Computational homology in dynamical systems

Marian Mrozek

Jagiellonian University, Kraków

National University of Ireland, Galway
29 June - 10 July 2009

Outline

- Dynamical systems
- Rigorous numerics of dynamical systems
- Homological invariants of dynamical systems
- Computing homological invariants
- **Homology algorithms for subsets of $\mathbb{R}^d$**
- Homology algorithms for maps of subsets of $\mathbb{R}^d$
- Applications

Cubical Chains

- Given an elementary cube Q we define the associated elementary chain by

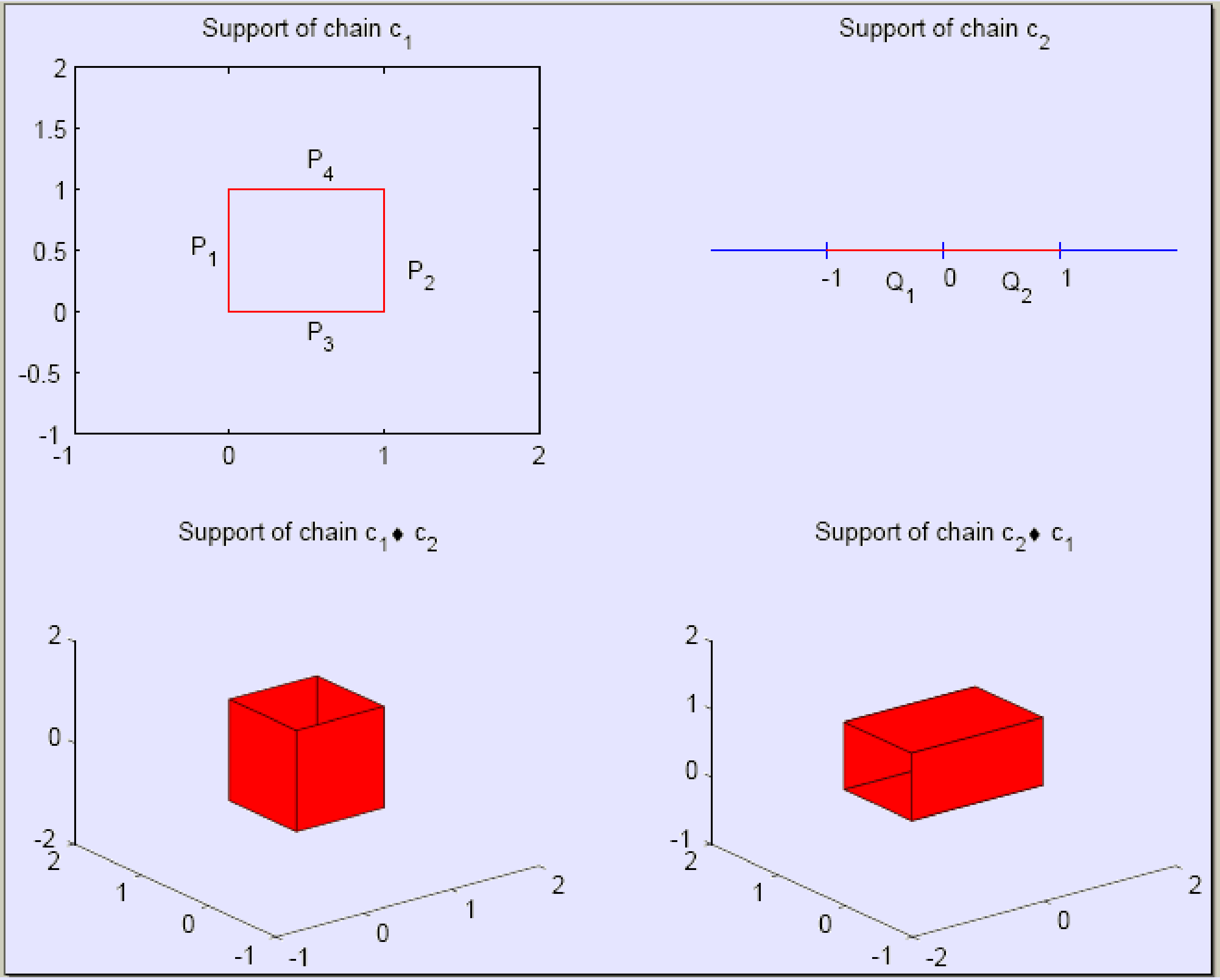
$$\widehat{Q}(P) = \begin{cases} 1 & \text{if } P = Q \\ 0 & \text{otherwise.} \end{cases}$$

- A cubical chain is a finite linear combination of elementary chains of the same dimension, called the dimension of the chain.
- All cubical chains of dimension q form an Abelian group, denoted C_q and called the group of q-chains.

Cubical Product

- Given two elementary chains $\widehat{P}, \widehat{Q}$, we define their cubical product by
$$\widehat{P} \diamond \widehat{Q} := \widehat{P \times Q}.$$
and we extend this definition linearly to arbitrary chains.

Cubical Product



Boundary Operator

- Boundary operator is a homomorphism $\partial : C_q \to C_{q-1}$ given on generators by

$$\partial\widehat{Q} := \begin{cases} 0 & \text{if } Q = [l], \\ \widehat{[l+1]} - \widehat{[l]} & \text{if } Q = [l, l+1]. \\ \partial\widehat{I} \diamond \widehat{P} + (-1)^{\dim I}\widehat{I} \diamond \partial\widehat{P} & \text{if } Q = I \times P. \end{cases}$$

Theorem.

$$\partial \circ \partial = 0$$

Chain groups of a cubical set

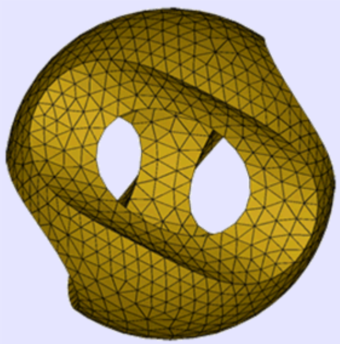
- For an elementary chain $c = \sum_{i=1}^{n} \alpha_i \widehat{Q}_i$ we define its support by
$$|c| := \bigcup \{ Q_i \mid \alpha_i \neq 0 \}$$
- Given a cubical set X we define the group of q-chains of X by
$$C_q(X) := \{ c \in C_q \mid |c| \subset X \}.$$
- Is is easy to verify that we have the induced boundary operator
$$\partial_q^X : C_q(X) \to C_{q-1}(X).$$

Cubical Homology

- The kernel of ∂_q^X is called the group of q-cycles of X and denoted by $Z_q(X)$.
- The image of ∂_{q+1}^X is called the group of q-boundaries of X and denoted by $B_q(X)$.
- One can verify that $B_q(X) \subset Z_q(X)$, which allows us to define the qth homology group of X by
$$H_q(X) := Z_q(X)/B_q(X)$$
- By homology of X we mean the collection of all homology groups $H(X) := \{H_q(X)\}$.

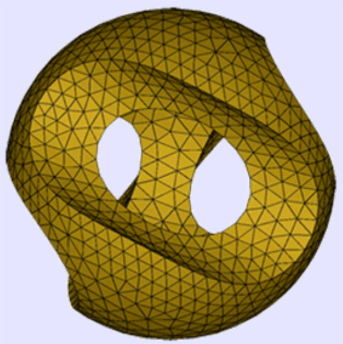
Homology algorithms - standard approach

Immediate algebraization:



Immediate algebraization:

- triangulate the space

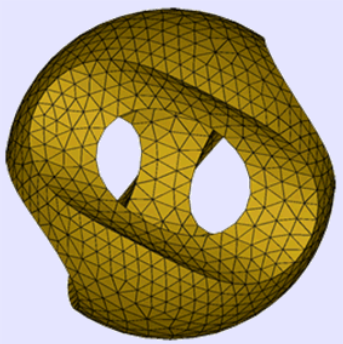


Immediate algebraization:

- triangulate the space
- construct the boundary maps

$$D_k = \begin{bmatrix} \mathbf{1} & -\mathbf{1} & 0 & 0 & \ldots \\ \mathbf{1} & 0 & \mathbf{1} & 0 & \ldots \\ -\mathbf{1} & \mathbf{1} & 0 & 0 & \ldots \\ 0 & \mathbf{1} & 0 & 0 & \ldots \\ . & . & . & . & . \end{bmatrix}$$

Homology algorithms - standard approach



$$D_k = \begin{bmatrix} \mathbf{1} & -\mathbf{1} & 0 & 0 & \dots \\ \mathbf{1} & 0 & \mathbf{1} & 0 & \dots \\ -\mathbf{1} & \mathbf{1} & 0 & 0 & \dots \\ 0 & \mathbf{1} & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix}$$

$$B_k = Q^{-1} D_k R$$

$$B_k = \begin{bmatrix} \mathbf{2} & 0 & 0 & 0 & \dots \\ 0 & \mathbf{1} & 0 & 0 & \dots \\ 0 & 0 & \mathbf{1} & 0 & \dots \\ 0 & 0 & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix}$$

Immediate algebraization:

- triangulate the space
- construct the boundary maps
- find Smith diagonalization and read Betti numbers

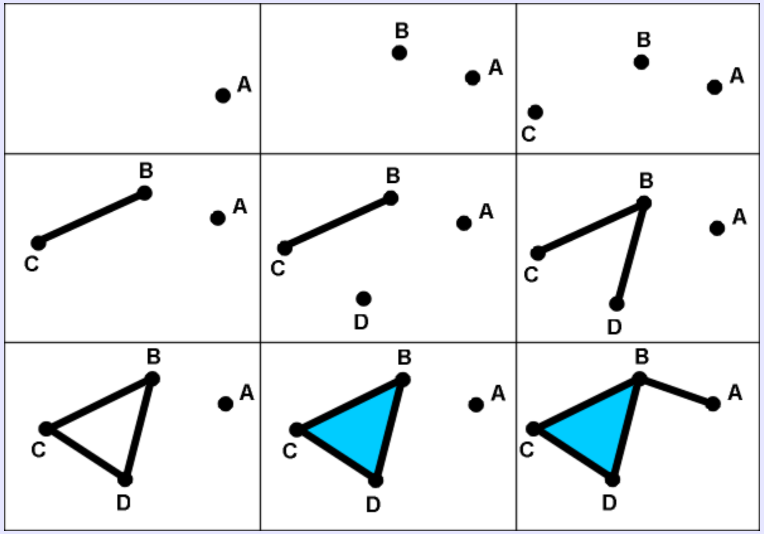
Advantages:

- standard linear algebra
- may be easily adapted to homology generators

Problems:

- building triangulation may increase data size
- complexity: Cn^3
- sparseness of matrices may not help (fill-in process)
- C large for sparse matrices (dynamic storage allocation)

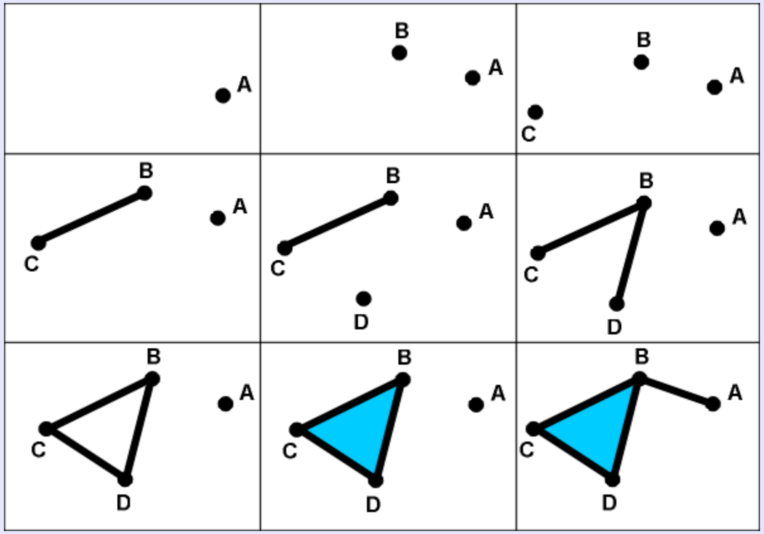
Delfinado-Edelsbrunner algorithm (1995)



Incremental Algorithm

- a filter $\{\sigma_1, \sigma_2, \ldots, \sigma_n\}$ of a triangulation of S^3 on input

Delfinado-Edelsbrunner algorithm (1995)



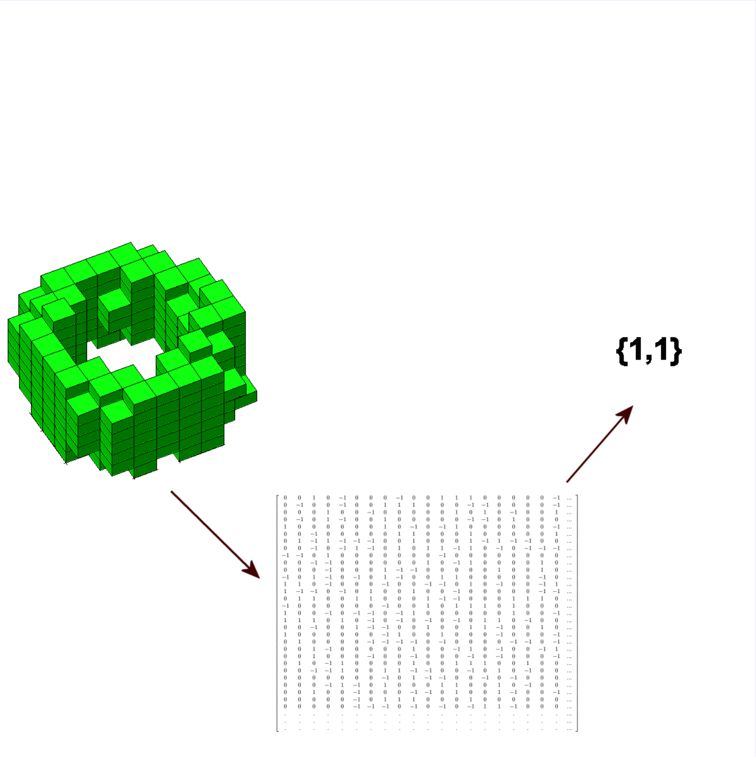
for $j := 0$ **to** 3 **do**
  $\beta_j := 0;$
endfor;
for $i := 1$ **to** n **do**
  $k := \dim \sigma_i;$
  if σ_i belongs to a k-cycle **then**
    $\beta_k := \beta_k + 1$
  else
    $\beta_{k-1} := \beta_{k-1} - 1$
  endif;
endfor;

Incremental Algorithm

- a filter $\{\sigma_1, \sigma_2, \ldots, \sigma_n\}$ of a triangulation of S^3 on input
- computes Betti numbers $\beta_0, \beta_1, \beta_2, \beta_3$ of subpolyhedra of S^3
- complexity: $Cn\alpha(n)$
- replaces algebra by combinatorics

Problems:

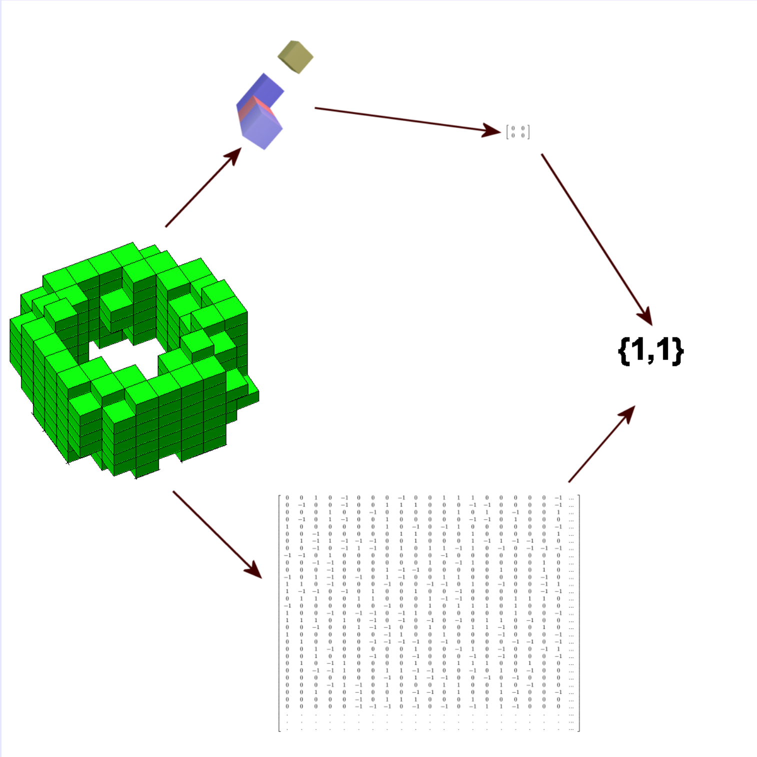
- requires the triangularization of the complement
- no homology generators



Standard Approach

- build chain complex
- compute homology

Reduction algorithms



Standard Approach

- build chain complex
- compute homology

Reduction Approach

- Reduce the set so that
  - the representation used is preserved
  - the homology is not changed
- build chain complex
- compute homology

Advantages:

- bypassing the construction of a big chain complex
- applying the algebraization to a much smaller set
- benefits possible only when:
  - the complexity of reduction is Cn with small C
  - the set after reduction is significantly smaller

Free face reductions

- free face - a generator with exactly one generator in coboundary

Free face reductions

foreach σ **do**
  if $\mathrm{cbd}(\sigma) = \{\tau\}$ **then**
    remove(σ);
    remove(τ);
  endif;
endfor;

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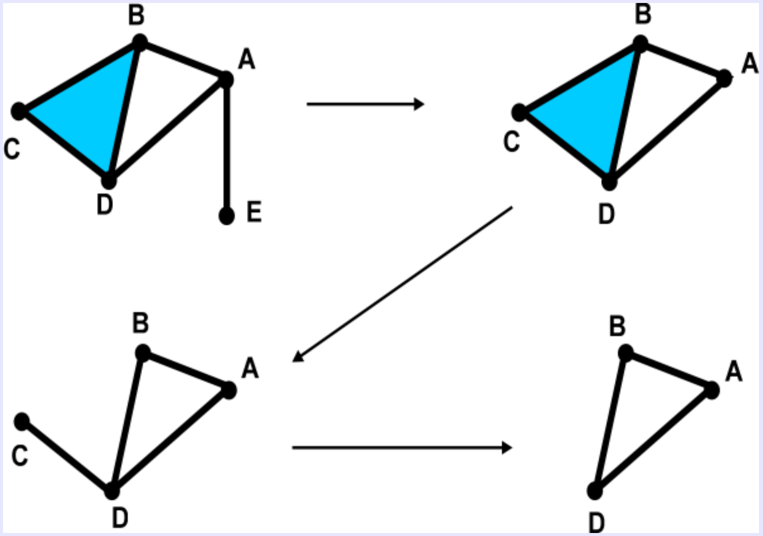

- free face - a generator with exactly one generator in coboundary
- a combinatorial counterpart of deformation retraction

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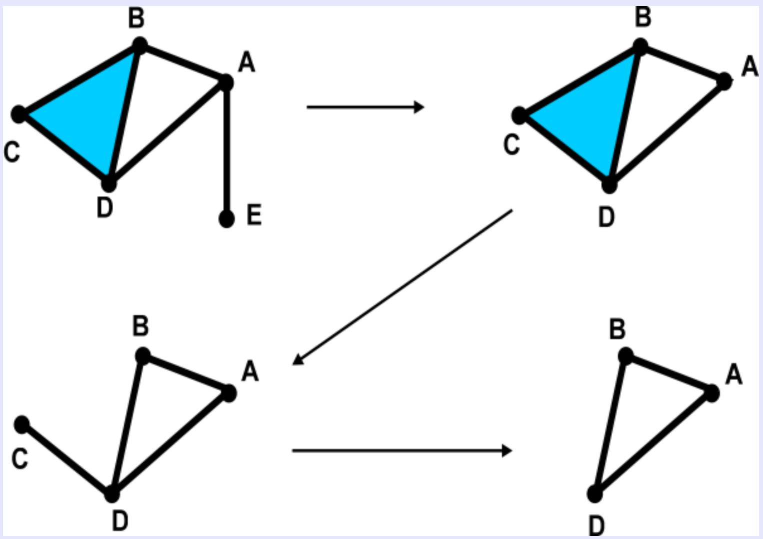


- free face - a generator with exactly one generator in coboundary
- a combinatorial counterpart of deformation retraction
- on algebraic level:

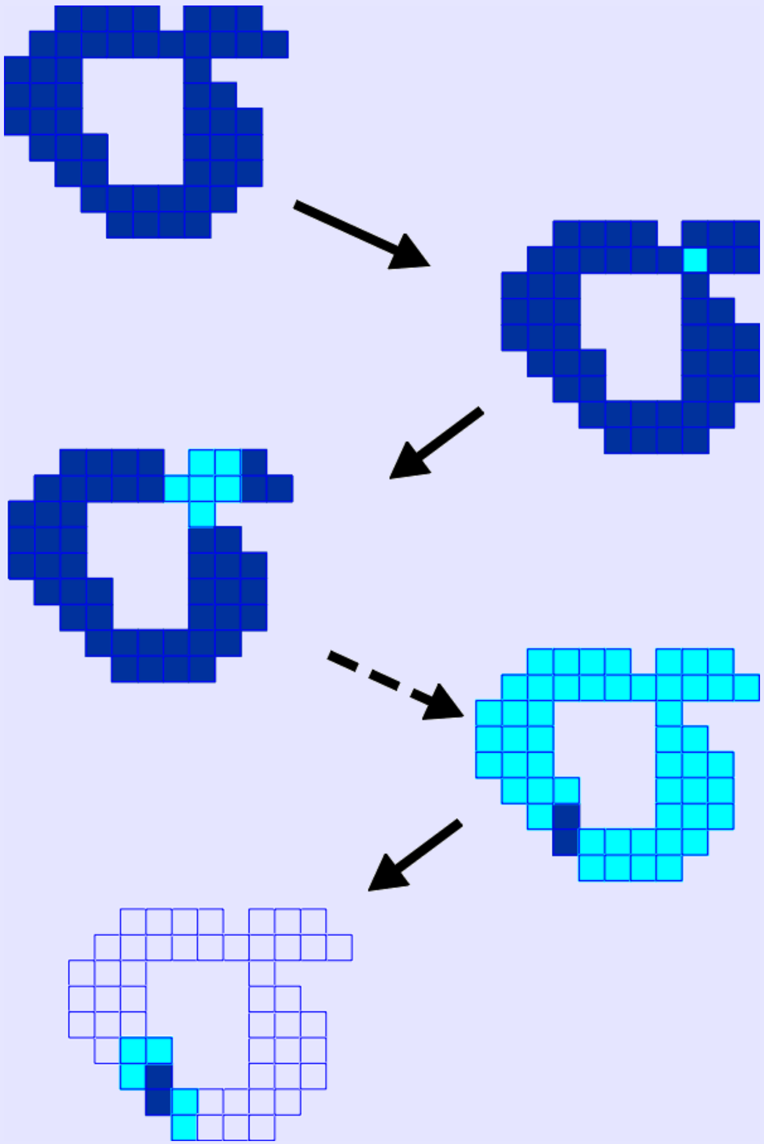
$$\begin{bmatrix}
1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & \cdots \\
1 & 1 & 1 & 0 & 0 & 1 & 0 & 0 & \cdots \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\
0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & \cdots \\
0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & \cdots \\
0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & \cdots \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & \cdots \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & \cdots \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & \cdots \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & \cdots \\
. & . & . & . & . & . & . & . & \cdots \\
. & . & . & . & . & . & . & . & \cdots \\
. & . & . & . & . & . & . & . & \cdots
\end{bmatrix}$$

Acyclic subspace

- If X is cubical and $A \subset X$ is acyclic then

$$H_n(X) \cong \begin{cases} H_n(X,A), & \text{for } n \geq 1 \\ \mathbb{Z} \oplus H_n(X,A), & \text{for } n = 0 \end{cases}$$

Acyclic subspace



- If X is cubical and $A \subset X$ is acyclic then

$$H_n(X) \cong \begin{cases} H_n(X,A), & \text{for } n \geq 1 \\ \mathbb{Z} \oplus H_n(X,A), & \text{for } n = 0 \end{cases}$$

- breadth-first search construction
- acyclicity tests via lookup tables:
  - 2^{3^d-1} entries
  - extremely fast in dimension 2 and 3
  - not enough memory for dimension above 3
  - partial acyclicity tests in higher dimensions

Dual reductions?

$$
\begin{bmatrix}
\mathbf{1} & \mathbf{1} & 0 & \mathbf{1} & \mathbf{1} & 0 & \mathbf{1} & 0 & \ldots \\
\mathbf{1} & \mathbf{1} & \mathbf{1} & 0 & 0 & \mathbf{1} & 0 & 0 & \ldots \\
0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 & \ldots \\
0 & \mathbf{1} & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & \ldots \\
0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & \ldots \\
0 & 0 & \mathbf{1} & 0 & 0 & 0 & \mathbf{1} & 0 & \ldots \\
0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & \mathbf{1} & \ldots \\
0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & \ldots \\
0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & \ldots \\
0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & \ldots \\
. & . & . & . & . & . & . & . & \ldots \\
. & . & . & . & . & . & . & . & \ldots \\
. & . & . & . & . & . & . & . & \ldots
\end{bmatrix}
$$

- free coface - a generator with exactly one generator in boundary
- one space homology theory with compact supports for locally compact sets (Steenrod 1940, Massey 1978)
- combinatorial version (MM, B. Batko, 2006)

S-complexes

- $R(A)$ - free module over R generated by A
- S be a finite set with a gradation S_q
- $\dim s = q$ iff $s \in S_q$
- $\kappa : S \times S \to R$ s.t.

$$\kappa(s,t) \neq 0 \;\Rightarrow\; \dim s = \dim t + 1$$

- (S, κ) is an S-complex if $(R(S), \partial^\kappa)$ with $\partial^\kappa : R(S) \to R(S)$ given by

$$\partial^\kappa(s) := \sum_{t \in S} \kappa(s,t)t$$

  is a free chain complex with base S

> We assume that the coding of S carries the information about κ.

Subcomplexes

$$\begin{aligned} \mathrm{bd}_S\, A &:= \{\, t \in S \mid\ \kappa(s,t) \neq 0 \text{ for some } s \in A. \,\} \\ \mathrm{cbd}_S\, A &:= \{\, s \in S \mid\ \kappa(s,t) \neq 0 \text{ for some } t \in A. \,\} \\ S' &\subset S \\ \kappa' &:= \kappa|_{S' \times S'} \end{aligned}$$

Theorem. If $S' \subset S$ is such that for all $t_1, t_2 \in S'$ and $s \in S$

(1) $\qquad s \in \mathrm{bd}_S\, t_1$ and $t_2 \in \mathrm{bd}_S\, s$ implies $s \in S'$,

then (S', κ') is an S-complex.

- $S' \subset S$ satisfying (1) is regular
- $S' \subset S$ is closed in S if $\mathrm{bd}_S\, S' \subset S'$
- $S' \subset S$ is open in S if $S \setminus S'$ is closed in S

Theorem. If $S' \subset S$ is closed in S, then S' and $S \setminus S'$ are regular.

Exact sequence

Theorem. Assume $S' \subset S$ is closed in S. Let $S'' := S \setminus S'$ and $\kappa'' := \kappa|_{S'' \times S''}$. Then the inclusion

$$\iota : (R(S'), \partial^{\kappa'}) \to (R(S), \partial^{\kappa})$$

and the projection

$$\pi : (R(S), \partial^{\kappa}) \to (R(S''), \partial^{\kappa''})$$

are chain maps. Moreover, we have the following short exact sequence

$$0 \to R(S') \xrightarrow{\iota} R(S) \xrightarrow{\pi} R(S'') \to 0$$

and the following long exact sequence of homology modules

$$...H_q(R(S')) \xrightarrow{\iota_q} H_q(R(S)) \xrightarrow{\pi_q} H_q(R(S'')) \xrightarrow{\partial_k} H_{q-1}(R(S'))...$$

Theorem. If S' is closed in S then

$$H(R(S'')) \cong H(R(S), R(S')).$$

Reduction and coreduction pairs

$T \subset S$ is a nullset of S if T is closed or open in S and $H(R(T)) = 0$.

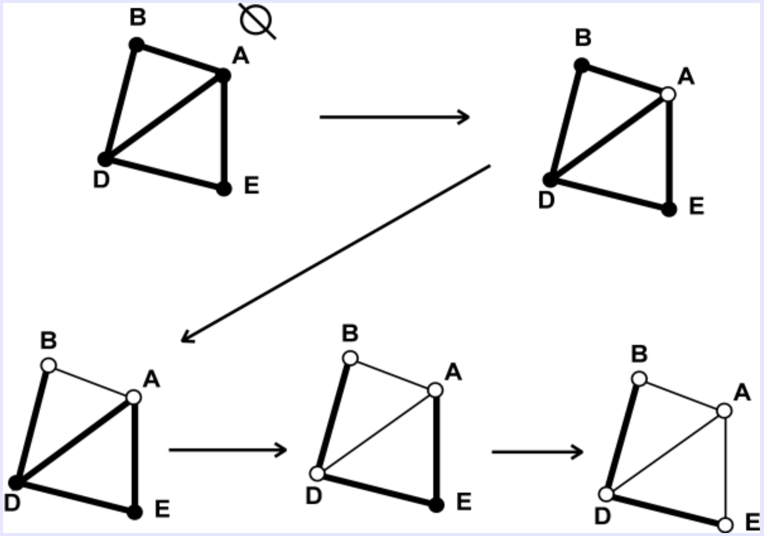
Theorem. If T is a nullset of S then $H(R(S))$ and $H(R(S \setminus T))$ are isomorphic.

- (a, b) is a reduction pair if $\kappa(a, b)$ is invertible
- a is a free face of b in S if (a, b) is a reduction pair and $\mathrm{cbd}_S\, a = \{b\}$
- b is a free coface of a in S if (a, b) is a reduction pair and $\mathrm{bd}_S\, b = \{a\}$

Theorem. Assume $a, b \in S$. If a is a free face of b or b is a free face of a then $\{a, b\}$ is a nullset.

Coreduction algorithm

$Q :=$ empty queue;
enqueue(Q,s);
while $Q \neq \emptyset$ **do**
  s:=dequeue(Q);
  if $\mathrm{bd}_S\, s = \{t\}$ **then**
    remove(s);
    remove(t);
    foreach $u \in \mathrm{cbd}_S\, t$ **do**
    if $u \notin Q$ **then**
      enqueue(Q, u);
    endif;
  else if $\mathrm{bd}_S\, s = \emptyset$ **then**
    foreach $u \in \mathrm{cbd}_S\, s$ **do**
    if $u \notin Q$ **then**
      enqueue(Q, u);
    endif;
  endif;
endwhile ;



Coreduction algorithm complexity

- X - a cubical set
- $|X|$ - size of its representation
- X' - the output of the Free Coface Reduction Algorithm applied to X

Proposition. Assume that for a certain class of cubical sets and some $\kappa \in (0,1)$ we have

$$|X'| = O(|X|^{\kappa})$$

Then the complexity of finding homology in this class by means of Free Coface Reduction Algorithm followed by another homology algorithm applied to X' is

$$O(|X|^{\max(1,\alpha\kappa)})$$

if the complexity of the other homology algorithm is $O(|X|^{\alpha})$.

Coreduction algorithm complexity

Conjecture. Consider a class of q-dimensional cubical sets such that any two of them are homeomorphic under a certain class of homeomorphisms. Then for X in this class

$$|X'| = O(|X|^{\frac{q-1}{q}}).$$

- For some fixed integer $n > 0$ put

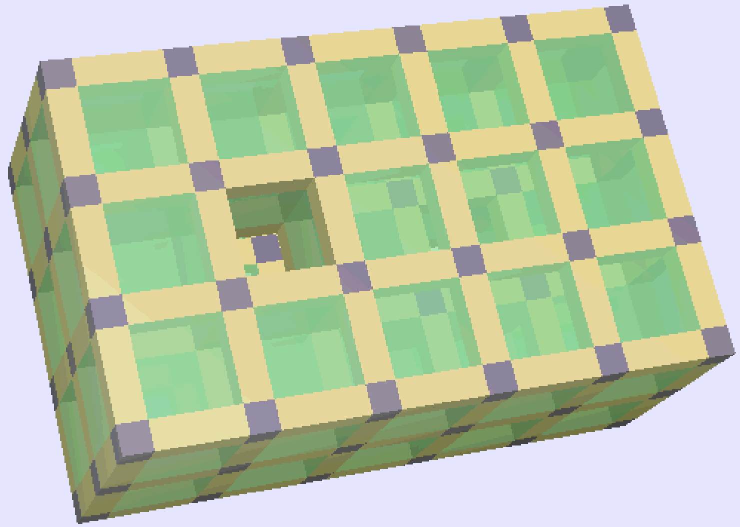
$$R_n : \mathbb{R}^d \ni x \to nx \in \mathbb{R}^d$$

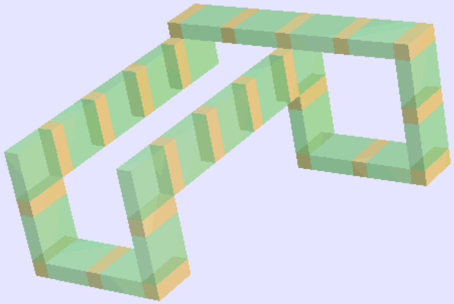
- By an n-rescaling of a cubical set X we mean the image of X under R_n.

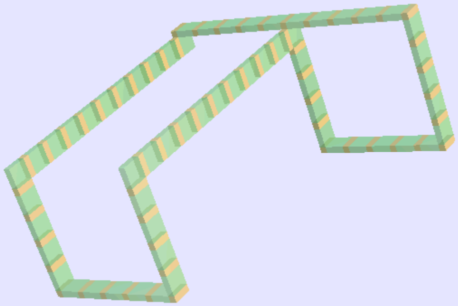
Theorem. (MM, B. Batko, 2008) The class of all n-rescalings of a fixed q-dimensional cubical set X_0 satisfies the conjecture. In particular, the complexity of finding homology in this class is

$$O(|X|^{\alpha\frac{q-1}{q}}).$$

Coreduction algorithm complexity







Reduction Algorithms and their implementations

- Free face collapses algorithm (K. Mischaikow, MM, 1993)
- Algebraic elementary reductions algorithm (T. Kaczynski, MM, M. Ślusarek, 1998)
- Geometrically controlled algebraic reductions (W.D. Kalies, K. Mischaikow, G. Watson, 1999)
  - [**BK**] W.D. Kalies (1999-2005)
- Acyclic intersection algorithm (P. Pilarczyk, 2001)
  - [**PP**] P. Pilarczyk (1999-2005)
- Lookup tables in dimension 3 (A. Szymczak, 2003)
- Acyclic intersection algorithm via lookup tables and decision trees in dimension 3 (M. Gameiro, W.D. Kalies, P. Pilarczyk, 2005)
  - [**BKLT**] M. Gameiro, W.D. Kalies, V. Nanda, A. Szymczak 2005
- Algebraically controlled algebraic reductions (MM, M. Ślusarek, 2005)
  - [**AR**] MM, 2005
- Acyclic subspace algorithm (MM, P. Pilarczyk, N. Żelazna, 2005)
  - [**AS**] MM, 2005
  - [**ASLT**] MM, 2005
  - [**ASPP**] P. Pilarczyk, 2005
- Free coface collapses algorithm (MM, B. Batko, 2005)
  - [**CR**] MM, 2005
- Reduction Trees Algorithm (M. Allili, D. Corriveau, 2006)
  - [HRT] D. Corriveau, 2006

Numerical examples

Size	BBM	CR	ASLT	BK
28800	7.99	0.14	0.13	12.0
51200	15.2	0.23	0.20	24.0
115200	36.7	0.55	0.39	60.0
204800	65.0	0.97	0.63	122.
320000	104.	1.56	0.96	246.
Torus (dim=2, emb=3)				

Size	BBM	CR	ASLT	BK
74341	16.7	0.44	0.27	32.
132321	36.8	0.80	0.39	58.
206901	71.5	1.27	0.61	76.
298081	105.	1.80	0.84	182.
405861	163.	2.52	1.23	221.
Bing's House (dim=2, emb=3)				

Enviroment: 3.6 GHz Pentium 4, 2GB memory, Windows XP

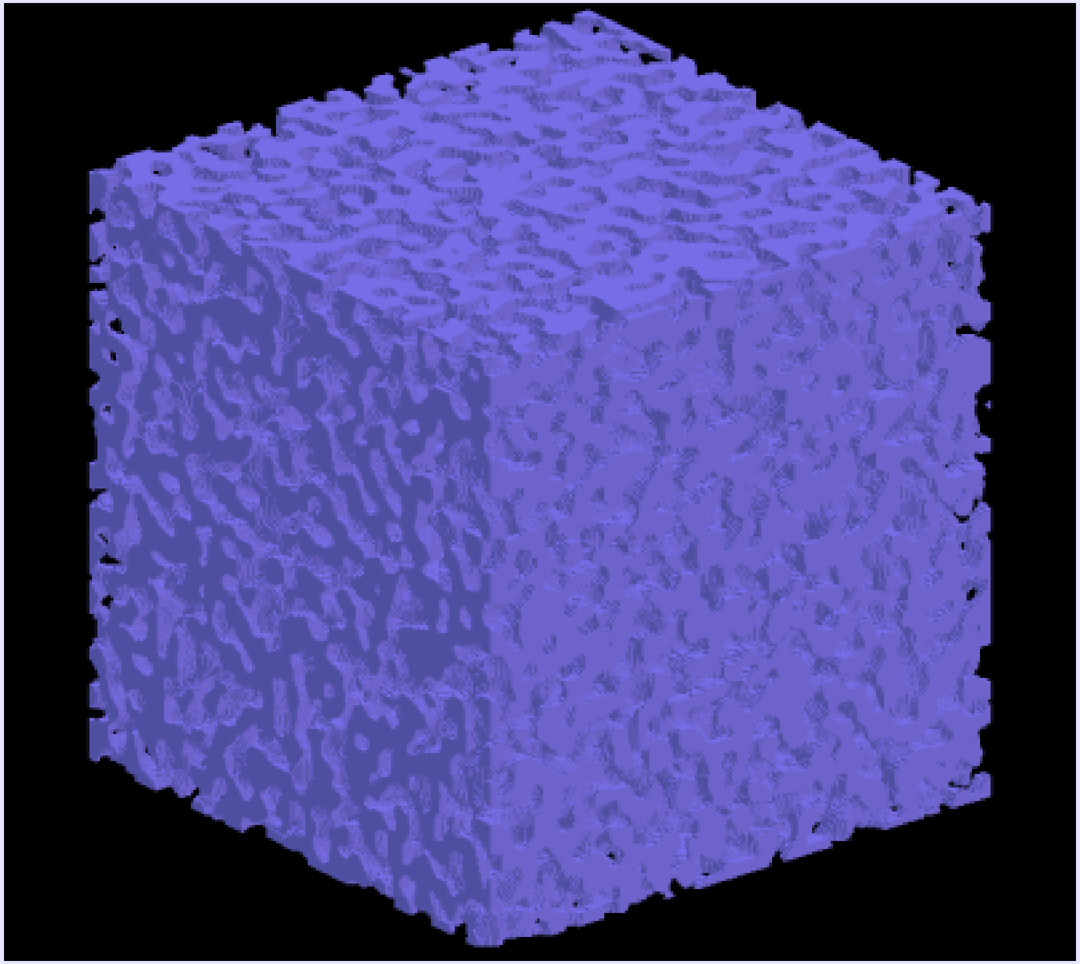
Size	BBM	CR	AS	BK
12522	14.	0.26	1.7	173.
22280	36.	0.51	3.0	1086.
34830	86.	0.90	4.8	716.
50172	184.	1.4	7.0	1677.
68306	326.	2.1	10	1532.
Klein bottle (dim=2, emb=4)				

Size	BBM	CR	AS	BK
937	0.56	0.01	0.30	4.0
3745	3.1	0.07	1.9	25.
8425	8.6	0.15	4.1	69.
14977	18.	0.30	5.4	232.
23401	39.	0.48	8.7	322.
Projective plane (dim=2, emb=4)				

Enviroment: 2.2 GHz Pentium 4, 1GB memory, Linux

- BBM- building boundary matrices

A 4D example from Cahn-Hillard equation



Data provided by Marcio Gameiro

A 4D example from Cahn-Hillard equation

- A four dimensional set of circa 350 000 000 cubes was obtained by gluing together 41 consecutive time slices from the Cahn-Hillard equation
- **CR** algorithm needed 12 min 47 sec to find the Betti numbers

$$\beta_0 = 1$$
$$\beta_1 = 1509$$
$$\beta_2 = 0$$
$$\beta_3 = 0$$

Non-full cubical sets

- Free Coface Collapses Algorithm is perfect in applications to cubical sets, which are not full.
- The following examples are cubical sets in $\mathbb{R}^{12}$, which appear as energy sublevel sets for a randomly chosen k-SAT problem with 12 variables and 50 clauses.

Size	9050	27494	65298	135351	230471	332309
$\beta_0(X)$	1	1	1	1	1	1
$\beta_1(X)$	1	0	0	0	0	0
$\beta_2(X)$	13	8	0	0	0	0
$\beta_3(X)$	1	7	11	1	0	0
$\beta_4(X)$	0	0	4	4	2	0
$\beta_5(X)$	0	0	0	5	3	1
$\beta_6(X)$	0	0	0	0	1	1
CR	0.031	0.11	0.328	0.766	1.547	1.922

Remarks

- Direct algebraization need not be the quickest way to compute homology.
- Reduction algorithms operating directly on sets substantially speed up homology computations.
- There is potential for further improvement in homology computations.

Software

- **CR** and **AS** constitute a part of HomAlg software package in

  Computational Homology Project (CHOMP)
  http://chomp.rutgers.edu/

  Computer Assisted Proofs in Dynamics (CAPD)
  http://capd.wsb-nlu.edu.pl/

  libraries
- extract (**CR** and **AS** only) available from
  http://www.ii.uj.edu.pl/˜ mrozek/software/homology.html

References

- **C.J.A. Delfinado and H. Edelsbrunner**, An incremental algorithm for Betti numbers of simplicial complexes on the 3-sphere, *Computer Aided Geometric Design* (**1995**).
- **T. Kaczynski, M. Mrozek, M. Ślusarek**, Homology computation by reduction of chain complexes, *Computers and Math. Appl.* (**1998**).
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- **MM, B. Batko**, Coreduction homology algorithm, *Discrete and Computational Geometry* (**2009**).