Ripser

Efficient computation of Vietoris–Rips persistence barcodes

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TUM

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DFG Deutsche Forschungsgemeinschaft
German Research Foundation

DGD | SFB TRR 109 | Discretization in Geometry and Dynamics

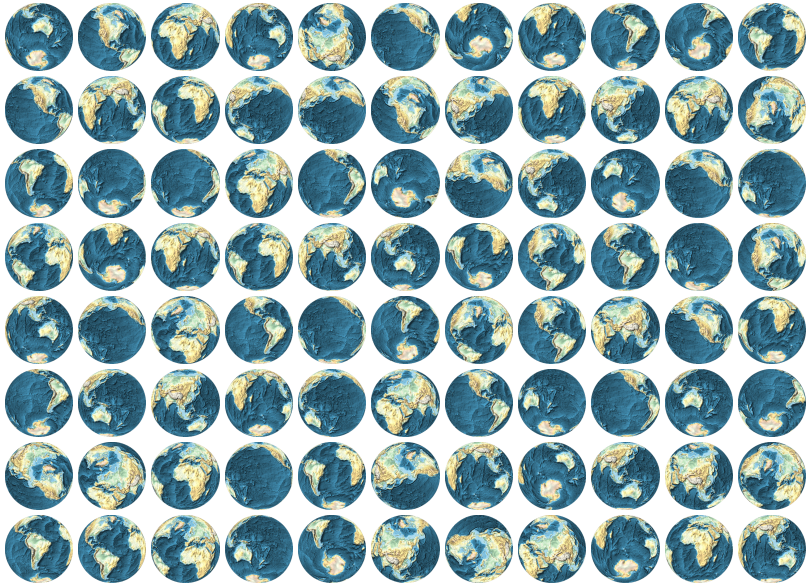
Technical University of Munich

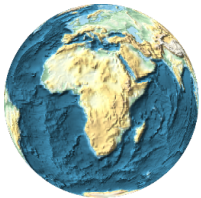
MDSI

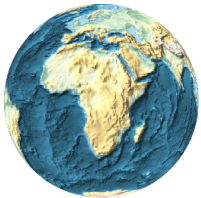
MCML Munich Center for Machine Learning

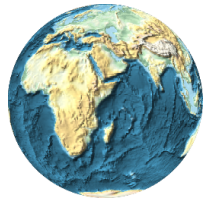
Finding topology in data sets

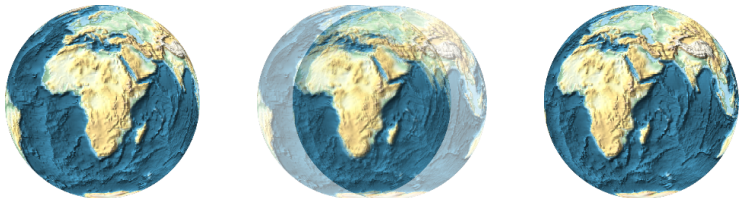
(Columbia Object Image Library)

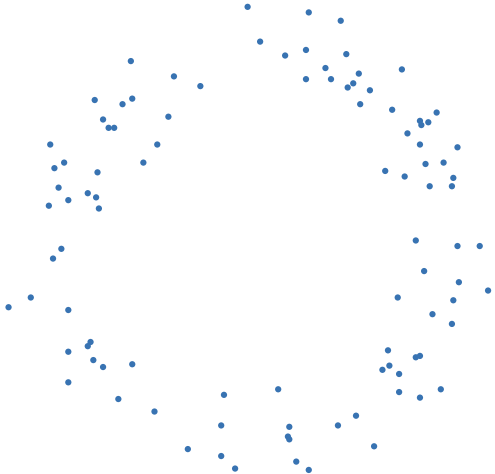


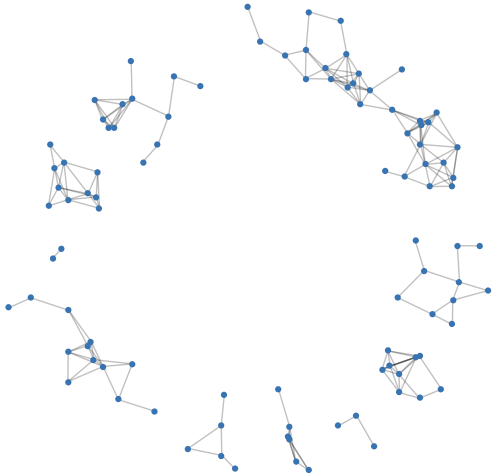


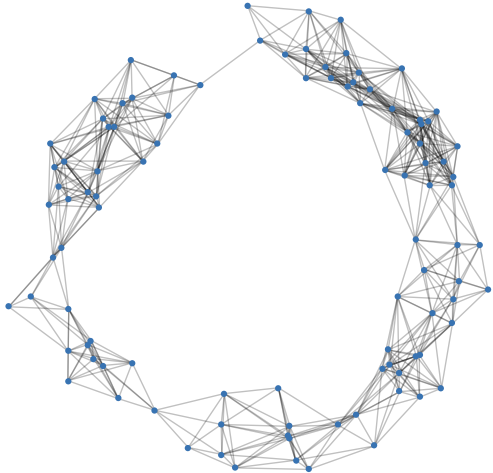


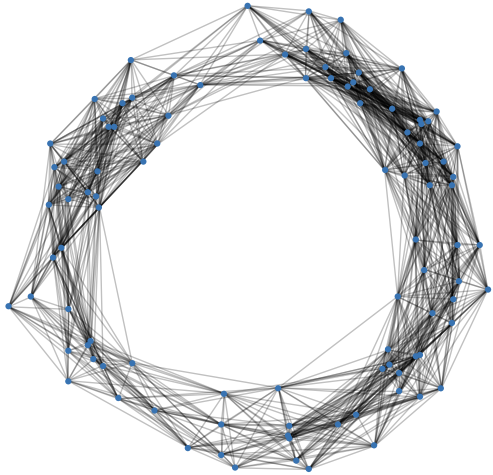


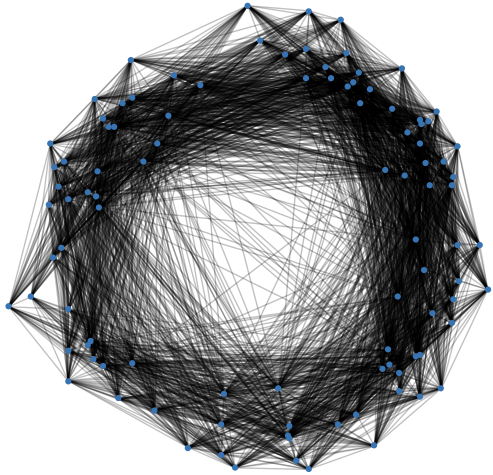


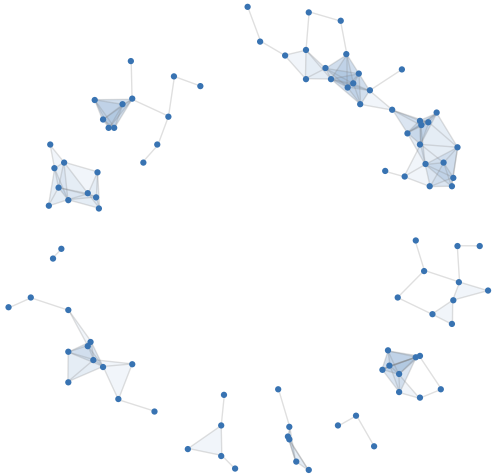


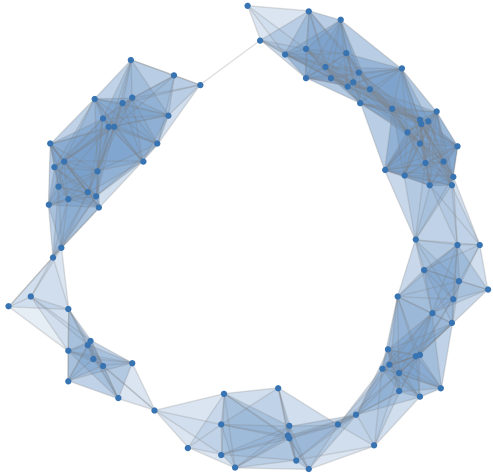


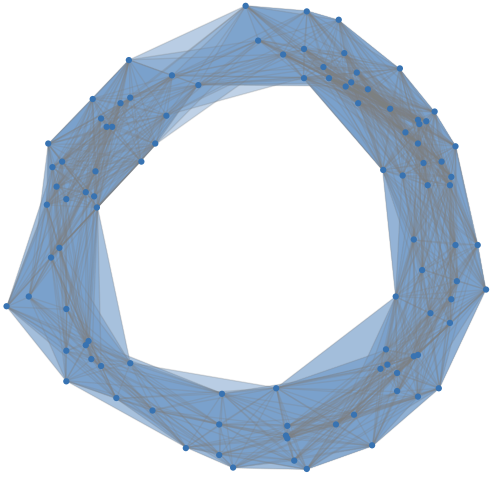


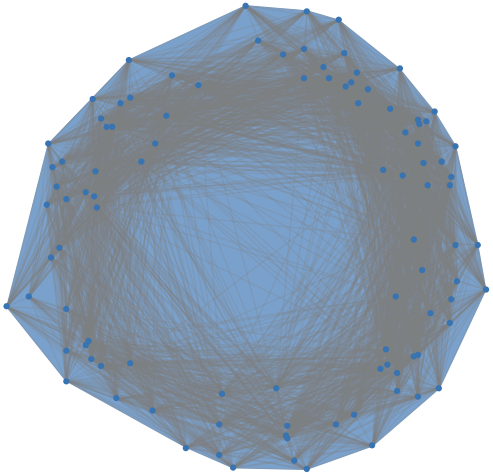












Vietoris–Rips complexes

Consider a finite metric space (X, d).

The *Vietoris–Rips complex* is the simplicial complex

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

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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!

An example computation

Example data set:

- 192 points on $\mathbb{S}^2$
- persistent homology barcodes up to dimension 2
- over 56 mio. simplices in 3-skeleton

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Demo: live.ripser.org

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- Ripser: 0.6 seconds, 160 MB

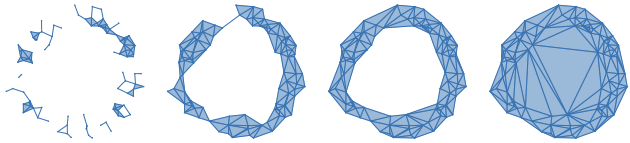
Ripser

A software for computing Vietoris–Rips persistent homology

- 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`), based on
  - WebAssembly (C++ within the browser)
  - D3.js (JavaScript visualization toolbox)
- 2016 ATMCS Best New Software Award (joint with RIVET by M. Lesnick and M. Wright)

Persistent homology

What is persistent homology?



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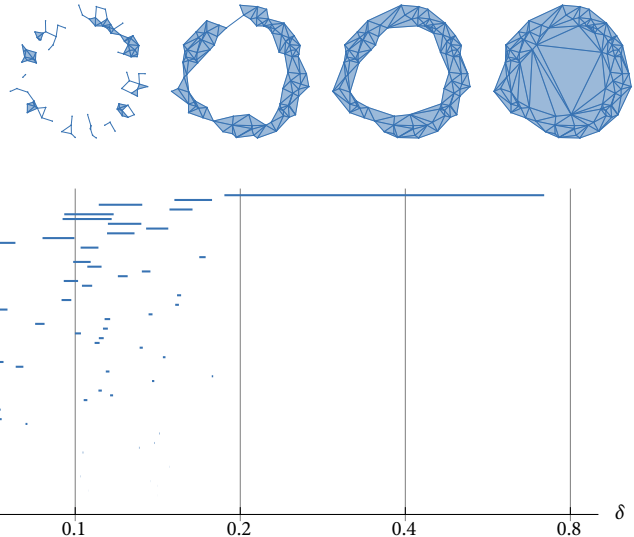

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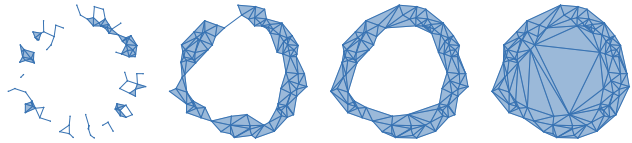

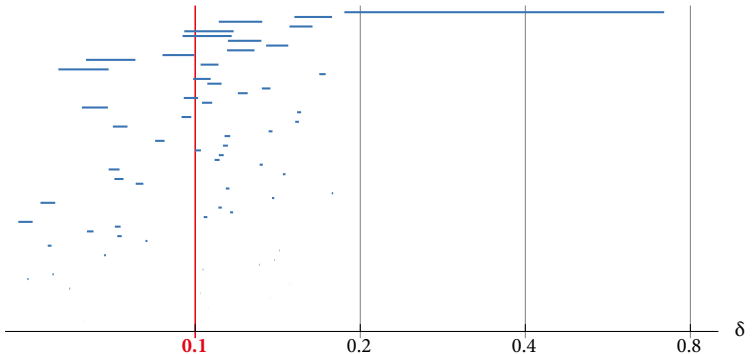

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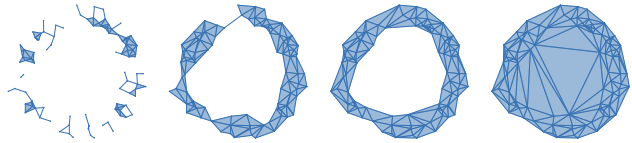

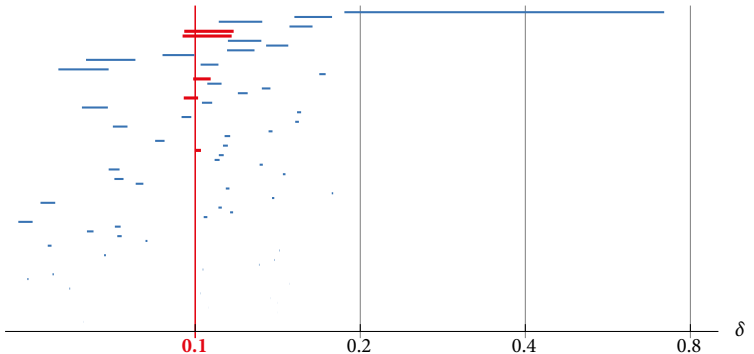

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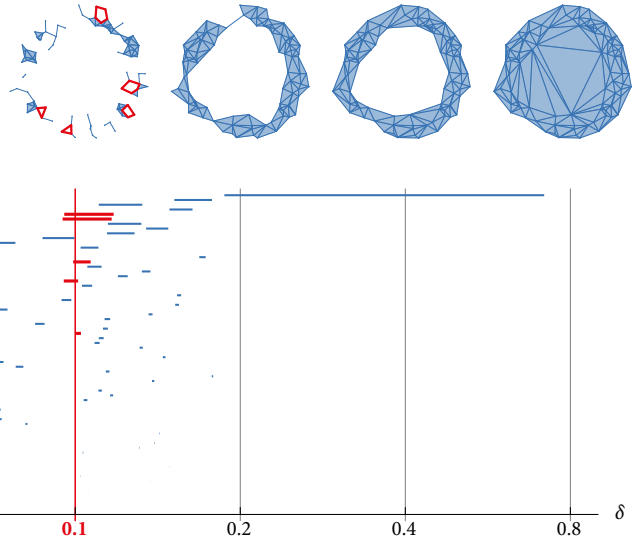

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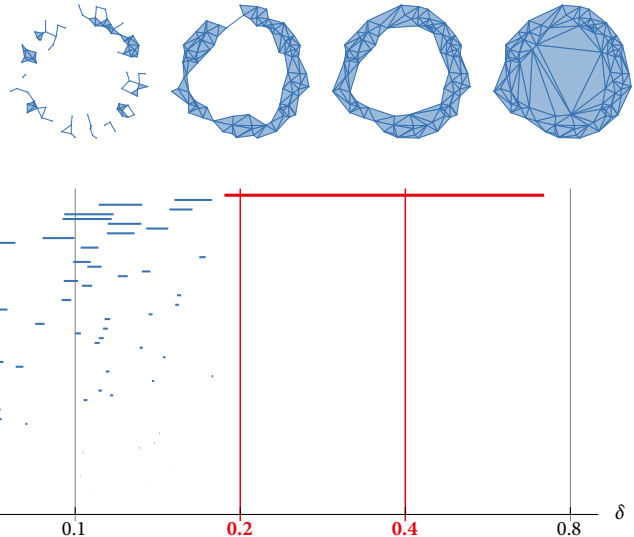

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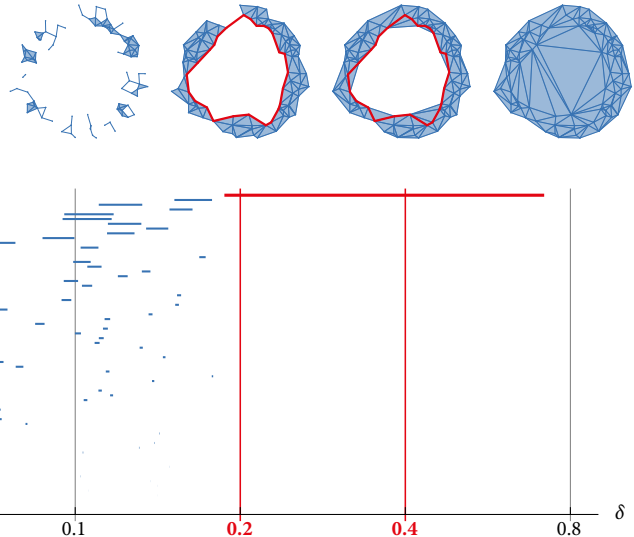
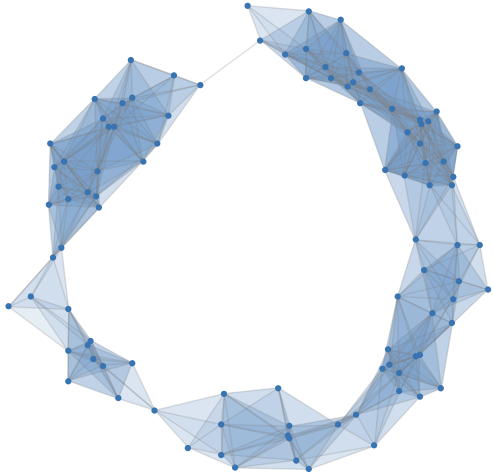
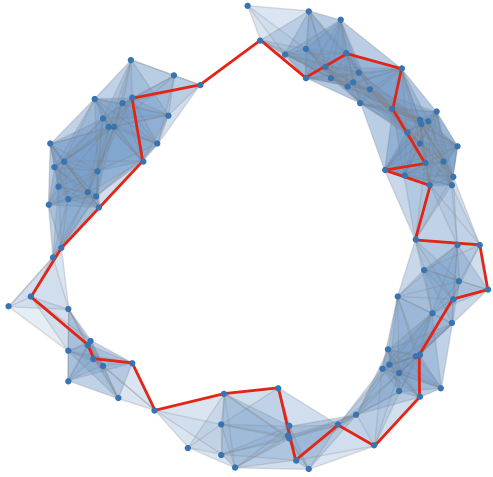
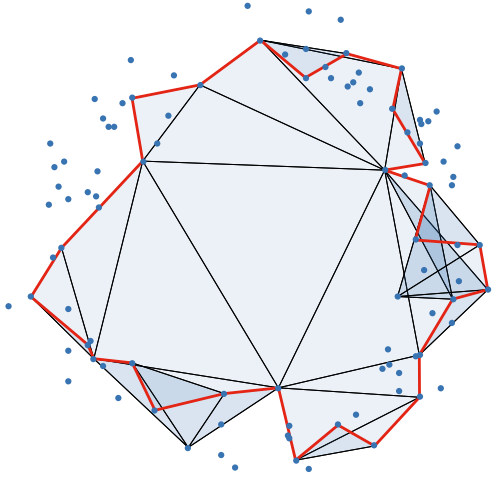
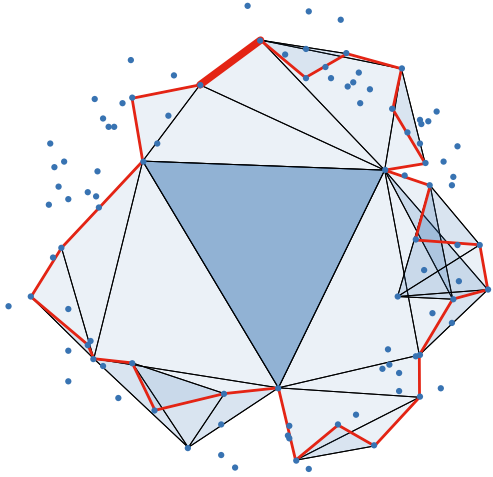








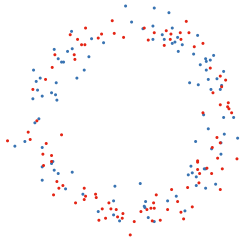


Stability of Vietoris–Rips persistence barcodes

If two finite metric spaces are close, then their barcodes are also close:

Theorem (Cohen-Steiner, Edelsbrunner, Harer 2005; Chazal et al. 2009)

Let X, Y be finite metric spaces with Gromov–Hausdorff distance $d_{GH}(X, Y) = \frac{\delta}{2}$.



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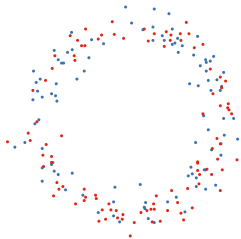

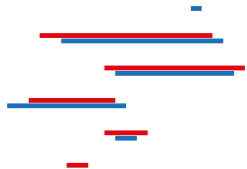

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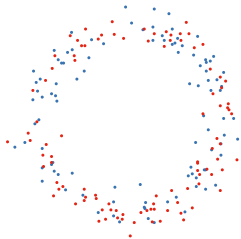

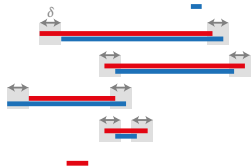

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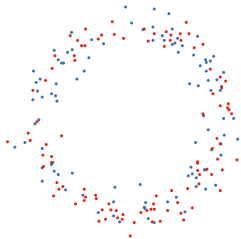
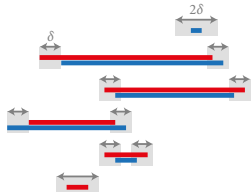
- *matched intervals have endpoints within distance $\leq \delta$, and*
- *unmatched intervals have length $\leq 2\delta$.*





Matrix reduction

Computing homology

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

- compute basis for boundaries $B_* = \operatorname{im} \partial_*$
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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:

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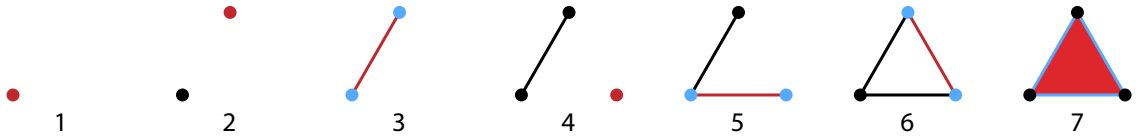
Notation:

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

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
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2		1					
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V

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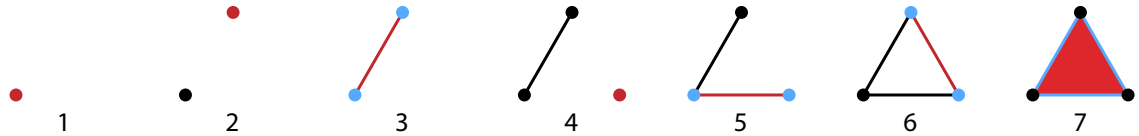

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4					1	1	
5							1
6							1
7							

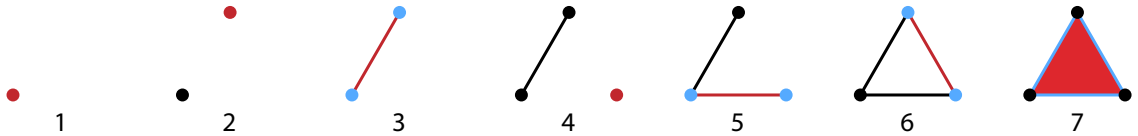
R

$= D \cdot$

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

V

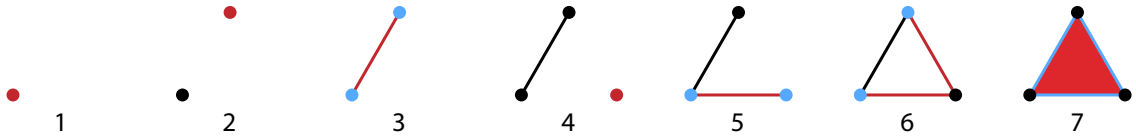
Matrix reduction



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

R $\qquad$ V

Matrix reduction



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

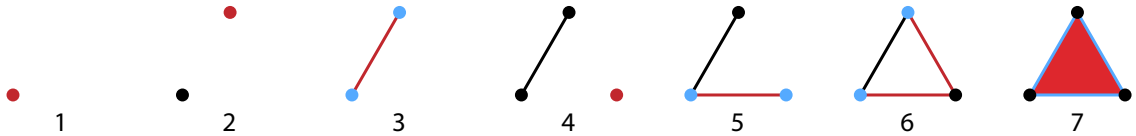
R

$= D \cdot$

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

V

Matrix reduction



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

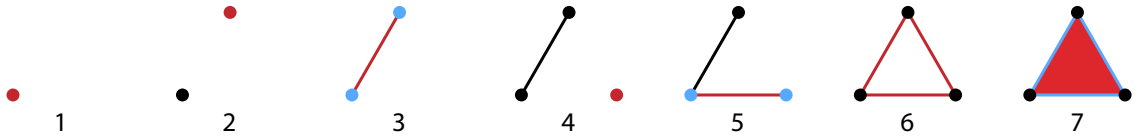
R

$= D \cdot$

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

V

Matrix reduction



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

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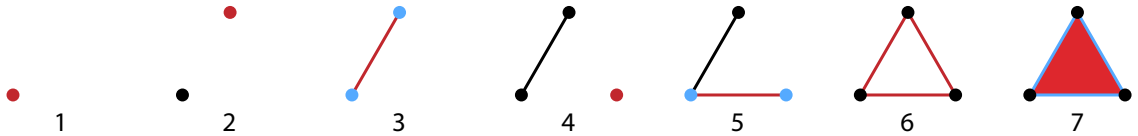
$= D \cdot$

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

V

Matrix reduction



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

R

$= D \cdot$

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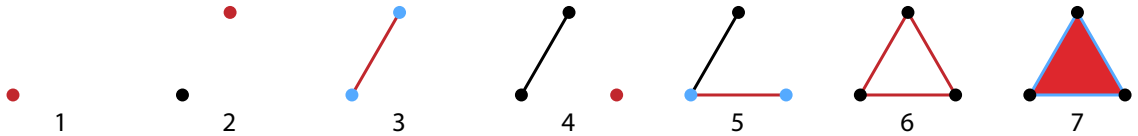
1	1						
2		1					
3			1			1	
4				1			
5					1	1	
6						1	
7							1

V

Matrix reduction



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

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$= D \cdot$

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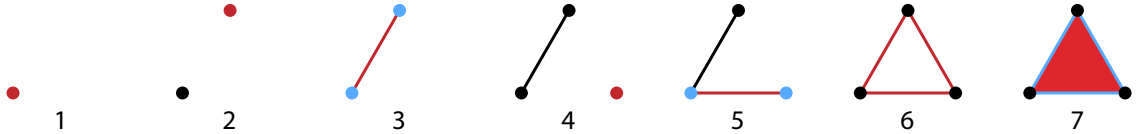
2		1					
3			1			1	
4				1			
5					1	1	
6						1	
7							1

V

Matrix reduction



	1	2	3	4	5	6	7
1			1		1		
2			1				
3							1
4					1		
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1	1						
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3			1			1	
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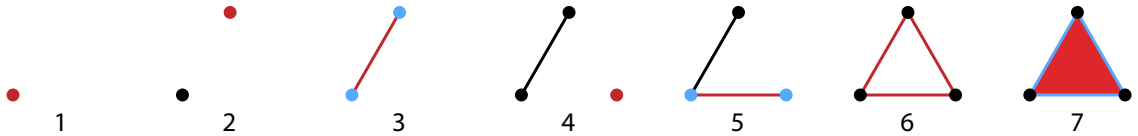
Matrix reduction



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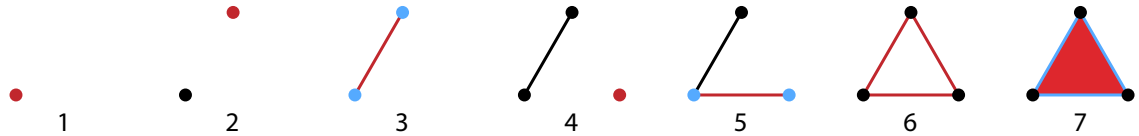

	1	2	3	4	5	6	7
1			1		1		
2			1				
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1	1						
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V

Matrix reduction algorithm

Require: D: $I \times J$ matrix

Ensure: $R = D \cdot V$: reduced, V: regular upper triangular

$R := D$

$V := I$

for $j \in J$ in increasing order **do**

  while $\exists k < j$ with $\operatorname{PivotIndex} R_k = \operatorname{PivotIndex} R_j$ **do**

    $\lambda := \operatorname{PivotEntry} R_j / \operatorname{PivotEntry} R_k$

    $R_j := R_j - \lambda \cdot R_k$ ▷ elimintates $\operatorname{PivotEntry} R_j$

    $V_j := V_j - \lambda \cdot V_k$

  if $(i := \operatorname{PivotIndex} R_j) \neq 0$ **then**

    append (i, j) to persistence pairs ▷ persistence interval $[i, j)$

  else

    append (j, ∞) to persistence pairs ▷ persistence interval $[j, \infty)$

Compatible basis cycles

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

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

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

$$I_e = I_b \setminus \operatorname{PivotIndices} R \qquad \textit{essential} \text{ indices.}$$

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Optimizations

The four special ingredients of Ripser

Main improvements to the standard algorithm:

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

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Lessons from previous work:

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

Clearing

Clearing non-essential positive columns

Recall:

- Columns with indices $\mathrm{PivotIndices}\, R$ (non-essential birth indices) not used at all

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Note:

- reducing *birth* columns typically harder than death columns:
  - $O(j^2)$ (birth) vs. $O((j-i)^2)$ (death)
- clearing avoids all non-essential birth columns (many, hard),
- reducing only death columns (easy) and *essential* birth columns

Counting homology column reductions

Number of columns in boundary matrix (n vertices, homology up to dimension k):

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

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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

Persistent (co)homology

Idea: compute persistent cohomology instead of persistent homology.

- Cohomology is the vector space dual of homology.

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What's the deal?

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

- Number of columns in coboundary matrix:

$$\underbrace{\sum_{d=0}^{k}\binom{n}{d+1}}_{\text{total}} = \underbrace{\sum_{d=0}^{k}\binom{n-1}{d+1}}_{\text{death}} + \underbrace{\sum_{d=0}^{k}\binom{n-1}{d}}_{\text{birth}}$$

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

Observations

When reducing $R = D \cdot V$, for a typical input:

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

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- most death columns of D are already reduced

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

Implicit matrix reduction

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- (Co)boundary matrix D for filtration-ordered basis
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  - 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

Implicit boundary matrix reduction algorithm

Require: D: $I \times J$ matrix

Ensure: $R = D \cdot V$: reduced, V: regular upper triangular

$R := D$

$V := I$

for $j \in J$ in increasing order **do**

  while $\exists k < j$ with $\operatorname{PivotIndex} R_k = \operatorname{PivotIndex} R_j$ **do**

    $\lambda := \operatorname{PivotEntry} R_j / \operatorname{PivotEntry} R_k$

    $R_j := R_j - \lambda \cdot R_k$ ▷ elimintates $\operatorname{PivotEntry} R_j$

    $V_j := V_j - \lambda \cdot V_k$

  if $(i := \operatorname{PivotIndex} R_j) \neq 0$ **then**

    append (i, j) to persistence pairs ▷ persistence interval $[i, j)$

  else

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Enumerating (co)faces in lexicographic order

There is an order-preserving bijection

$$\begin{array}{ccccccccc} [v_2, v_1, v_0] & [v_3, v_1, v_0] & [v_3, v_2, v_0] & [v_3, v_2, v_1] & [v_4, v_1, v_0] & \cdots & [v_{n-3}, v_{n-2}, v_{n-1}] \\ \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & & \downarrow \\ 0 & 1 & 2 & 3 & 4 & \cdots & \binom{n}{k+1} - 1 \end{array}$$

from k-simplices (ordered lexicographically) to natural numbers (called *combinatorial number system*).

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from k-simplices (ordered lexicographically) to natural numbers (called *combinatorial number system*).

- One direction is given by

$$[v_{i_k}, \ldots, v_{i_0}] \mapsto \sum_{j=0}^{k} \binom{i_j}{j+1}$$

- The other direction can also be computed quickly
- Using this bijection, faces and cofaces can be efficiently enumerated in (decreasing) lexicographic order

Filtrations and refinements

Simplexwise filtrations

Call a filtration $K_\bullet = (K_i)_i$ of simplicial complexes *simplexwise* if all $K_i \neq \emptyset$ are of the form $K_i = K_{i-1} \cup \{\sigma_i\}$ for some $\sigma_i \in K$.

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- These properties are natural assumptions for computation.
- The *Vietoris–Rips filtration* (indexed by $\mathbb{R}$) is not simplexwise.
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Ripser use the *lexicographic refinement*: simplices ordered by

- diameter, then
- dimension, then
- (decreasing) lexicographic order of vertices $\{v_{i_k}, \ldots, v_{i_0}\}$
  (induced by fixed total order $v_0 < \cdots < v_{n-1}$ on vertices)

Apparent pairs

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- σ is the youngest facet of τ, and
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- Can be identified *during* construction of a column in the coboundary matrix, *without even enumerating all cofacets* (shortcut for computation)
  - Relies on use of lexicographic refinement

Speedup from apparent pairs shortcut

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

- Only $53 + 601 = 654$ out of $18\,337 + 1\,179\,808$ columns fully constructed (without shortcut)
- Only $164\,214 + 3\,392\,039 = 3\,556\,253$ out of $3\,447\,550 + 216\,052\,515 = 219\,500\,065$ nonzero entries of the coboundary matrix are enumerated

Speedup: $0.6\,s$ vs. $6.1\,s$ (factor 10)

	n	d	non-zero pairs	non-shortcut pairs	persistence pairs
sphere3	192	1	53	53	18 145
		2	1	601	1 143 135
o3	4 096	1	2466	2466	230 051
		2	811	15 829	4 112 971
		3	33	123 035	39 738 338
torus4	50 000	1	14 006	14 006	2 192 209
		2	136	60 603	37 145 478
dragon	2 000	1	576	576	1 386 646
fractal-r	512	1	438	438	122 324
		2	659	6612	18 979 158

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Theorem (B, 2021)

Let (X, d) be a finite metric space with distinct pairwise distances, and consider the simplexwise refinement of the Vietoris–Rips filtration for X. In dimension 1, the apparent pairs are precisely the zero persistence pairs.

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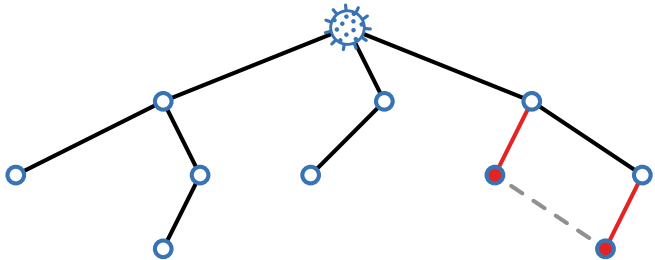
- *Output-sensitive*: only simplices contributing to the barcode incur a computational cost.

Topology of viral evolution



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

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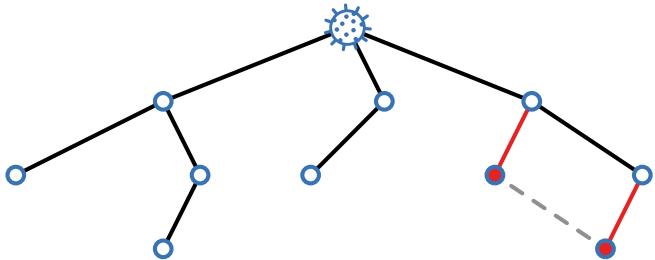

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Observation: Ripser runs unusually fast on genetic distance data

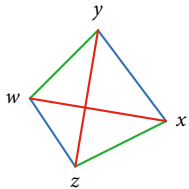
- SARS-CoV2 RNA sequences (spike protein)
- 25556 data points (2.8×10^{12} simplices in 2-skeleton)
- 120 s computation time (with data points ordered appropriately)

Gromov-hyperbolicity

Definition (Gromov 1988)

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

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



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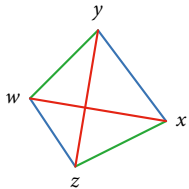

- The hyperbolic plane is $(\ln 2)$-hyperbolic.

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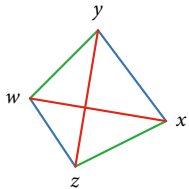

- The hyperbolic plane is $(\ln 2)$-hyperbolic.

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

Rips Contractibility

Theorem (Rips; Gromov 1988)

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

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- Connection to computation of persistent homology?

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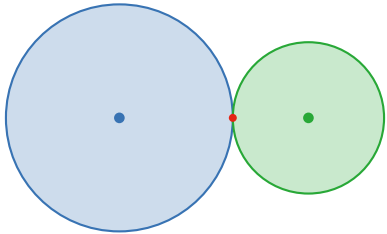
Theorem (B, Roll 2022)

Let X be a finite δ-hyperbolic space. Then there is a single discrete gradient encoding the collapses

$$\mathrm{Rips}_u(X) \searrow \mathrm{Rips}_t(X) \searrow \{*\}$$

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

Geodesic defect



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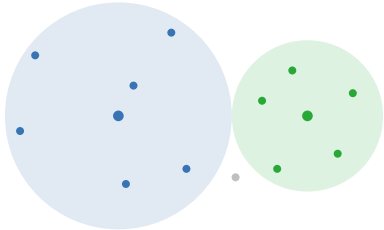

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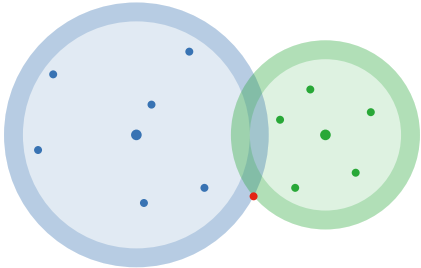

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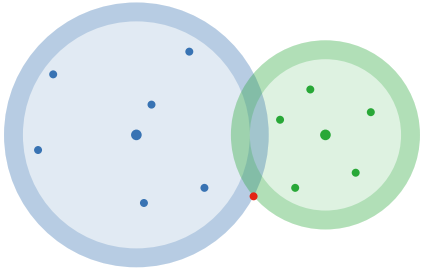

Definition (Bonk, Schramm 2000)

A metric space X is *v-geodesic* if for all points $x, y \in X$ and all $r, s \geq 0$ with $r + s = d(x, y)$ we have

$$B_{r+v}(x) \cap B_{s+v}(y) \neq \emptyset.$$

The infimum of all such v is the *geodesic defect* of X.

Tree metrics beyond the generic case

Why is Ripser particularly fast on genetic distances (tree-like)?

- Consider a weighted finite tree $T = (V, E)$, viewed as a metric space X.
- Choose an arbitrary root and extend the rooted tree partial order to a total order.

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The apparent pairs gradient for this total order induces the same collapses as in the generic case:

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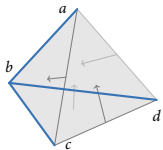

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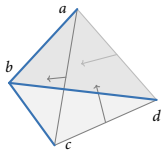

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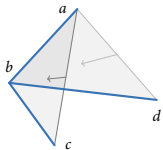

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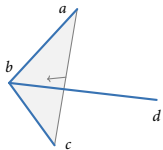

Thanks for your attention!