Computing Homology Cycles with Certified Geometry

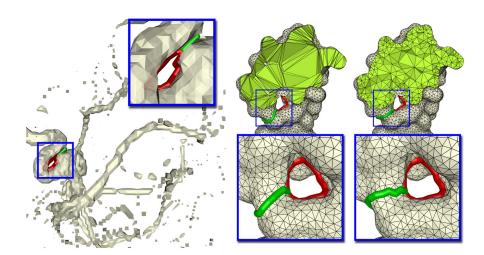


Tamal K. Dey

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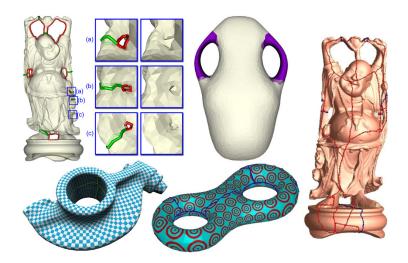
Cycles: Medical Imaging & Molecular Biology



Cycles: Computer-Aided Design

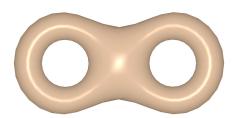


Cycles: Computer Graphics

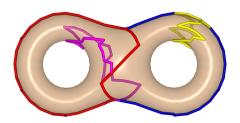


- Rank: Smith-Normal-Form; Special cases [DE95]
- Representative cycles:
 - Surfaces [VY90,DS95]
 - Volumes: [DG96]
 - General case: Persistence algorithm [ELZ00]
 - All are geometry-oblivious

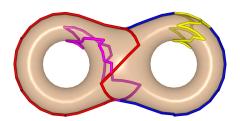
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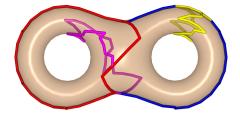
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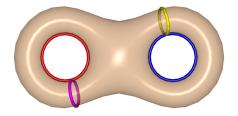


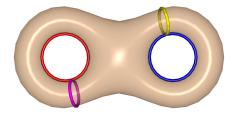
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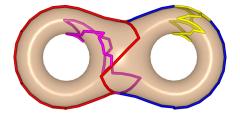
• Goal: 'Geometry-oblivious' to 'Geometry-aware'

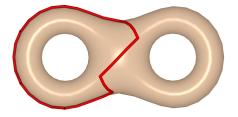


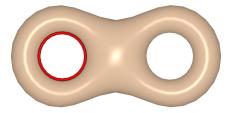




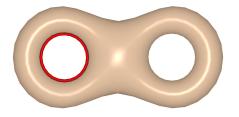
- First solution for surfaces: Erickson-Whittlesey [SODA05]
- General problem NP-hard: Chen-Freedman [SODA10]
- H₁ basis for simplicial complexes: D.-Sun-Wang [SoCG10]







• Compute an optimal cycle in a given class.



- Surfaces: Colin de Verdière-Lazarus [DCG05], Colin de Verdière-Erickson [SODA06], Chambers-Erickson-Nayyeri [SoCG09]
- General problem NP-hard: Chen-Freedman [SODA10]
- Special cases: D.-Hirani-Krishnamoorthy [STOC10]

Fields Institute (2011)

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Definition

A smallest basis of $H_p(\mathcal{T})$ is a set of *p*-cycles with minimal weight that generates $H_p(\mathcal{T})$

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• Given a *p*-cycle in a simplicial complex, compute a smallest cycle in its class.

Theorem 1 [D.-Sun-Wang 10]

Theorem

Let $\mathcal K$ be a finite simplicial complex with non-negative weights on edges. A smallest basis for $H_1(\mathcal K)$ can be computed in $O(n^4)$ time where $n=|\mathcal K|$

Greedy Set

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Definition

The greedy set G is an *ordered* set of cycles $\{c_1, \ldots, c_k\}$ satisfying the following conditions:

- (a) c_1 is the smallest cycle in $\mathcal L$ nontrivial in $\mathsf H_1(\mathcal K)$
- (b) c_{i+1} is the smallest cycle in \mathcal{L} independent of c_1, \ldots, c_i

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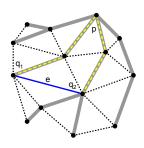
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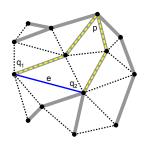
- (a) c_1 is the smallest cycle in $\mathcal L$ nontrivial in $\mathsf H_1(\mathcal K)$
- (b) c_{i+1} is the smallest cycle in $\mathcal L$ independent of c_1,\ldots,c_i
- If a set of cycles $\mathcal L$ in $\mathcal K$ contains a smallest basis, then the *greedy* set $\mathcal G$ chosen from $\mathcal L$ is a smallest basis by matroid theory

• Let T be a shortest path tree in $\mathcal K$ rooted at p

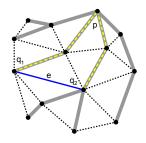
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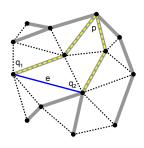
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Definition

The canonical cycle for a non-tree edge e is defined as

$$T(e) = \operatorname{sp}_T(q_1, q_2) \circ e$$



Candidate Cycles

Proposition

Let C_p be the set of all canonical cycles with respect to p:

$$C_p = \{T(e) : e \in E \setminus E_T\}$$

 $\cup_{p\in P} C_p$ contains a smallest basis

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 $\bigcup_{p\in P} G_p$ from $\bigcup_{p\in P} C_p$ and a smallest basis from $\bigcup_{p\in P} G_p$ can be computed by persistence algorithm in time $O(n^4)$.

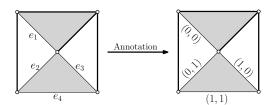
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Definition

An annotation for *p*-simplices is a function $a: \mathcal{K}_p \to (\mathbb{Z}_2)^g$ where any two *p*-cycles are homologous iff $\Sigma_{\sigma \in c} a(\sigma) = \Sigma_{\sigma \in c'} a(\sigma)$.

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Theorem (Busaryev-Cabello-Chen-D.-Wang 11)

For a simplicial complex with n simplices, annotations can be computed in $O(n^{\omega})$ time.

 ω : two $n \times n$ matrices can be multiplied in $O(n^{\omega})$ time, $\omega < 2.376$, used in improving persistence algorithms [MMS11,CK11].

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Theorem (BCCDW 11)

For a simplicial complex $\mathcal K$ with n simplices, a smallest basis for $H_1(\mathcal K)$ can be computed in time $O(n^\omega + n^2 g^{\omega-1})$ using simplex annotations where g is the dimension of $H_1(\mathcal K)$.

• Let $P \subset \mathbb{R}^d$ be a point set sampled from a smooth closed manifold $\mathcal{M} \subset \mathbb{R}^d$ embedded isometrically

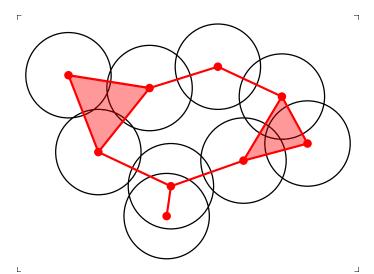
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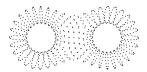
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- Compute a smallest basis of $H_1(\mathcal{K})$
- Argue that if P is *dense*, a subset of computed 1-cycles approximate a smallest basis of $H_1(\mathcal{M})$ within constant factors

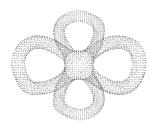
Rips complex $\mathcal{R}^r(P)$



Fields Institute (2011) Homology Cycles

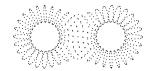
$PCD \rightarrow complex$



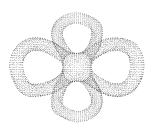


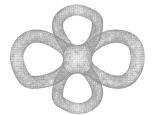
Point cloud

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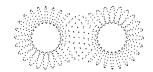




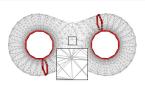
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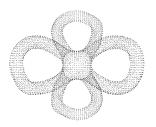
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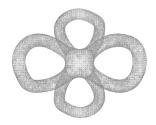
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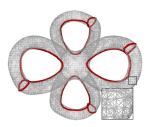












Point cloud

Rips complex

1-cycles

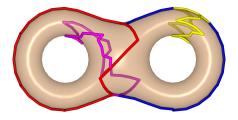
Approximation Theorem [DSW10]

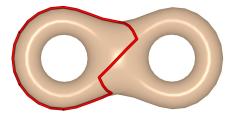
Theorem

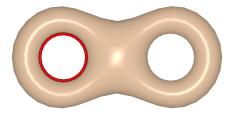
Let $\mathcal{M} \subset \mathbb{R}^d$ be a smooth, closed manifold with ℓ as the length of a smallest basis of $H_1(\mathcal{M})$ and $k = \operatorname{rank} H_1(\mathcal{M})$. Given a set $P \subset \mathcal{M}$ of n points which is an ε -sample of \mathcal{M} and $4\varepsilon \leq r \leq \min\{\frac{1}{2}\sqrt{\frac{3}{5}}\rho(\mathcal{M}), \rho_c(\mathcal{M})\}$, one can compute a set of k 1-cycles G within r/2 Hausdorff distance of a basis of $H_1(\mathcal{M})$ in $O(nn_e^2n_t)$ time where

$$\frac{1}{1+\frac{4r^2}{3\rho^2(\mathcal{M})}}\ell \leq \mathsf{Len}(\mathsf{G}) \leq (1+\frac{4\varepsilon}{\mathsf{r}})\ell.$$

Here n_e , n_t are the number of edges and triangles in $\mathcal{R}^{2r}(P)$







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- Are the solutions integral?
- Yes, if the constraint matrix is totally unimodular
- We characterize the complexes for which this is true
- For such complexes, the optimal cycle can be computed in polynomial time ©

Total Unimodularity

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Theorem

Let A be an $m \times n$ totally unimodular matrix and \mathbf{b} an integral vector, i.e. $\mathbf{b} \in \mathbb{Z}^m$. Then the polyhedron $\mathcal{P} = \{\mathbf{x} \in \mathbb{R}^n | A\mathbf{x} = \mathbf{b}, \mathbf{x} \geq 0\}$ is integral meaning that \mathcal{P} is the convex hull of the integral vectors contained in \mathcal{P} . In particular, the extreme points (vertices) of \mathcal{P} are integral. Similarly the polyhedron $\mathcal{Q} = \{\mathbf{x} \in \mathbb{R}^n | A\mathbf{x} \geq \mathbf{b}\}$ is integral.

Optimization

• Consider an integral vector $\mathbf{b} \in \mathbb{Z}^m$ and a real vector $\mathbf{f} \in \mathbb{R}^n$.

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Program

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Corollary

Let A be a totally unimodular matrix. Then the integer linear program above can be solved in time polynomial in the dimensions of A.

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- Convert it to an integer linear program by introducing some extra variables and constraints.
- Find the conditions under which the constraint matrix of the program is totally unimodular.
- For this class of problems, relax the integer linear program to a linear program by dropping the constraint that the variables be integral.

Optimization Program

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Program

$$\begin{aligned} & \min ||W\mathbf{x}||_1 \\ \text{such that} & \quad \mathbf{x} = \mathbf{c} + [\partial_{p+1}]\mathbf{y} \\ & \quad \text{and} & \quad \mathbf{x} \in \mathbb{Z}^m, \mathbf{y} \in \mathbb{Z}^n. \end{aligned}$$

Integer Linear Program

Program

$$\begin{aligned} \min & \sum_i |w_i| \big(x_i^+ + x_i^-\big) \\ \text{subject to} & & \mathbf{x}^+ - \mathbf{x}^- = \mathbf{c} + [\partial_{p+1}] \mathbf{y} \\ & & & \mathbf{x}^+, \mathbf{x}^- \geq 0 \\ & & & & \mathbf{x}^+, \mathbf{x}^- \in \mathbb{Z}^m, \mathbf{y} \in \mathbb{Z}^n. \end{aligned}$$

Linear Program

Program

$$\begin{aligned} \min \sum_{i} |w_{i}| (x_{i}^{+} + x_{i}^{-}) \\ \text{subject to} \quad \mathbf{x}^{+} - \mathbf{x}^{-} &= \mathbf{c} + [\partial_{p+1}] \mathbf{y} \\ \mathbf{x}^{+}, \mathbf{x}^{-} &\geq 0 \end{aligned}$$

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Lemma

If $B = [\partial_{p+1}]$ is totally unimodular then so is [I - I - B B].

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Lemma

If $B = [\partial_{p+1}]$ is totally unimodular then so is $[I - I - B \ B]$.

Theorem

If the boundary matrix $[\partial_{p+1}]$ of a finite simplicial complex of dimension greater than p is totally unimodular, the optimal homologous chain problem for p-chain can be solved in polynomial time.

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Orientable Manifolds

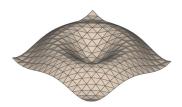
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Corollary

For a finite simplicial complex triangulating a (p+1)-dimensional compact orientable manifold, OHCP can be solved for p-chains in polynomial time.

Total Unimodularity and Relative Torsion

Definitions

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A pure subcomplex is a subcomplex that is a pure simplicial complex.

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Theorem (DHK10)

 $[\partial_{p+1}]$ is totally unimodular if and only if $H_p(\mathcal{L}, \mathcal{L}_0)$ is torsion-free, for all pure subcomplexes $\mathcal{L}_0, \mathcal{L}$ of \mathcal{K} of dimensions p and p+1, respectively, where $\mathcal{L}_0 \subset \mathcal{L}$. Hence, OHCP for p-chains in such complexes are polynomial time solvable by linear programs.

A Special Case

Theorem

Let $\mathcal K$ be a finite simplicial complex embedded in $\mathbb R^{d+1}$. Then, $H_d(\mathcal L,\mathcal L_0)$ is torsion-free for all pure subcomplexes $\mathcal L_0$ and $\mathcal L$ of dimensions d and d+1 respectively, such that $\mathcal L_0\subset\mathcal L$.

A Special Case

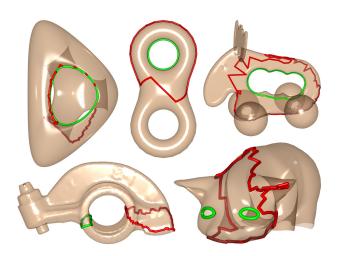
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Corollary

Given a d-chain \mathbf{c} in a weighted finite simplicial complex embedded in \mathbb{R}^{d+1} , an optimal chain homologous to \mathbf{c} can be computed by a linear program.

Computed Optimal Cycles



• $O(n^{\omega}+n^2g^{\omega-1})$ algorithm for OHBP for simplicial complexes. Can it be improved?

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- What about efficient updates?

Thank You