Ripser

Efficient Computation of Vietoris–Rips Persistence Barcodes

Ulrich Bauer

TUM

July 18, 2017

Workshop Topology, Computation, and Data Analysis
Schloss Dagstuhl

Vietoris–Rips persistence

Vietoris-Rips filtrations

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

$$Rips_t(X) = \{ S \subseteq X \mid diam S \le t \}$$

- 1-skeleton: all edges with pairwise distance $\leq t$
- all possible higher simplices (flag complex)

Vietoris-Rips filtrations

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

$$Rips_t(X) = \{ S \subseteq X \mid diam S \le t \}$$

- 1-skeleton: all edges with pairwise distance $\leq t$
- all possible higher simplices (flag complex)

Goal:

• compute persistence barcodes for $H_d(\operatorname{Rips}_t(X))$ (in dimensions $0 \le d \le k$)

Demo: Ripser

Example data set:

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

Demo: Ripser

Example data set:

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

Comparison with other software:

- javaplex: 3200 seconds, 12 GB
- Dionysus: 533 seconds, 3.4 GB
- GUDHI: 75 seconds, 2.9 GB
- DIPHA: 50 seconds, 6 GB
- Eirene: 12 seconds, 1.5 GB

Demo: Ripser

Example data set:

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

Comparison with other software:

- javaplex: 3200 seconds, 12 GB
- Dionysus: 533 seconds, 3.4 GB
- GUDHI: 75 seconds, 2.9 GB
- DIPHA: 50 seconds, 6 GB
- Eirene: 12 seconds, 1.5 GB

Ripser: 1.2 seconds, 152 MB

Ripser

A software for computing Vietoris–Rips persistence barcodes

- about 1000 lines of C++ code, no external dependencies
- support for
 - coefficients in a prime field \mathbb{F}_p
 - sparse distance matrices for distance threshold
- open source (http://ripser.org)
 - released in July 2016
- online version (http://live.ripser.org)
 - launched in August 2016
- most efficient software for Vietoris–Rips persistence
 - computes H² barcode for 50 000 random points on a torus in 136 seconds / 9 GB (using distance threshold)
- 2016 ATMCS Best New Software Award (jointly with RIVET)

Design goals

Goals for previous projects:

- PHAT [B, Kerber, Reininghaus, Wagner 2013]: fast persistence computation (matrix reduction only)
- DIPHA [B, Kerber, Reininghaus 2014]: distributed persistence computation

Design goals

Goals for previous projects:

- PHAT [B, Kerber, Reininghaus, Wagner 2013]: fast persistence computation (matrix reduction only)
- DIPHA [B, Kerber, Reininghaus 2014]: distributed persistence computation

Goals for Ripser:

- Use as little memory as possible
- Be reasonable about computation time

The four special ingredients

The improved performance is based on 4 insights:

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

The four special ingredients

The improved performance is based on 4 insights:

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

Lessons from PHAT:

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

Matrix reduction

Matrix reduction algorithm

Setting:

- finite metric space X, n points
- persistent homology $H_d(\text{Rips}_t(X); \mathbb{F}_2)$ in dimensions $d \leq k$

Notation:

- D: boundary matrix of filtration
- R_i : *i*th column of R

Matrix reduction algorithm

Setting:

- finite metric space X, n points
- persistent homology $H_d(\text{Rips}_t(X); \mathbb{F}_2)$ in dimensions $d \leq k$

Notation:

- D: boundary matrix of filtration
- R_i : *i*th column of R

Algorithm:

- R = D, V = I
- while $\exists i < j$ with pivot R_i = pivot R_j
 - add R_i to R_j , add V_i to V_j

Matrix reduction algorithm

Setting:

- finite metric space X, n points
- persistent homology $H_d(\text{Rips}_t(X); \mathbb{F}_2)$ in dimensions $d \leq k$

Notation:

- D: boundary matrix of filtration
- R_i : *i*th column of R

Algorithm:

- R = D, V = I
- while $\exists i < j$ with pivot R_i = pivot R_j
 - add R_i to R_j , add V_i to V_j

Result:

- $R = D \cdot V$ is reduced (unique pivots)
- V is full rank upper triangular

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

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

positive indices,

 $N=\left\{ j:R_{j}\neq0\right\}$

negative indices,

 $E = P \setminus \text{pivots } R$

essential indices.

Then

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

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

positive indices,

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

negative indices,

$$E = P \setminus \text{pivots } R$$

essential indices.

Then

$$\widetilde{\Sigma}_Z = \{ V_i \mid i \in P \}$$

is a basis of Z_* ,

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

$$P = \{i : R_i = 0\}$$
 positive indices,

$$N = \{j : R_j \neq 0\}$$
 negative indices,

$$E = P \setminus \text{pivots } R$$
 essential indices.

Then

$$\widetilde{\Sigma}_Z = \{ V_i \mid i \in P \}$$

$$\Sigma_B = \left\{ R_j \mid j \in N \right\}$$

is a basis of Z_* ,

is a basis of B_* ,

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

$$P = \{i : R_i = 0\}$$
 positive indices,

$$N = \{j : R_j \neq 0\}$$
 negative indices,

$$E = P \setminus \text{pivots } R$$
 essential indices.

Then

$$\widetilde{\Sigma}_Z = \{ V_i \mid i \in P \}$$
 is a basis of Z_* ,

$$\Sigma_B = \{R_j \mid j \in N\}$$
 is a basis of B_* ,

$$\Sigma_Z = \Sigma_B \cup \{V_i \mid i \in E\}$$
 is another basis of Z_* .

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

$$P = \{i : R_i = 0\}$$
 positive indices,
 $N = \{j : R_j \neq 0\}$ negative indices,

 $E = P \setminus \text{pivots } R$ essential indices.

Then

$$\begin{split} \widetilde{\Sigma}_Z &= \big\{ V_i \ | \ i \in P \big\} & \text{is a basis of } Z_*, \\ \Sigma_B &= \big\{ R_j \ | \ j \in N \big\} & \text{is a basis of } B_*, \\ \Sigma_Z &= \Sigma_B \cup \big\{ V_i \ | \ i \in E \big\} & \text{is another basis of } Z_*. \end{split}$$

Persistent homology is generated by the basis cycles Σ_Z .

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

$$P = \{i : R_i = 0\}$$
 positive indices,
 $N = \{j : R_j \neq 0\}$ negative indices,
 $E = P \setminus \text{pivots } R$ essential indices.

Then

$$\widetilde{\Sigma}_Z = \{ V_i \mid i \in P \}$$
 is a basis of Z_* ,
$$\Sigma_B = \{ R_j \mid j \in N \}$$
 is a basis of B_* ,
$$\Sigma_Z = \Sigma_B \cup \{ V_i \mid i \in E \}$$
 is another basis of Z_* .

Persistent homology is generated by the basis cycles Σ_Z .

- Persistence intervals: $\{[i,j) \mid i = \text{pivot } R_j\} \cup \{[i,\infty) \mid i \in E\}$
- · Columns with non-essential positive indices never used!

Clearing

Idea [Chen, Kerber 2011]:

- Don't reduce at non-essential positive indices
- Reduce boundary matrices of $\partial_d : C_d \to C_{d-1}$ in decreasing dimension $d = k + 1, \dots, 1$
- Whenever $i = \operatorname{pivot} R_j$ (in matrix for ∂_d)
 - Set R_i to 0 (in matrix for ∂_{d-1})

Idea [Chen, Kerber 2011]:

- Don't reduce at non-essential positive indices
- Reduce boundary matrices of $\partial_d : C_d \to C_{d-1}$ in decreasing dimension $d = k + 1, \dots, 1$
- Whenever $i = \operatorname{pivot} R_j$ (in matrix for ∂_d)
 - Set R_i to 0 (in matrix for ∂_{d-1})
 - Set V_i to R_j

Idea [Chen, Kerber 2011]:

- Don't reduce at non-essential positive indices
- Reduce boundary matrices of $\partial_d : C_d \to C_{d-1}$ in decreasing dimension $d = k + 1, \dots, 1$
- Whenever $i = \operatorname{pivot} R_j$ (in matrix for ∂_d)
 - Set R_i to 0 (in matrix for ∂_{d-1})
 - Set V_i to R_j
- Still yields $R = D \cdot V$ reduced, V full rank upper triangular

Idea [Chen, Kerber 2011]:

- Don't reduce at non-essential positive indices
- Reduce boundary matrices of $\partial_d : C_d \to C_{d-1}$ in decreasing dimension $d = k + 1, \dots, 1$
- Whenever $i = \operatorname{pivot} R_j$ (in matrix for ∂_d)
 - Set R_i to 0 (in matrix for ∂_{d-1})
 - Set V_i to R_j
- Still yields $R = D \cdot V$ reduced, V full rank upper triangular

Note:

- reducing positive columns typically harder than negative
- with clearing: need only reduce essential positive columns

Cohomology

Persistent cohomology

We have seen: many columns of $R = D \cdot V$ are not needed

Skip those inessential columns in matrix reduction

Persistent cohomology

We have seen: many columns of $R = D \cdot V$ are not needed

Skip those inessential columns in matrix reduction

For persistence barcodes in low dimensions $d \le k$:

- Number of skipped indices for reducing D^T (cohomology) is much larger than for D (homology)
 - reducing boundary matrix produces basis for $H_{k+1}(K_{k+1})$, which is not needed (and very expensive)
- The resulting persistence barcode is the same [de Silva et al. 2011]

Persistent cohomology

We have seen: many columns of $R = D \cdot V$ are not needed

Skip those inessential columns in matrix reduction

For persistence barcodes in low dimensions $d \le k$:

- Number of skipped indices for reducing D^T (cohomology) is much larger than for D (homology)
 - reducing boundary matrix produces basis for $H_{k+1}(K_{k+1})$, which is not needed (and very expensive)
- The resulting persistence barcode is the same [de Silva et al. 2011]

Example (k = 2, n = 192):

Observations

For a typical input:

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

Observations

For a typical input:

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

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

Only 845 out of 1161 471 columns have to be reduced

Implicit matrix reduction

Implicit matrix reduction

Standard approach:

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

Implicit matrix reduction

Standard approach:

- Boundary matrix D for filtration-ordered basis
 - Explicitly generated and stored in memory
- Matrix reduction: store only reduced matrix R
 - transform D into R by column operations

Implicit matrix reduction

Standard approach:

- Boundary matrix D for filtration-ordered basis
 - Explicitly generated and stored in memory
- Matrix reduction: store only reduced matrix R
 - transform D into R by column operations

Approach for Ripser:

- Boundary matrix D for lexicographically ordered basis
 - Implicitly defined and recomputed when needed

Implicit matrix reduction

Standard approach:

- Boundary matrix D for filtration-ordered basis
 - Explicitly generated and stored in memory
- Matrix reduction: store only reduced matrix R
 - transform D into R by column operations

Approach for Ripser:

- ullet Boundary matrix D for lexicographically ordered basis
 - Implicitly defined and recomputed when needed
- Matrix reduction in Ripser: store only coefficient matrix V
 - recompute previous columns of $R = D \cdot V$ when needed
 - Typically, V is much sparser and smaller than R

Oblivious matrix reduction

Algorithm variant:

- R = D
- for j = 1, ..., n
 - while $\exists i < j$ with pivot $R_i = \text{pivot } R_j$
 - add D_i to R_j

Oblivious matrix reduction

Algorithm variant:

- R = D
- for j = 1, ..., n
 - while $\exists i < j$ with pivot $R_i = \text{pivot } R_j$
 - add D_i to R_j

Computing the persistence intervals requires only:

- current column R_i
- pivots of previous columns R_i

Oblivious matrix reduction

Algorithm variant:

- R = D
- for j = 1, ..., n
 - while $\exists i < j$ with pivot $R_i = \text{pivot } R_j$
 - add D_i to R_j

Computing the persistence intervals requires only:

- current column R_j
- pivots of previous columns R_i

Corollary

The rank of an $m \times n$ matrix can be computed in O(n) memory.

Apparent and emergent pairs

Natural filtration settings

Typical assumptions on the filtration:

 general filtration 	persistence (in theory)
--	-------------------------

- filtration by singletons or pairs
- simplexwise filtration

discrete Morse theory

persistence (computation)

Natural filtration settings

Typical assumptions on the filtration:

•	general filtration	persistence (in theory)
•	filtration by singletons or pairs	discrete Morse theory
•	simplexwise filtration	persistence (computation)

Conclusion:

 Discrete Morse theory sits in the middle between persistence and persistence (!)

Apparent pairs

Definition

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

- σ is the youngest face of τ
- τ is the oldest coface of σ

Apparent pairs

Definition

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

- σ is the youngest face of τ
- τ is the oldest coface of σ

Lemma

Any apparent pairs is a persistence pair.

Lemma

The apparent pairs form a discrete gradient.

 Generalizes a construction proposed by [Kahle 2011] for the study of random Rips filtrations

Emergent persistent pairs

Consider the *lexicographically refined Rips filtration*:

- increasing diameter, refined by
- lexicographic order

This is the simplexwise filtration for computations in Ripser.

Emergent persistent pairs

Consider the lexicographically refined Rips filtration:

- increasing diameter, refined by
- lexicographic order

This is the simplexwise filtration for computations in Ripser.

Lemma

Assume that

- τ is the lexicographically minimal proper coface of σ with $diam(\tau) = diam(\sigma)$,
- and τ is not already in a persistence pair (ρ, τ) with $\rho > \sigma$.

Then (σ, τ) is an emergent persistence pair.

Emergent persistent pairs

Consider the *lexicographically refined Rips filtration*:

- increasing diameter, refined by
- lexicographic order

This is the simplexwise filtration for computations in Ripser.

Lemma

Assume that

- τ is the lexicographically minimal proper coface of σ with $diam(\tau) = diam(\sigma)$,
- and τ is not already in a persistence pair (ρ, τ) with $\rho > \sigma$.

Then (σ, τ) is an emergent persistence pair.

- Includes all apparent pairs with persistence 0
- Can be identified *without* enumerating all cofaces of σ
 - Provides a shortcut for computation

Ripser Live: users from 156 different cities

