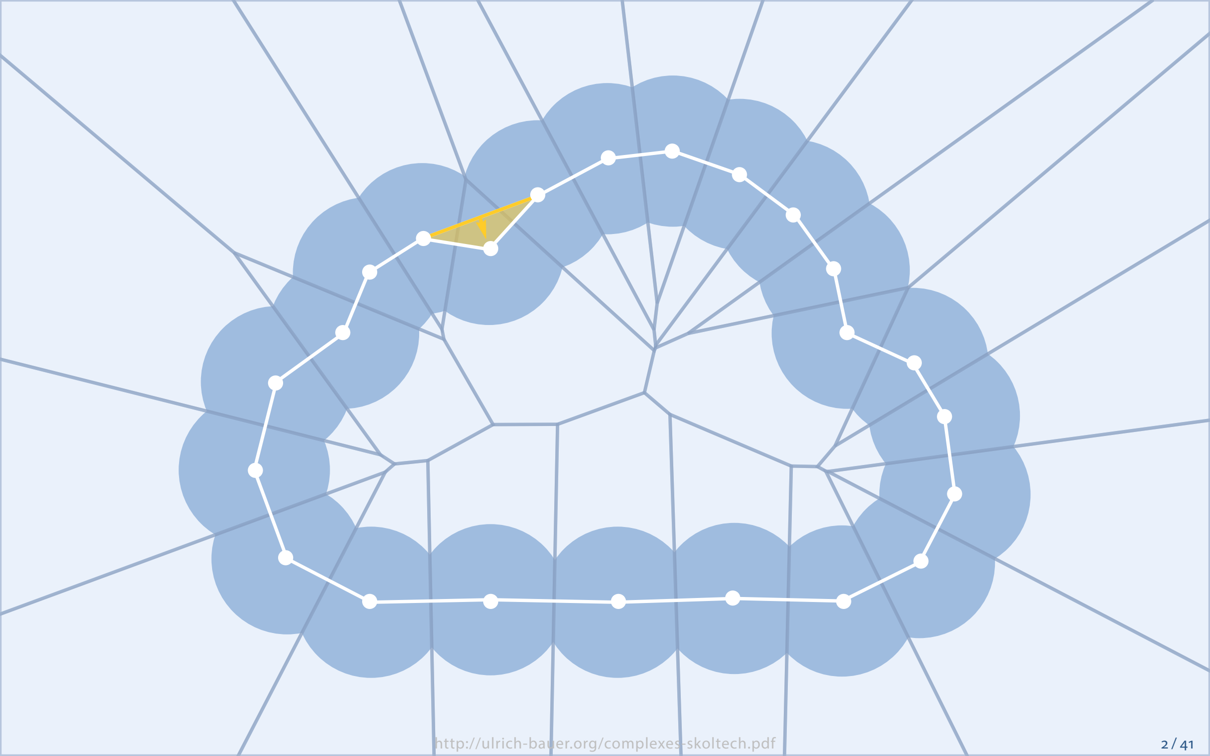


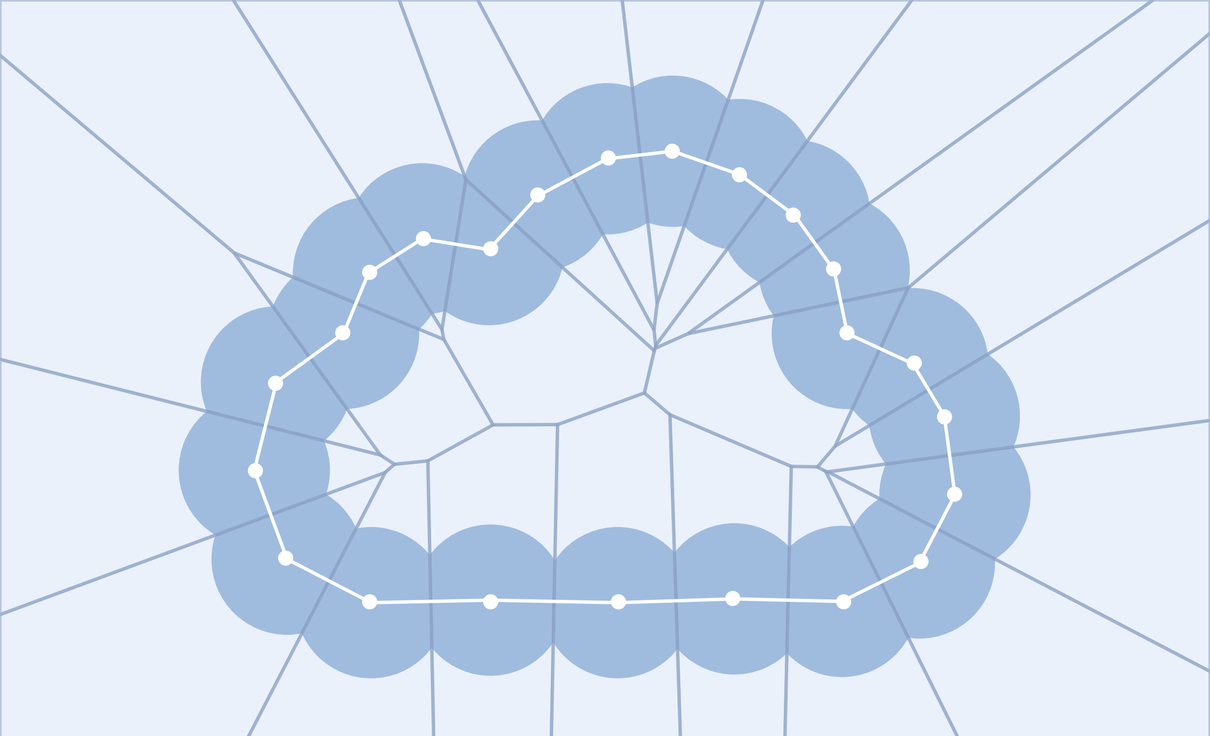


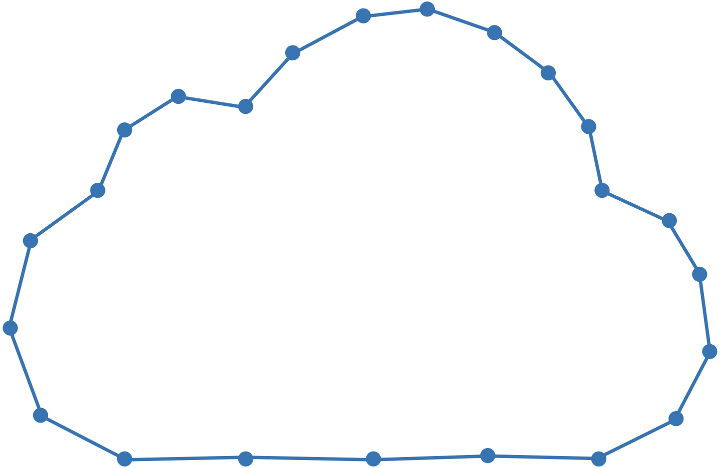












Connecting Čech and Delaunay complexes

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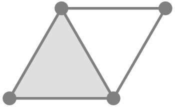
- Are all three complexes homotopy equivalent?
- Are they related by a sequence of *simplicial collapses*?

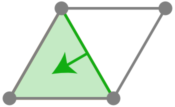
Simplicial collapses



Definition (Whitehead 1938)

Let K be a simplicial complex.

Simplicial collapses



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- A *free face* of K is a simplex that has a unique proper coface.

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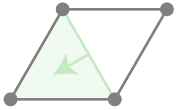

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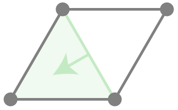

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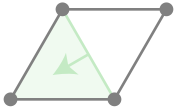

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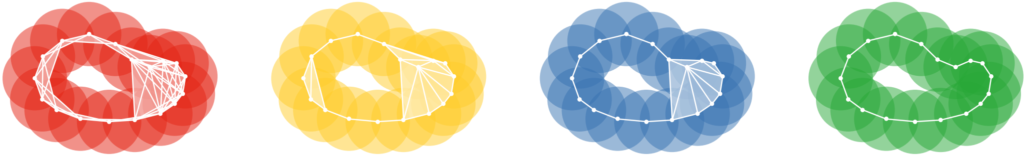
If there is a sequence of such elementary collapses from K to M, we say that K *collapses* to M (written $K \searrow M$).

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

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



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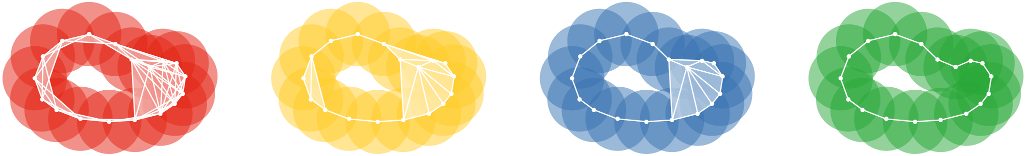
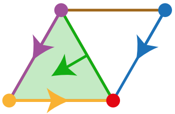


- Extends to weighted Delaunay triagulations
- All collapses are induced by a single *discrete gradient field*
- This yields explicit isomorphims in persistent homology

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.



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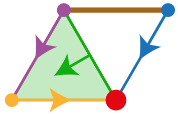

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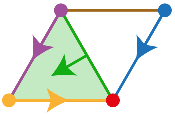

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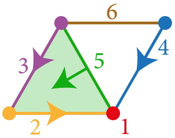
A function $f : K \to \mathbb{R}$ on a simplicial complex is a *discrete Morse function* if for all $t \in \mathbb{R}$:

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



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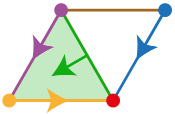

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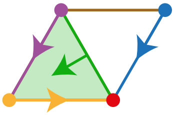

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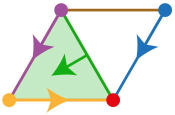

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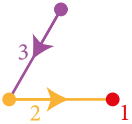

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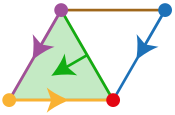

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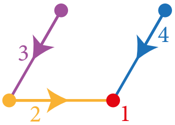

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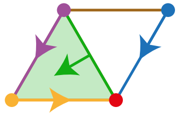

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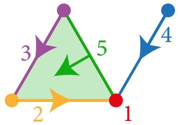

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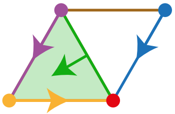

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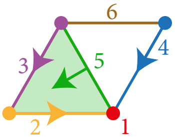

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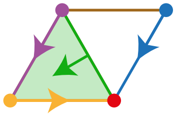

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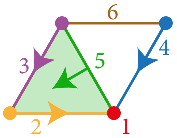

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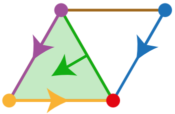

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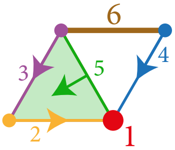

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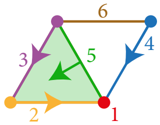
If $f^{-1}(t) = \{Q\}$ then t is a *critical value.*

Collapses from Morse functions and gradients

Let f be a discrete Morse function on a simplicial complex K.



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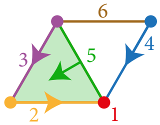

Theorem (Forman 1998)

If $(s, t]$ contains no critical value of f, then $K_t \searrow K_s$.

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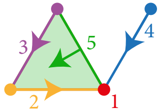

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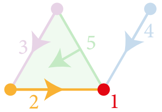

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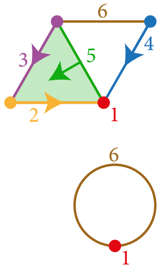
Corollary

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



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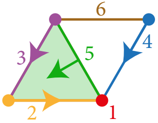

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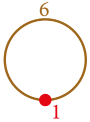

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Let V be a discrete gradient field on a simplicial complex K, and let L be a subcomplex of K.

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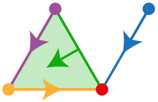
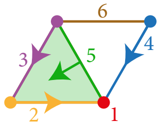


If $K \setminus L$ is a union of pairs of V, then $K \searrow L$.

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

Collapses from Morse functions and gradients

Let f be a discrete Morse function on a simplicial complex K.



Theorem (Forman 1998)

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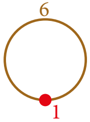

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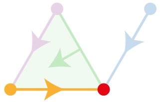

Čech and Delaunay functions

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$X \subset \mathbb{R}^d$: finite point set (in general position)

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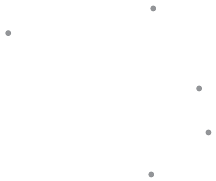

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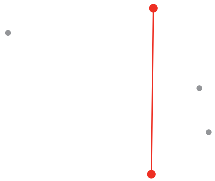

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- *Čech radius function* $f_{\mathrm{Cech}}(Q)$:
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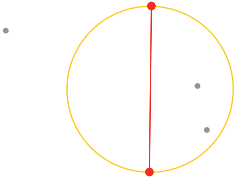

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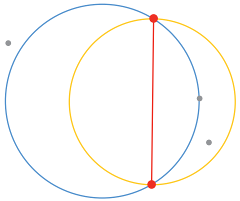
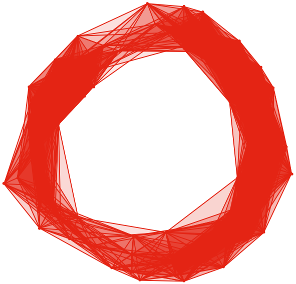
    - defined only on $\mathrm{Del}(X)$



Čech and Delaunay complexes from functions

For any radius r:

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



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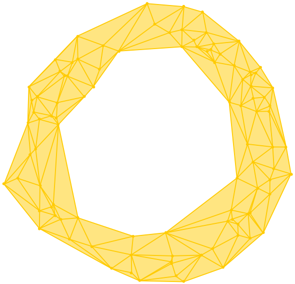

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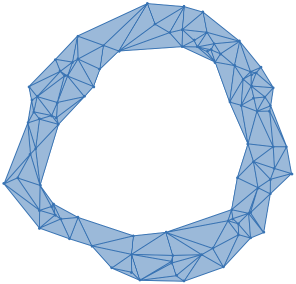

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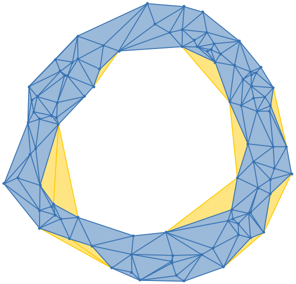

Unfortunately…

Neither the Čech nor the Delaunay functions
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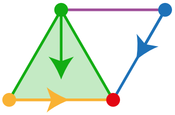
- Example: two simplices Q, Q' with $f_{\text{Cech}}(Q) = f_{\text{Cech}}(Q')$ where neither is a face of the other:

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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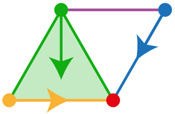

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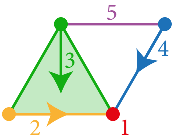
A *generalized discrete Morse function* $f : K \to \mathbb{R}$ satisfies:

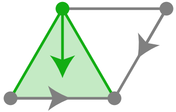
- the sublevel sets $K_t = f^{-1}(-\infty, t]$ are subcomplexes (for all $t \in \mathbb{R}$)
- the level sets $f^{-1}(t)$ form a generalized vector field (the *discrete gradient* of f)



Refining generalized vector fields

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

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



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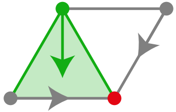

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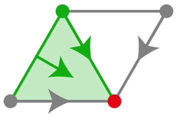
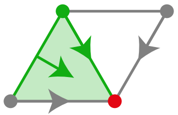


Refining generalized vector fields



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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.

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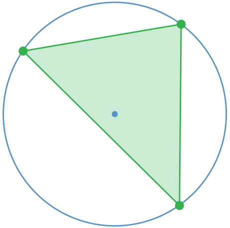
The Čech function and the Delaunay function are generalized discrete Morse functions.

The following are equivalent:

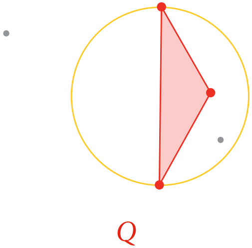
- *Q is a critical simplex of* f_{Cech}
- *Q is a critical simplex of* f_{Del}
- $f_{\mathrm{Cech}}(Q) = f_{\mathrm{Del}}(Q)$
- *Q is a* centered *Delaunay simplex (containing the circumcenter in the interior)*



Čech 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



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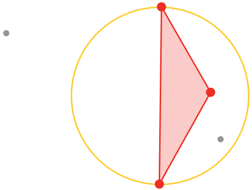

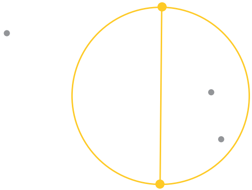

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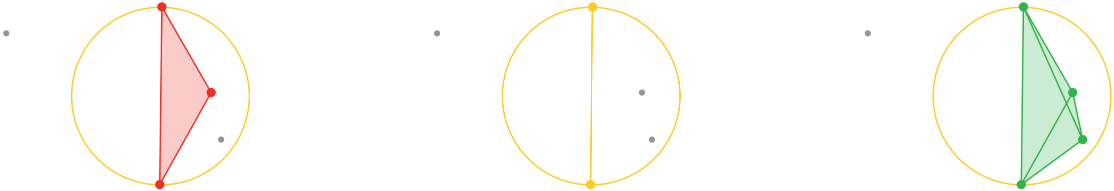

Q $\quad$ $\operatorname{On} S$ $\quad$ $\operatorname{Encl} S$

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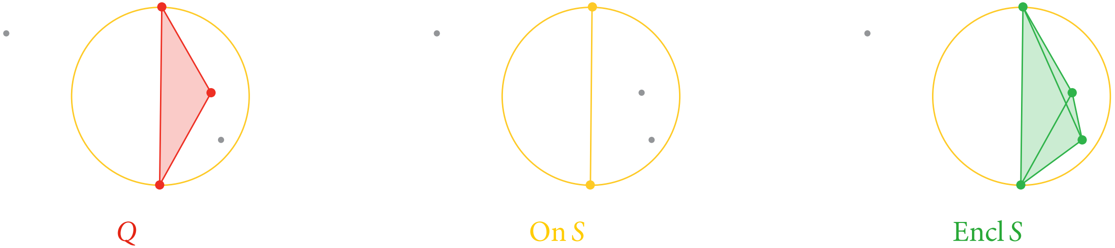

The front and back faces of a simplex

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

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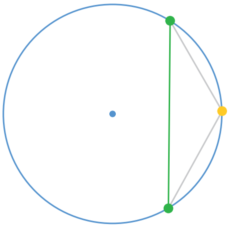

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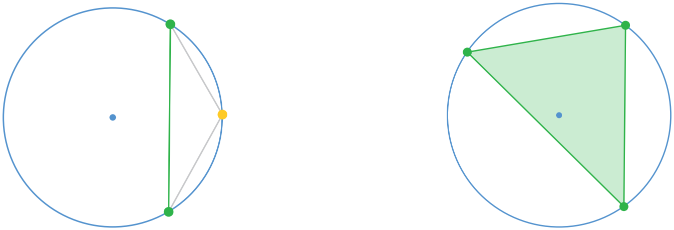
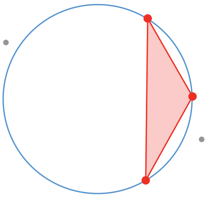


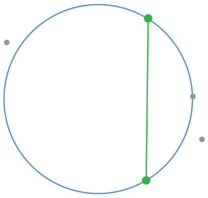
Delaunay face intervals

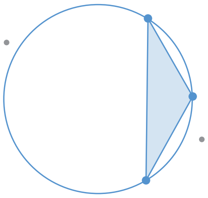
Lemma

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

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







Selective Delaunay complexes

Sphere optimization problems

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

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

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

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- Čech function: choose $E = \varnothing$
- Delaunay function: choose $E = X$

Sphere optimization problems

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

$$\begin{aligned} \underset{r,z}{\text{minimize}} \quad & r^2 & \\ \text{subject to} \quad & \|z - q\|^2 \le r^2, & q \in Q, \\ & \|z - e\|^2 \ge r^2, & e \in E. \end{aligned}$$

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

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$$
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& && 2\langle z, e\rangle - a - \|e\|^2 \leq 0, && \forall e \in E.
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The Karush–Kuhn–Tucker optimality conditions

Consider an optimization problem of the form

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

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

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

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

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

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

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

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 $\mathrm{On}\, S$,*
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Corollary

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

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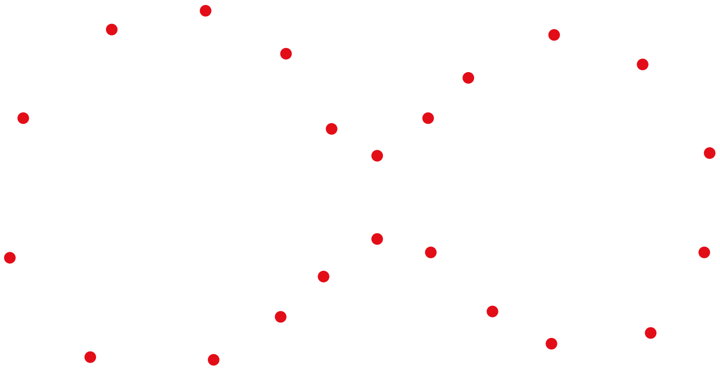
- *The Čech face intervals are of the form $[\mathrm{On}\, S, \mathrm{Encl}\, S]$.*
- *The Delaunay face intervals are of the form $[\mathrm{Front}\, S, \mathrm{On}\, S]$.*

The Delaunay gradient



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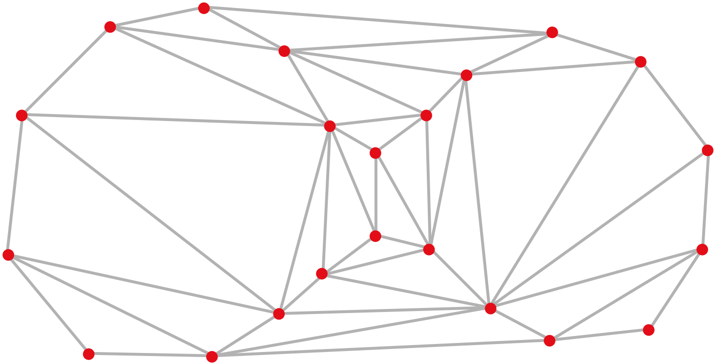

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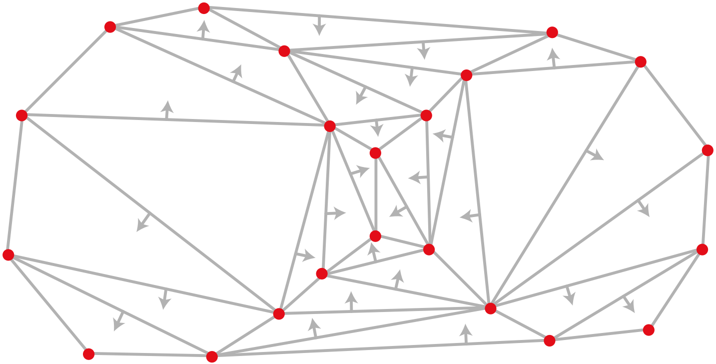

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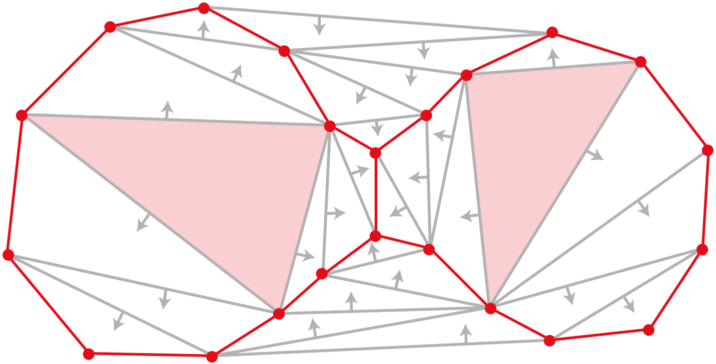

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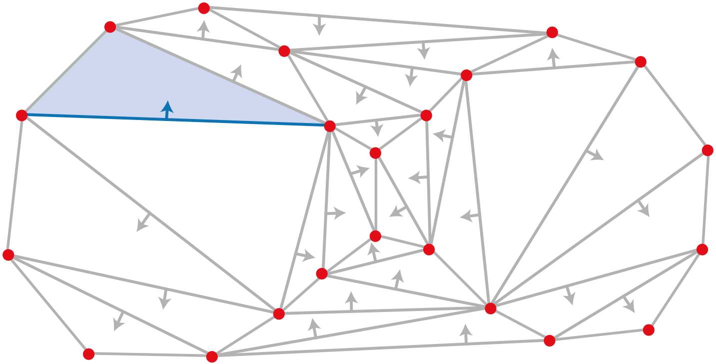

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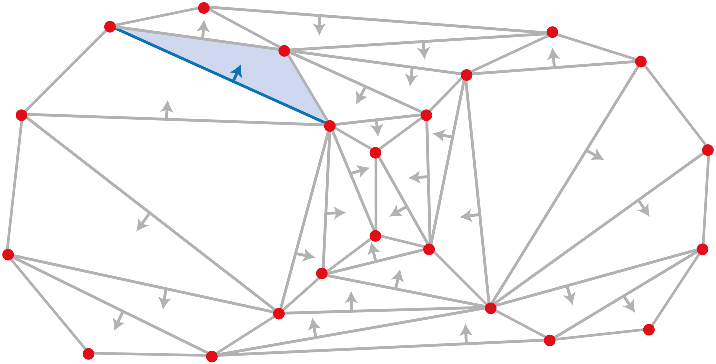

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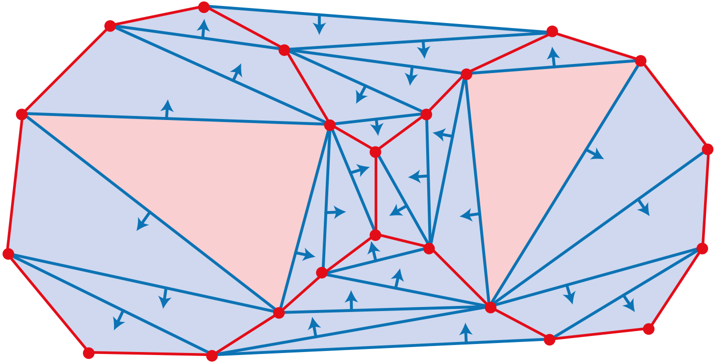

Wrap complexes

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

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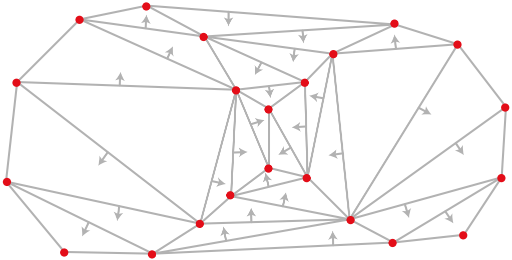

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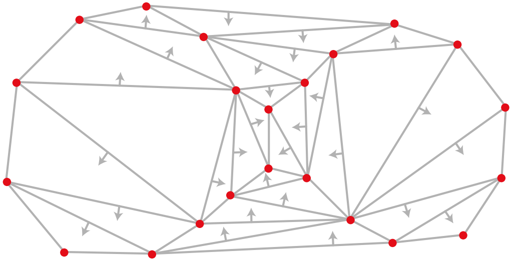

Define $\mathrm{Wrap}_r(X)$ as the smallest subcomplex of $\mathrm{Del}\, X$ that

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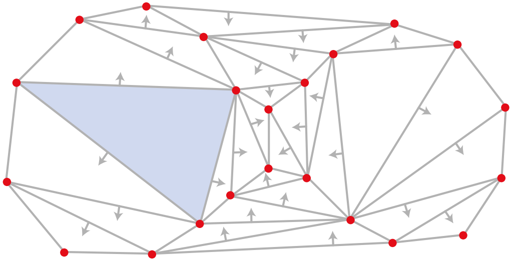

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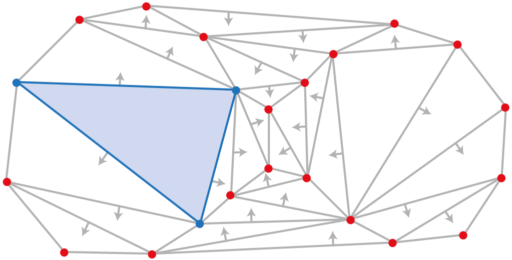

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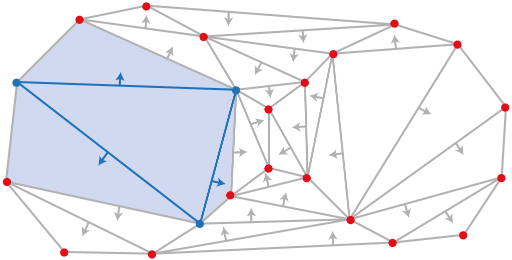

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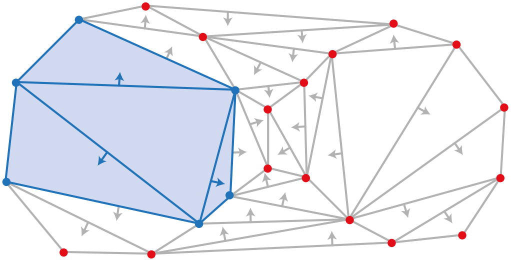

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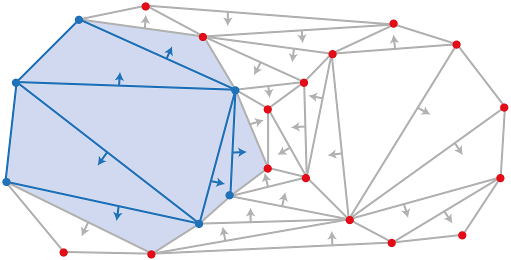

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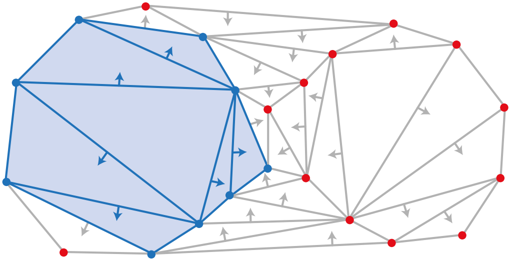

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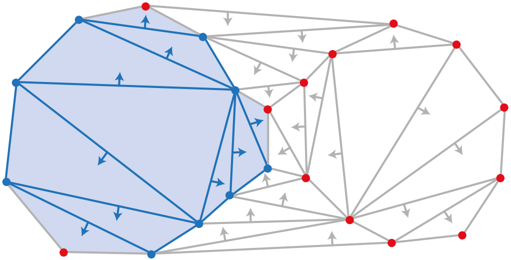

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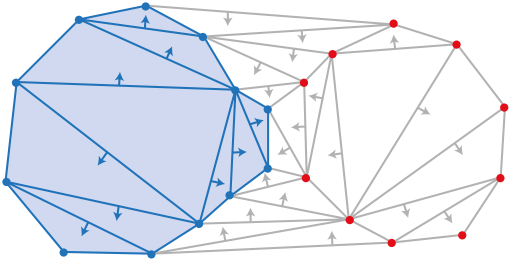

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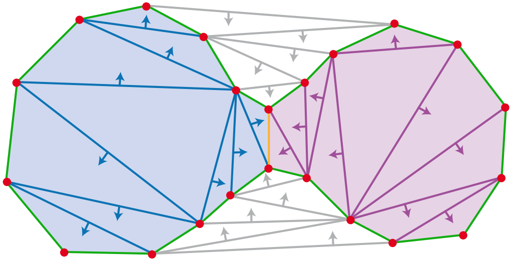

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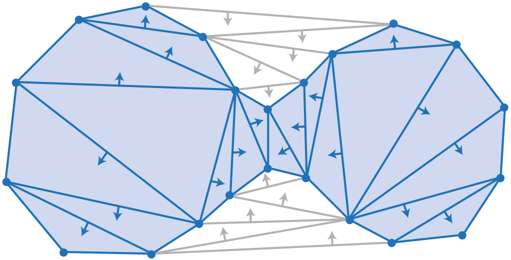

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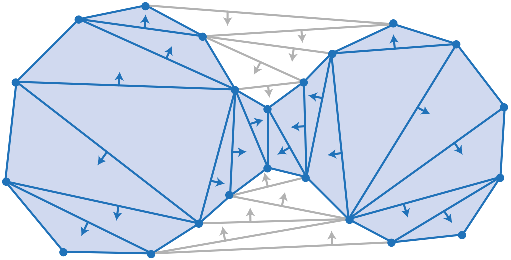

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Corollary

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

Vietoris–Rips complexes

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Consider a finite metric space (X, d).

The *Vietoris–Rips complex* is the simplicial complex

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

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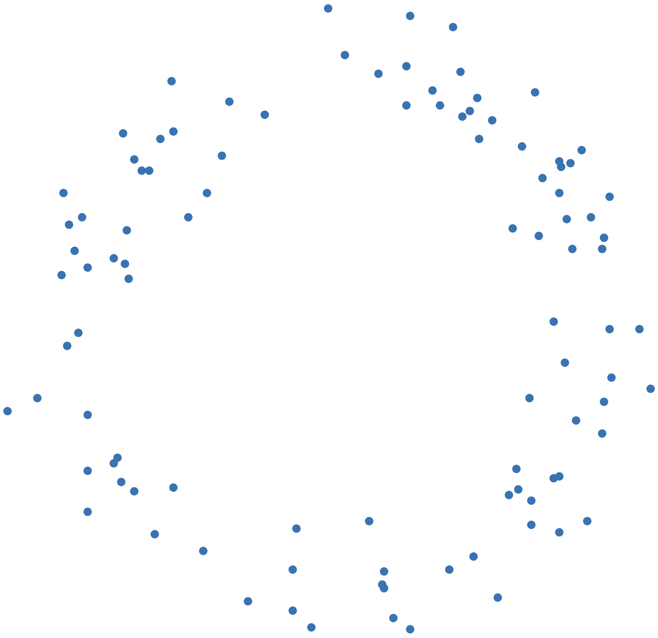
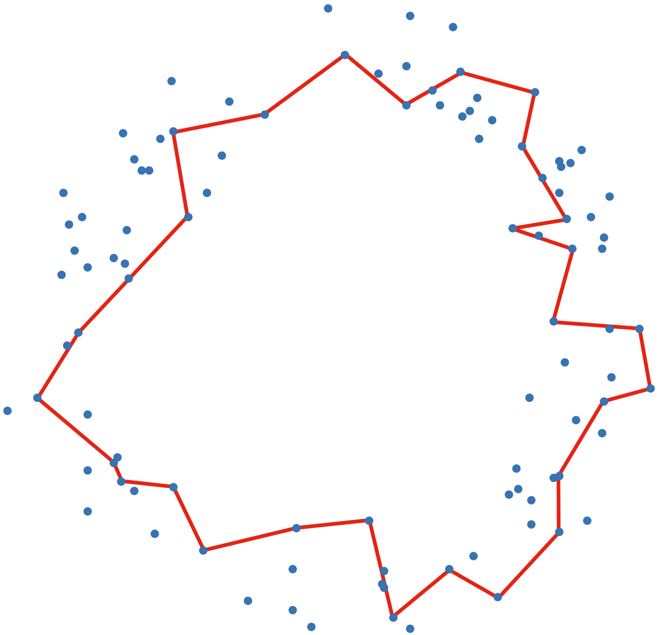
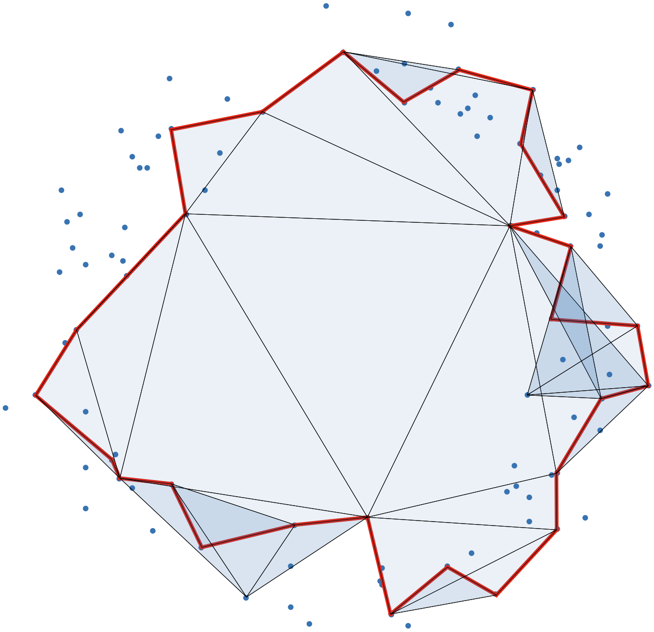
- all edges with pairwise distance $\leq t$
- all possible higher simplices

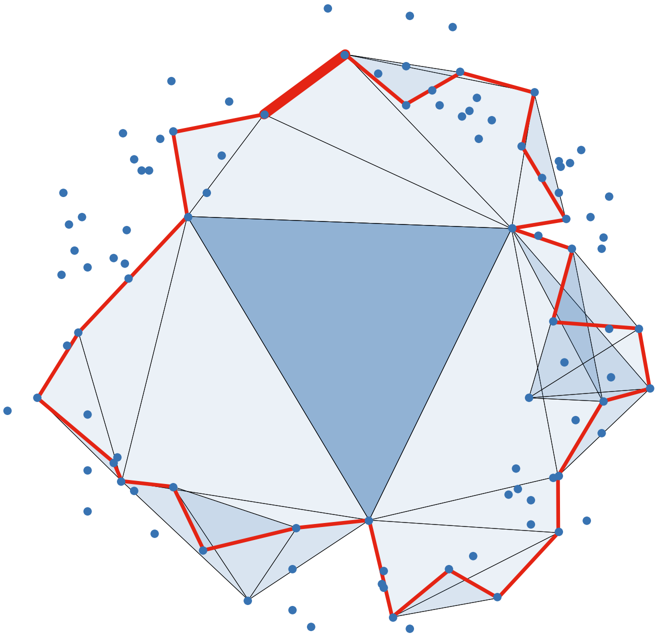
For large t, $\mathrm{Rips}_t(X)$ is the full simplex with vertices X

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









Another example data set

coil100-obj14-grid.pdf

Ripser

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 conjuction!

Matrix reduction

Computing homology

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

- compute basis for boundaries $B_* = \operatorname{im} \partial_*$
- extend to basis for cycles $Z_* = \ker \partial_*$
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Computing *persistent* homology $H_* = Z_*/B_*$ (for a simplexwise filtration $K_i \subseteq K$):

- compute *filtered* basis for boundaries $B_* = \operatorname{im} \partial_*$
- 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 $d = 0, \ldots, k$

Notation:

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

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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

$$I_b = \{i : R_i = 0\} \qquad \textit{birth indices},$$

$$I_d = \{j : R_j \neq 0\} \qquad \textit{death indices},$$

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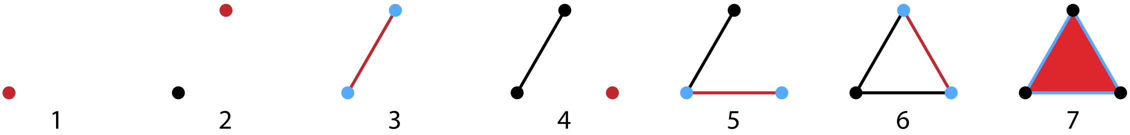
Matrix reduction



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

R

$= D \cdot$

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

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

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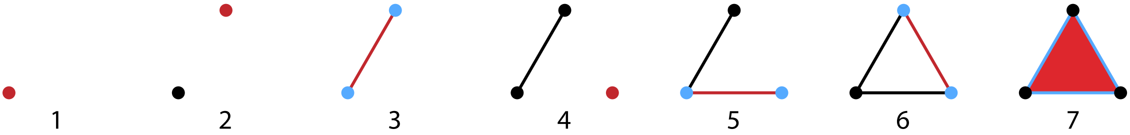

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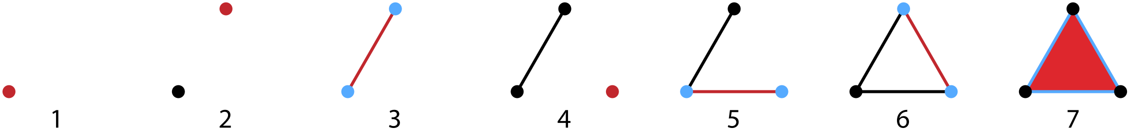

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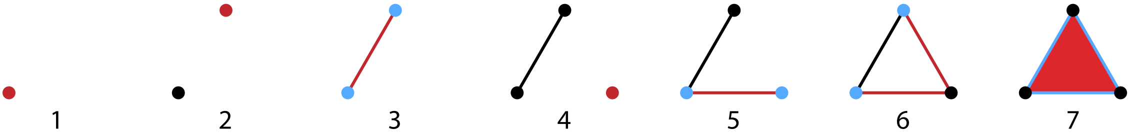

	1	2	3	4	5	6	7
1			1		1	1	
2			1			1	
3							1
4					1	0	
5							1
6							1
7							

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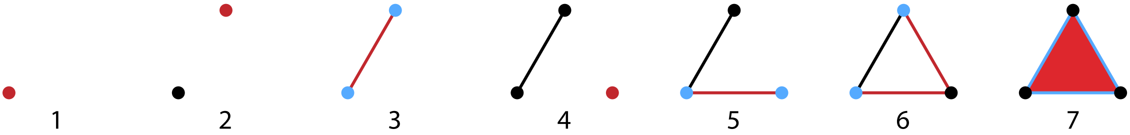

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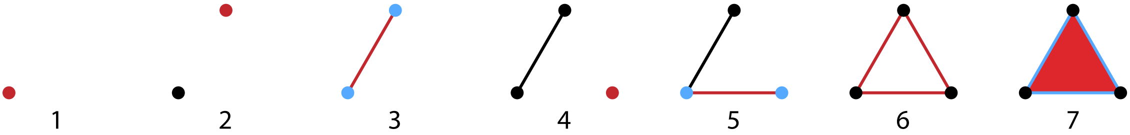

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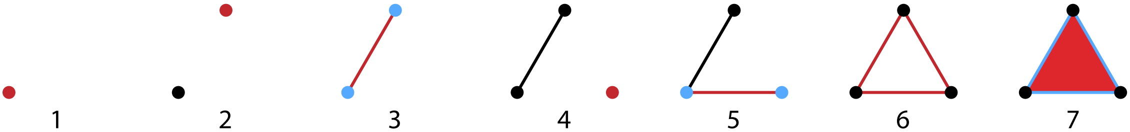

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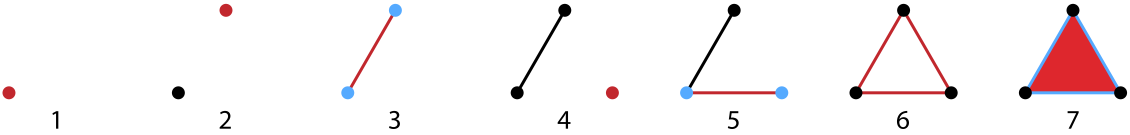

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Algorithm (over $\mathbb{Z}/2\mathbb{Z}$):

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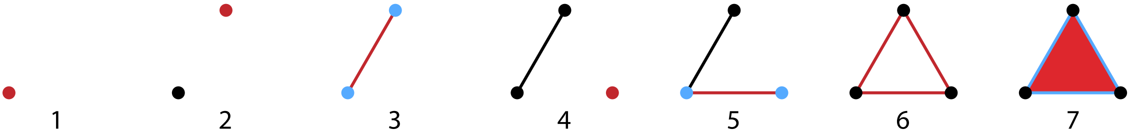

	1	2	3	4	5	6	7
1			1		1		
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R

$= D \cdot$

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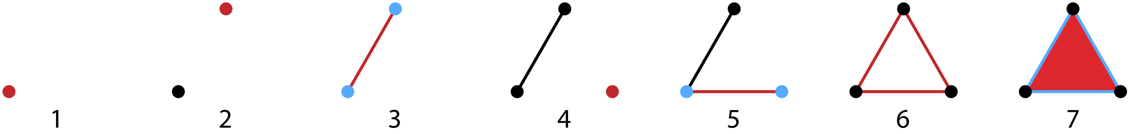

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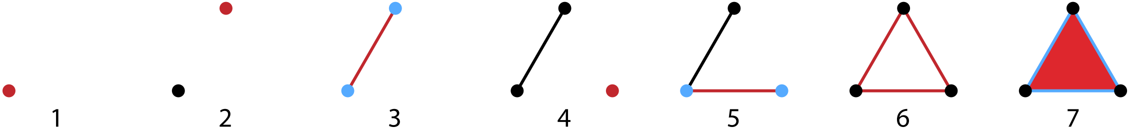

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Clearing

Clearing non-essential positive columns

Recall:

- Columns with indices $\operatorname{PivotIndices} R$ (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: $i = \operatorname{PivotIndex} R_j$ 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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$k = 2, n = 192$: $\quad 56\,050\,096 = 1\,161\,471 + 53\,727\,345 + 1\,161\,280$

- 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

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

- Number of columns in coboundary matrix:

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- $k = 2, n = 192$: $\quad 1\,179\,808 = 1\,161\,471 + 1 + 18\,336$

Observations

For a typical input:

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

- Only $79 + 42 + 1 = 122$ out of $192 + 18\,145 + 1\,143\,135 = 1\,161\,471$ columns are actually modified in matrix reduction

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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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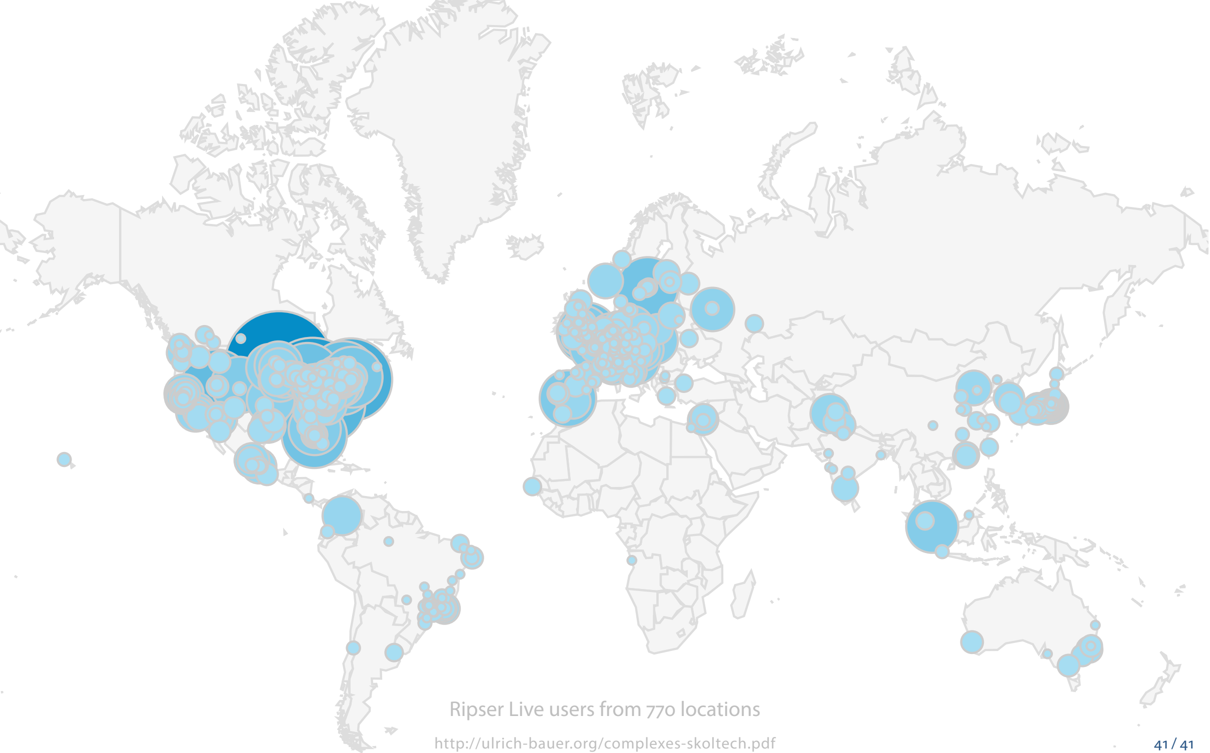
Theorem

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



Ripser Live users from 770 locations

Ulrich Bauer.
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Submitted, Aug. 2019. arXiv:1908.02518
Software available at http://ripser.org.

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