An introduction to persistent homology

Part 3: Computation

Ulrich Bauer

TUM

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Vietoris–Rips complexes

Consider a finite metric space (X, d).
The *Vietoris–Rips complex* is the simplicial complex

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

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

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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!

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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Some previous software:

- javaplex (Stanford): 3200 seconds, 12 GB
- Dionysus (Duke): 615 seconds, 3.4 GB
- DIPHA (IST Austria): 50 seconds, 6 GB
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Demo: live.ripser.org

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- Ripser: 1.2 seconds, 160 MB

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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- Apparent and emergent pairs

Lessons from previous work:

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

Filtrations and refinements

Simplexwise filtrations

Call a filtration $K_\bullet = (K_i)_{i \in I}$ of simplicial complexes (I totally ordered)

- *essential* if $i \neq j$ implies $K_i \neq K_j$,
- *simplexwise* if all $K_i \neq \varnothing$ are of the form $K_i = K_j \cup \{\sigma_i\}$ for some $j < i \in I$ and $\sigma_i \in K$.

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Note:

- These properties are natural assumptions for computation.
- The *Vietoris–Rips filtration* (indexed by $\mathbb{R}$) is not simplexwise (and not essential).
- To compute Vietoris–Rips persistence, we have to reindex and refine.

Reindexing and refinement

A filtration $K : I \to \mathbf{Simp}$ is a *reindexing* of another filtration $F : R \to \mathbf{Simp}$ if $F = K \circ r$ for some monotonic map $r : R \to I$.

- If r is injective, we call K a *refinement* of F;
- if r is surjective, we call K a *condensation* of F.

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The Vietoris–Rips filtration can be reindexed:

- condensed to an essential filtration (over the finite set of pairwise distances), and further
- refined to a simplexwise filtration.

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Ripser use the *lexicographic refinement*: simplices ordered by

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

Enumerating (co)faces in lexicographic order

There is an order-preserving bijection

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

from k-simplices (as ordered tuples, 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

Persistence barcodes through reindexing

Proposition

Consider a filtration $F : \mathbb{R} \to \mathbf{Simp}$ *with reindexing* $F = K \circ r$, $K : I \to \mathbf{Simp}$, $r : \mathbb{R} \to I$.
The persistence barcode of $K_\bullet$ *determines the persistence barcode of* $F_\bullet$*:*

$$B(H_*(F_\bullet)) = \{r^{-1}[i,j) \neq \varnothing \mid [i,j) \in B(H_*(K_\bullet))\}.$$

Matrix reduction

Computing homology

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

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

Persistence by matrix reduction

Given:

- D: matrix of boundary ∂_d for a simplexwise filtration $(K_i)_i$ (for canonical basis in filtration order, indexed by $I \times J$)

Wanted:

- persistence barcode of homology $H_d(K_i; \mathbb{F})$ for some (prime) field $\mathbb{F}$, in dimensions $d = 0, \ldots, k$

Notation:

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

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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

$$I_b = \{i : R_i = 0\} \qquad \textit{birth} \text{ indices ,}$$
$$I_d = \{j : R_j \neq 0\} \qquad \textit{death} \text{ indices,}$$
$$I_e = I_b \setminus \operatorname{PivotIndices} R \qquad \textit{essential} \text{ indices.}$$

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- Persistent homology is generated by the basis cycles Σ_Z.

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- Persistent homology is generated by the basis cycles Σ_Z.
- Persistence intervals: $\{[i, j) \mid i = \operatorname{PivotIndex} R_j\} \cup \{[i, \infty) \mid i \in I_e\}$

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					
3			1				
4				1			
5					1		
6						1	
7							1

V

Matrix reduction

	1	2	3	4	5	6	7
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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
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3			1				
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V

Matrix reduction

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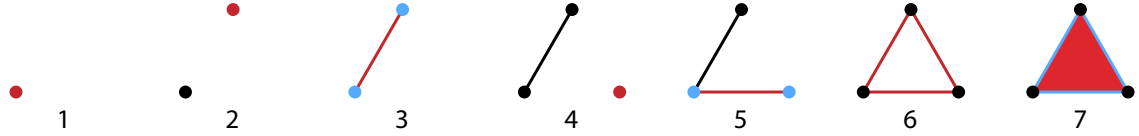
Matrix reduction



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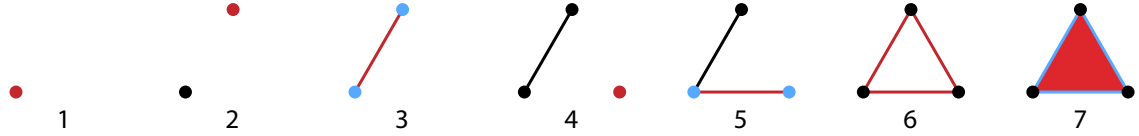

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V

Matrix reduction algorithm

Require: D: $I \times J$ matrix

Ensure: $R = D \cdot V$: reduced, V: regular upper triangular, P: persistence pairs, E: essential

$P := \varnothing$

$R := D$

$V := I$

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 P ▷ persistence interval $[i, j)$

  else

    append j to E ▷ persistence interval $[j, \infty)$

Clearing

Clearing non-essential positive columns

Idea [Chen, Kerber 2011]:

- Don't reduce at non-essential birth indices
- Use the fact that $i = \operatorname{PivotIndex} R_j$ implies $R_i = 0$
  - Reduce matrices of $\partial_d : C_d \to C_{d-1}$ for $d = k+1, \dots, 1$
  - Whenever $i = \operatorname{PivotIndex} R_j$ (in matrix for ∂_d): set R_i to 0 (in matrix for ∂_{d-1})

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  - Whenever $i = \operatorname{PivotIndex} R_j$ (in matrix for ∂_d): set R_i to 0 (in matrix for ∂_{d-1})

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:

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

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$$= \underbrace{\sum_{d=1}^{k+1}\binom{n-1}{d}}_{\text{death}} + \underbrace{\binom{n-1}{k+2}}_{\text{essential}} + \underbrace{\sum_{d=1}^{k}\binom{n-1}{d+1}}_{\text{cleared}}$$

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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

How is persistent cohomology related to persistent homology?

Proposition (de Silva et al 2011)

Persistent homology and persistent cohomology have the same barcode.

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Proof.

- Cohomology (over $\mathbb{F}$) is vector space dual to homology:

$$H^p(K) \cong H_p(K)^* = \mathrm{Hom}(H_p(K), \mathbb{F}).$$

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- Duality preserves ranks of linear maps (in finite dimensions): for $f : V \to W$ with dual $f^* : W^* \to V^*$,

$$\mathrm{rank}\, f^* = \mathrm{rank}\, f.$$

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$$\mathrm{rank}\, f^* = \mathrm{rank}\, f.$$

- The persistence barcode of a persistence module is uniquely determined by the ranks of the internal maps. □

Persistent (relative) homology

How is persistent relative homology related to persistent homology?

- Consider the short exact sequence of filtered chain complexes (with coefficients in $\mathbb{F}$)

$$0 \to C_p(K_\bullet) \to C_p(K) \to C_p(K, K_\bullet) \to 0$$

  (where $C_p(K)$ is the constant filtration).

- This induces a long exact sequence of persistence modules

$$\cdots \to H_{p+1}(K, K_\bullet) \to H_p(K_\bullet) \to H_p(K) \to H_p(K, K_\bullet) \to \cdots$$

  and analogously for persistent cohomology.

Persistent (relative) homology barcodes

Consider the long exact sequence of persistence modules

$$\cdots \to H_{p+1}(K) \xrightarrow{r} H_{p+1}(K, K_\bullet) \xrightarrow{\partial} H_p(K_\bullet) \xrightarrow{i} H_p(K) \to \cdots$$

We have:

- $B(\mathrm{im}(i)) = B^\infty(H_p(K_\bullet)) := \{[b, \infty) \in B(H_p(K_\bullet))\}$

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- $B(\mathrm{im}(i)) = B^\infty(H_p(K_\bullet)) := \{[b, \infty) \in B(H_p(K_\bullet))\}$
- $B(\mathrm{im}(\partial)) = B(\ker(i)) = B^\dagger(H_p(K_\bullet)) := \{[b, d) \in B(H_p(K_\bullet)) \mid d < \infty\}$

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The absolute *and* relative *persistence barcodes determine each other:*

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  - Can be computed by reduction of *filtration coboundary matrix*:
    - transpose of filtration boundary matrix,
    - with reversed index orders

Counting cohomology column reductions

Consider K: $k+1$-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

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

Implicit boundary matrix reduction algorithm

Require: D: $I \times J$ matrix

Ensure: $R = D \cdot V$: reduced, V: regular upper triangular, P: persistence pairs, E: essential

$P := \varnothing$

$R := D$

$V := I$

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

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

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

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

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Apparent and emergent pairs

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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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Remark

The apparent pairs also form a *discrete gradient* (in the sense of discrete Morse theory).

Emergent persistent pairs

A persistence pair (σ, τ) for a simplexwise filtration is

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Proposition

Let $K_\bullet$ be the lexicographically refined Rips filtration. Assume that

- *τ is the lexicographically minimal cofacet of σ with $\operatorname{diam}(\tau) = \operatorname{diam}(\sigma)$, and*
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Then (σ, τ) is a 0-persistence emergent coface pair of $K_\bullet$.

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Then (σ, τ) is a 0-persistence emergent coface pair of $K_\bullet$.

- Includes all apparent pairs with persistence 0 (most pairs are of this kind)
- Can be identified *without* enumerating all cofaces of σ (shortcut for computation)

Speedup from emergent 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

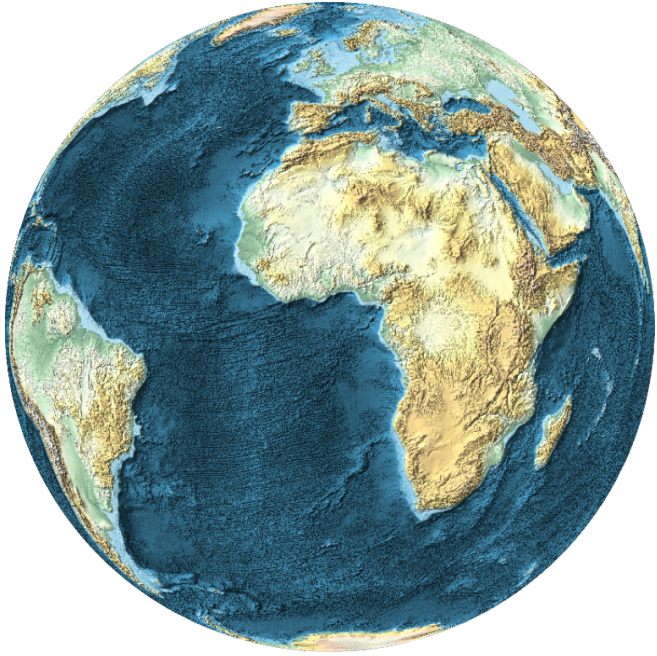
Speedup: $1.2\,s$ vs. $5.6\,s$ (factor 4.7)

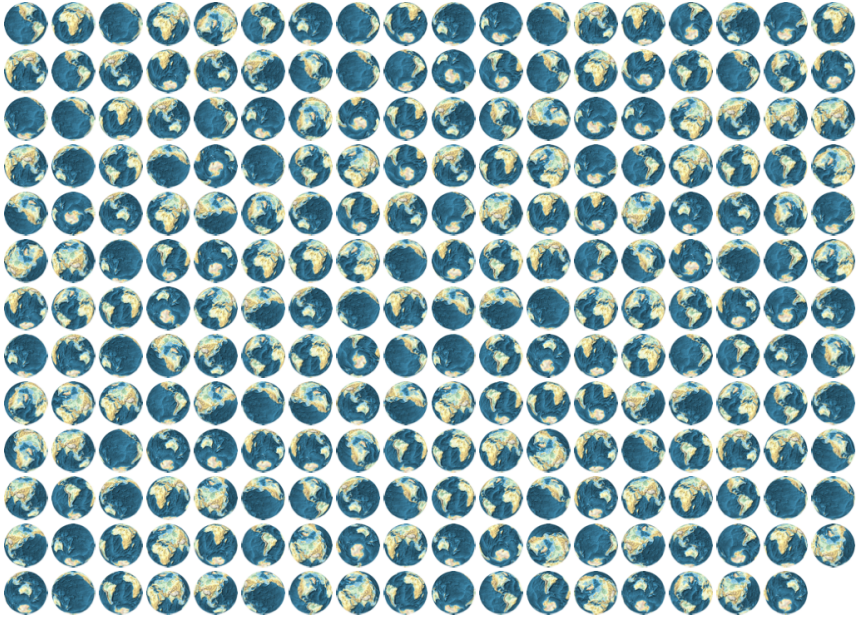
Apparent pairs in dimension 1

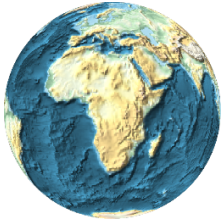
Theorem

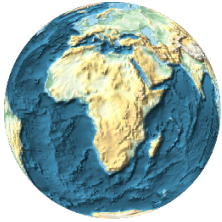
Let (X, d) be a finite metric space with distinct pairwise distances,
and let $K_\bullet$ be a simplexwise refinement of the Vietoris–Rips filtration for X.
In dimension 1, the zero persistence pairs of $K_\bullet$ are precisely the apparent pairs.

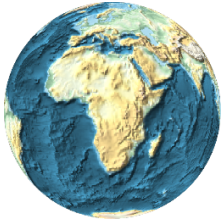
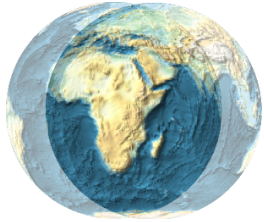
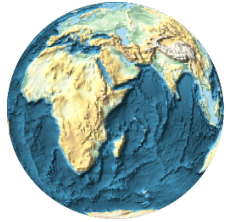
Around the world

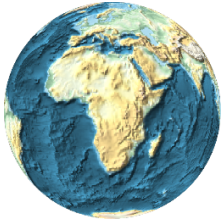
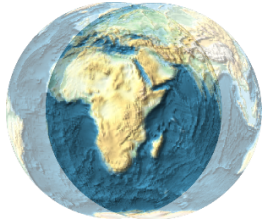
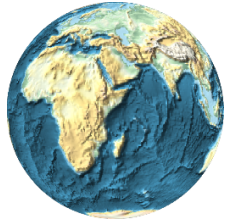




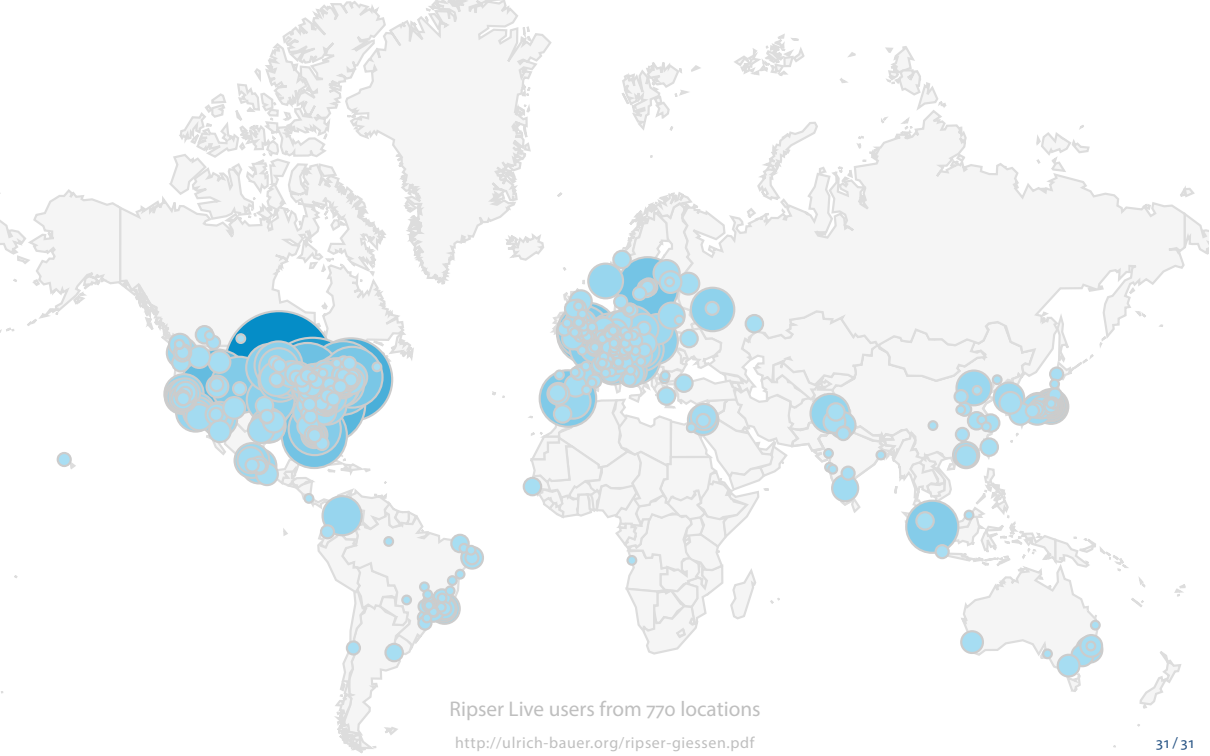




Demo (Ripser)



Ripser Live users from 770 locations