Multi-parameter persistent homology: applications and algorithms

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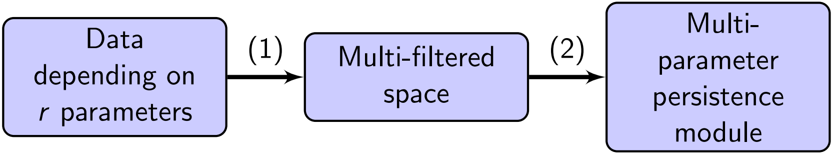
Multi-parameter persistent homology pipeline



Step (1): from data to multi-filtered spaces

Define the following partial order on $\mathbb{N}^r$:
$(u_1, \ldots, u_r) \leq (v_1, \ldots, v_r)$ iff $u_i \leq v_i$ for all $i = 1, \ldots, r$.

A *multi-filtered space K* is a set of spaces $\{K_u\}_{u \in \mathbb{N}^r}$ such that $K_u \subseteq K_v$ if $u \leq v$ for all $u, v \in \mathbb{N}^r$.

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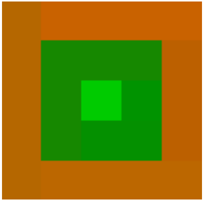
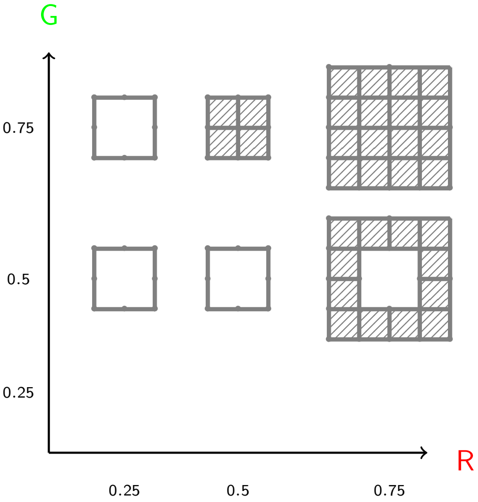
Map $f\colon X \to \mathbb{R}^r$ $\longrightarrow$ r-filtered simplicial complex

digital image with color vectors of length r $\longrightarrow$ r-filtered cubical complex

Step (1): from data to multi-filtered spaces: example



$\longrightarrow$



Step (2): from multi-filtered spaces to multi-parameter persistence modules

r-filtered space	$\xrightarrow{H_i}$	r-parameter persistence module

An *r-parameter persistence module* is a tuple $(\{M_i\}_{i\in\mathbb{N}^r}, \{\phi_{i,j}\}_{i\leq j\in\mathbb{N}^r})$ where:

- for each $i \in \mathbb{N}^r$ we have that M_i is a k-module
- for every $i \leq j$ we have that $\phi_{i,j}\colon M_i \to M_j$ is a k-module homomorphism such that whenever $i \leq k \leq j$ we have

$$\phi_{k,j} \circ \phi_{i,k} = \phi_{i,j}.$$

In other words, an r-parameter persistence module is a functor $F\colon \mathbb{N}^r \to k\mathrm{Mod}$.

Interlude: representation theory of quivers

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A *quiver* $Q = (Q_0, Q_1, s, t)$ consists of two non-empty sets Q_0, Q_1 and two maps $s, t \colon Q_1 \to Q_0$. A quiver is *finite* if both Q_0 and Q_1 are finite.

Whenever $s(u) = x$ and $t(u) = y$ we write $x \xrightarrow{u} y$. For example, the following are finite quivers:

$$\begin{tikzcd} x \arrow[loop left, "u"] \arrow[loop right, "v"] \end{tikzcd} \qquad \begin{tikzcd}[column sep=large] y \arrow[r, bend left, "s"] \arrow[r, bend right, "h"'] & w \arrow[l, "t"'] \end{tikzcd}$$

Representations of quivers

Let k be a field. A *representation of a quiver* (V, ϕ) consists of a family of k-vector spaces $V = \{V_i\}_{i \in Q_0}$ together with a family of k-linear maps $\phi = \{\phi_e \colon V_{s(e) \to V_{t(e)} | e \in Q_1}\}$. A representation (V, ϕ) is *finite-dimensional* if for all $i \in Q_0$ the vector space V_i is finite-dimensional.

A *morphism of representations* $f \colon (V, \phi) \to (V', \phi')$ is given by k-linear maps $f_i \colon V_i \to V'_i$ for all $i \in Q_0$ such that the following diagram

$$\begin{tikzcd}
V_{s(e)} \arrow[r, "\phi_e"] \arrow[d, "f_{s(e)}"'] & V_{t(e)} \arrow[d, "f_{t(e)}"] \\
V'_{s(e)} \arrow[r, "\phi'_{t(e)}"'] & V'_{t(e)}
\end{tikzcd}$$

commutes for all $e \in Q_1$.

Examples of quiver representations

$$x \xrightarrow{u} y$$

Two finite-dimensional representations $\phi\colon V' \to V$ and $\psi\colon W' \to W$ are isomorphic iff $\dim V' = \dim W'$ and $\dim V = \dim W$ and $\mathrm{rank}\phi = \mathrm{rank}\psi$.

$$\begin{tikzcd} x \arrow[loop above, "u"] \end{tikzcd}$$

Two finite-dimensional representations $\phi\colon V \to V$ and $\psi\colon W \to W$ are isomorphic iff ϕ and ψ have the same Jordan normal form.

$$\begin{tikzcd} x \arrow[loop left, "u"] \arrow[loop right, "v"] \end{tikzcd}$$

Studying isomorphism classes of representations of this quiver amounts to studying pairs of quadratic matrices up to simultaneous conjugation.

Indecomposable representations

The *direct sum* of two representations (ϕ, V) and (ψ, W) is the representation $(\phi \oplus \psi, V \oplus W)$ where $V \oplus W = V_i \oplus W_i$ for all $i \in Q_0$ and $(\phi \oplus \psi)_e = \begin{pmatrix} \phi_e & 0 \\ 0 & \psi_e \end{pmatrix}$.

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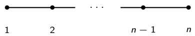
Example: indecomposable representations of the loop quiver are given by the Jordan blocks.

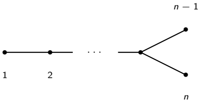
Theorem (Krull, Remak, Schmidt) Assume that Q is finite, then any finite-dimensional representation (V, ϕ) of Q can be written as a direct sum $(V, \phi) = (V_1, \phi_1) \oplus \cdots \oplus (V_r, \phi_r)$ where each (V_i, ϕ_i) is indecomposable, and the decomposition is unique up to isomorphism and permutation of the terms.

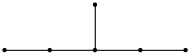
Classification of (representations of) quivers

Dynkin

($n \geq 2$)







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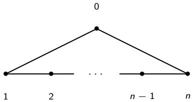
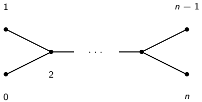
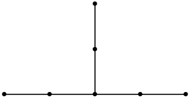
Extended Dynkin

($n \geq 2$)



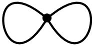




...

Wild

Everything else. For example:



Classification of representations of quivers

Suppose that k is algebraically closed. The number of isomorphism classes of indecomposable representations is:

Dynkin	**Extended Dynkin**	**Wild**
Finite.	Infinite; depends on one parameter.	Infinite; depends on $N > 1$ parameters, where N depends on the quiver.

G. Kac, *Infinite root systems, representations of graphs and invariant theory I - II*, 1980-2 and P. Gabriel, *Unzerlegbare darstellungen I*, 1972.

Classification of indecomposable representations of quivers: example

Conside again the loop quiver:

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Conside again the loop quiver:

Recall that two finite-dimensional representations $\phi \colon V \to V$ and $\psi \colon W \to W$ are isomorphic iff ϕ and ψ have the same Jordan normal form, and the isomorphism classes of indecomposable representations of the loop quiver are given by the Jordan blocks.

Each Jordan block depends on a continuous parameter given by the eigenvalue.

Back to multi-parameter persistent homology

A multi-parameter persistence module is a representation of a quiver of the following form:

$$
\begin{tikzcd}
\cdots & \cdots & \cdots & \\
\bullet \arrow[r] \arrow[u] & \bullet \arrow[r] \arrow[u] & \bullet \arrow[r] \arrow[u] & \cdots \\
\bullet \arrow[r] \arrow[u] & \bullet \arrow[r] \arrow[u] & \bullet \arrow[r] \arrow[u] & \cdots \\
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Such quivers are wild.

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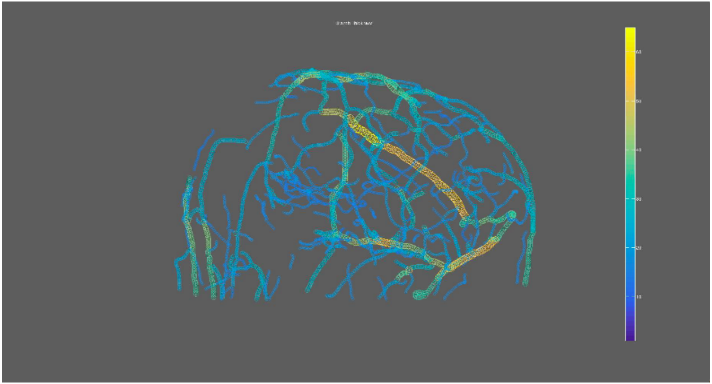
\end{tikzcd}$$

Such quivers are wild.

Our motivation/goal: find computable invariants for applications.

Application: Time evolution of blood vessel growth in presence of tumors



Roche, Oxford Oncology (B. Markelc), Mathematical Biology, University of Oxford (B. Stolz, H. Byrne, J. Grogan)

Persistence modules are modules

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- Recall that an $\mathbb{N}^r$-graded (or multi-graded) ring is a ring A together with a collection $\{A_u\}_{u \in \mathbb{N}^r}$ of subgroups of the underlying abelian group of A such that $A = \oplus_{u \in \mathbb{N}^r} A_u$ and for all $a \in A_m$ and $b \in A_n$ we have $ab \in A_{m+n}$.

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- Make the ring $A = k[x_1, \ldots, x_r]$ into an $\mathbb{N}^r$-graded ring by setting

$$A_u = k x_1^{u_1} \ldots x_r^{u_r} \text{ for all } u = (u_1, \ldots, u_r) \in \mathbb{N}^r.$$

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- A module M over an $\mathbb{N}^r$-graded ring A is *graded* if there is a collection $\{M_i\}_{i \in \mathbb{N}^r}$ of subgroups of the underlying abelian group of M such that $M = \oplus_{i \in \mathbb{N}^r} M_i$ and for all $a \in A_j$ we have $aM_i \subset M_{i+j}$.

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Correspondence Theorem of Persistent Homology (Carlsson, Zomorodian '09)
The functor category of r-parameter persistence modules is isomorphic to the category of graded $k[x_1, \ldots, x_r]$-modules and module homomorphisms respecting the grading.

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Theorem (Carlsson, Zomorodian, 2009)
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Therefore, studying the homology of r-filtered spaces amounts to studying graded modules over $k[x_1, \ldots, x_r]$.

Free resolutions and presentations

Let M be a finitely generated graded $k[x_1, \ldots, x_r]$-module. By the Hilbert Syzygy Theorem there is a free resolution by finitely generated $\mathbb{N}^r$-graded free $k[x_1, \ldots, x_r]$-modules of length at most r:

$$0 \longrightarrow F_m \xrightarrow{\phi_m} F_{m-1} \longrightarrow \ldots \longrightarrow F_1 \xrightarrow{\phi_1} F_0 \longrightarrow M \longrightarrow 0$$

with $\mathrm{image}(\phi_i) = \mathrm{kernel}(\phi_{i-1})$ and each F_i is a finitely generated graded free $k[x_1, \ldots, x_r]$-module and $m \leq r$.

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The first part

$$F_1 \xrightarrow{\phi_1} F_0 \longrightarrow M \longrightarrow 0$$

of a free resolution of a module is called *presentation*. If we are given a presentation of M, we can then explicitly write M as the quotient $F_0/\mathrm{im}\phi_1$.

Minimal presentations and resolutions

Resolutions and presentations are in general not unique.

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Example:[1] Let $M = (x_1x_2, x_1x_3) \subset k[x_1, x_2, x_3] = S$. The following are two free resolutions of M:

$$0 \longrightarrow S \xrightarrow{\begin{pmatrix} x_3 \\ -x_2 \end{pmatrix}} S^2 \xrightarrow{\begin{pmatrix} x_1x_2 & x_1x_3 \end{pmatrix}} M \longrightarrow 0$$

$$0 \xrightarrow{\begin{pmatrix} -x_2 \\ 1 \end{pmatrix}} S^2 \xrightarrow{\begin{pmatrix} x_3 & x_2x_3 \\ -x_2 & -x_2^2 \end{pmatrix}} S^2 \xrightarrow{\begin{pmatrix} x_1x_2 & x_1x_3 \end{pmatrix}} M \longrightarrow 0$$

However, minimal presentations of modules over local or graded rings are unique up to isomorphism.

[1] Bulletin of the AMS, July 2016

Invariants from resolutions and presentations

Minimal presentations are invariants of a module, and one can compute many invariants from minimal presentations and resolutions, such as:

- Betti numbers
- (Multi-graded) Hilbert series
- ...

Presentation of a persistence module: naïve Algorithm

Since the ith homology of the ith chain complex of a multi-filtered simplicial complex is defined as

$$H_i = \mathrm{kernel}(d_i)/\mathrm{image}(d_{i+1}),$$

an algorithm to compute a presentation of H_i is given by the following steps:

1. Compute a presentation of $\mathrm{image}(d_{i+1})$.

[1] G. Carlsson, G. Singh, A. Zomorodian, *Computing multidimensional persistence*, 2010.

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1. Compute a presentation of $\mathrm{image}(d_{i+1})$.
2. Compute a presentation of $\mathrm{kernel}(d_i)$.
3. Compute a presentation of the quotient H_i.

Problem: the known algorithms to compute $\mathrm{image}(d_{i+1})$ are exponential in time and space[1].

[1] G. Carlsson, G. Singh, A. Zomorodian, *Computing multidimensional persistence*, 2010.

Presentation of a module: algorithm by Carlsson, Singh and Zomorodian

In 2010 Carlsson, Singh and Zomorodian[2] put forward an optimisation of the algorithm to compute a presentation of homology of 'one-critical' multi-filtered complexes.

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Let $K = \{K_u\}_{u \in \mathbb{N}^r}$ be a multi-filtered simplicial complex. We assume that there exists $v \in \mathbb{N}^r$ such that K_v is a finite simplicial complex, and $K_u = K_v$ for all $u \geq v$. We denote the simplicial complex K_v by K_{tot}.

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For any $\sigma \in K_{\mathrm{tot}}$ define the set of *generators of* σ to be

$$\mathrm{gen}(\sigma) = \min\{v \in \mathbb{N}^r \mid \sigma \in K(v)\}.$$

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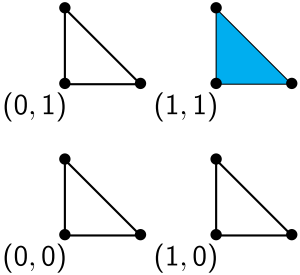
A multi-filtered simplicial complex is *one-critical* if the set of generators of every simplex has cardinality one.

[2] G. Carlsson, G. Singh, and A. Zomorodian, *Computing multidimensional persistence*, 2010.

One-critical multi-filtered simplicial complex: example

One-critical:



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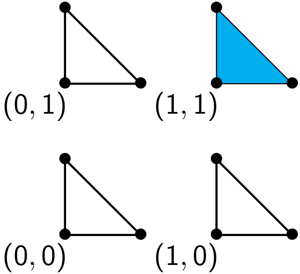
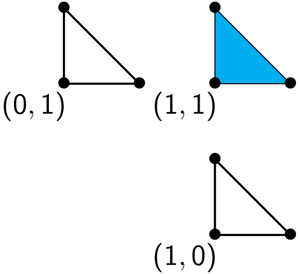


Not one-critical:



Optimization

For a one-critical multifiltered simplicial complex K:

- the chain modules are free modules, hence one can choose bases for them
- The standard basis is the basis of simplices in degree given by their generator
- The boundary maps can be written as homogeneous matrices with monomial entries
- Carlsson, Singh and Zomorodian show that this gives a polynomial bound on complexity.
- The resulting presentation is not an invariant, as it depends on a choice of basis.

Presentation of a module: algorithm by Chacholski-Scolamiero-Vaccarino (CSV)

In 2014 Chacholski, Scolamiero and Vaccarino[3] put forward a polynomial-time algorithm to compute a presentation of homology of arbitrary multi-filtered simplicial complexes.

[3] W. Chacholski, M. Scolamiero, and F. Vaccarino, *Combinatorial presentation of multidimensional persistent homology*, 2014.

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- For any $u \in \mathbb{N}^r$, denote by $K_{n,u}$ the set of n-simplices in K_u; the assignment $u \mapsto K_{n,u}$ induces a functor $K_n \colon \mathbb{N}^r \to \mathrm{Sets}$, where Sets is the category of sets.
- For any $v \in \mathbb{N}^r$ and any $i \in \{0, \ldots, n+1\}$ define the following map

$$d_i \colon K_{n+1,v} \longrightarrow K_{n,v} \colon \{x_0, \ldots, x_{n+1}\} \mapsto \{x_0, \ldots, \hat{x}_i, \ldots, x_{n+1}\}$$

  where $\hat{x}_i$ means that we omit the vertex x_i. The maps d_i give natural transformations $K_{n+1} \to K_n$.

[3] W. Chacholski, M. Scolamiero, and F. Vaccarino, *Combinatorial presentation of multidimensional persistent homology*, 2014.

CSV algorithm

Let $S = k[x_1, \ldots, x_r]$.There exists a sequence of free graded S-modules

$$\mathcal{RK}K_n \oplus \mathcal{RG}K_{n+1} \xrightarrow{\pi \oplus d} \mathcal{RG}K_n \xrightarrow{\alpha} \mathcal{R}D_{n-1}$$

such that $\alpha \circ (\pi \oplus d)$ is trivial, and the $k[x_1, \ldots, x_r]$-module $\mathrm{kernel}(\alpha)/\mathrm{im}(\pi \oplus d)$ is isomorphic to the homology in degree n of the multi-filtered simplicial complex K,

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- $\mathcal{RK}K_n = \bigoplus_{\sigma \in K_{\mathrm{tot},n}} \bigoplus_{v_0 \neq v_1 \in \mathrm{gen}(\sigma)} x^{\max\{v_0, v_1\}} S$,
- $\mathcal{RG}K_n = \bigoplus_{\sigma \in K_{\mathrm{tot},n}} \bigoplus_{v \in \mathrm{gen}(\sigma)} x^{v} S$, and
- $\mathcal{R}D_{n-1} = \bigoplus_{\sigma \in K_{\mathrm{tot},n-1}} S.$

with the notation $x^u := x_1^{u_1} \ldots x_r^{u_r}$.

CSV algorithm

The homomorphisms are defined as follows:

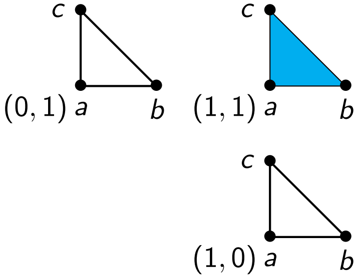
(π) For any $\sigma \in K_n$ and $v_0 \neq v_1 \in \mathrm{gen}(\sigma)$, the homomorphism $\pi\colon \mathcal{R}\mathcal{K}K_n \to \mathcal{R}\mathcal{G}K_n$ sends $x^{\max\{v_0,v_1\}}$ to $x^{v_0} - x^{v_1}$.

(d) For any $\sigma \in K_{n+1}$ and $v \in \mathrm{gen}(\sigma)$, the homomorphism $d\colon \mathcal{R}\mathcal{G}K_{n+1} \to \mathcal{R}\mathcal{G}K_n$ sends x^v to $\sum_{i=0}^{n+1}(-1)^i x^{\widetilde{d_i(\sigma)}}$, where $\widetilde{d_i(\sigma)}$ is the minimal element in the set $\{w \in \mathrm{gen}(d_i(\sigma)) \mid w \leq v\}$ with respect to the lexicographical order.

(α) For any $\sigma \in K_n$ and $v \in \mathrm{gen}(\sigma)$, the homomorphism $\alpha\colon \mathcal{R}\mathcal{G}K_n \to \mathcal{R}D_{n-1}$ sends x^v to $\sum_{i=0}^{n}(-1)^i d_i(\sigma)$.

CSV algorithm: example

We illustrate the algorithm for the computation of H_1 of the following 2-filtered simplicial complex K:



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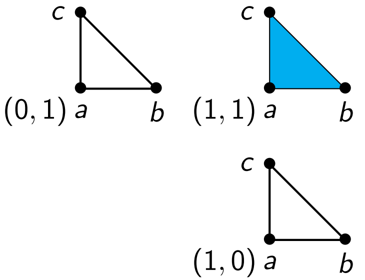

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$$\mathrm{gen}(\{a\}) = \{(0,1),(1,0)\}$$

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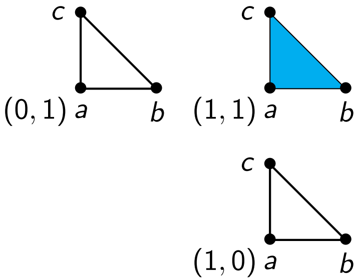

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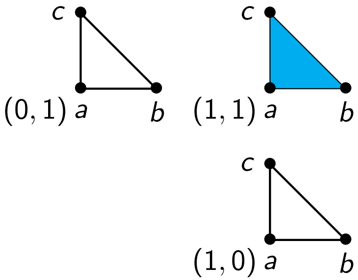

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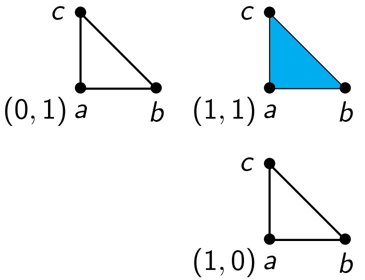

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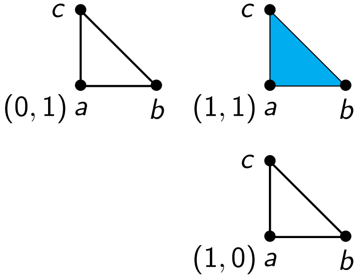

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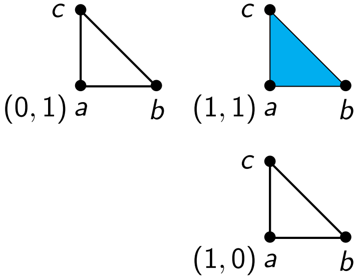

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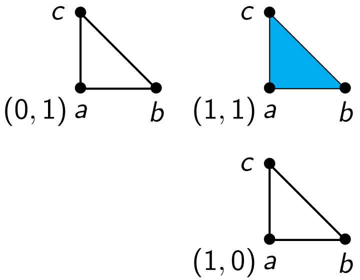

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CSV algorithm: example

Let $S = k[x_1, x_2]$. Then:

- $\mathcal{RK}K_1 = \bigoplus_{\sigma \in K_{\mathrm{tot},1}} \bigoplus_{v_0 \neq v_1 \in \mathrm{gen}(\sigma)} x^{\max\{v_0, v_1\}} S$

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- $\mathcal{RG}K_n = \bigoplus_{\sigma \in K_{\mathrm{tot},n}} \bigoplus_{v \in \mathrm{gen}(\sigma)} x^v S$, so
  $\mathcal{RG}K_2 = x_1x_2S$
  $\mathcal{RG}K_1 = x_1S \oplus x_2S \oplus x_1S \oplus x_2S \oplus x_1S \oplus x_2S$

CSV algorithm: example

Let $S = k[x_1, x_2]$. Then:

- $\mathcal{R}\mathcal{K}K_1 = \bigoplus_{\sigma \in K_{\mathrm{tot},1}} \bigoplus_{v_0 \neq v_1 \in \mathrm{gen}(\sigma)} x^{\max\{v_0, v_1\}} S$, so

  $\mathcal{R}\mathcal{K}K_1 = x_1x_2S \oplus x_1x_2S \oplus x_1x_2S$
- $\mathcal{R}\mathcal{G}K_n = \bigoplus_{\sigma \in K_{\mathrm{tot},n}} \bigoplus_{v \in \mathrm{gen}(\sigma)} x^v S$, so

  $\mathcal{R}\mathcal{G}K_2 = x_1x_2S$

  $\mathcal{R}\mathcal{G}K_1 = x_1S \oplus x_2S \oplus x_1S \oplus x_2S \oplus x_1S \oplus x_2S$
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- $\mathcal{R}D_0 = \bigoplus_{\sigma \in K_{\mathrm{tot},0}} k[x_1, \ldots, x_r]$, so

  $\mathcal{R}DK_0 = S \oplus S \oplus S$

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CSV algorithm: example

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$$\alpha = \begin{pmatrix} -1 & -1 & -1 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 & -1 & -1 \\ 0 & 0 & 1 & 1 & 1 & 1 \end{pmatrix}$$

CSV algorithm: example

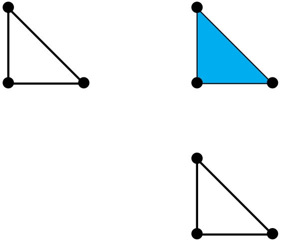
By using a computational algebra software package one can then compute the following minimal presentation:

$$0 \longrightarrow S^2 \xrightarrow{\begin{pmatrix} x_1 & 0 \\ 0 & x_2 \end{pmatrix}} S^2 \xrightarrow{\begin{pmatrix} x_2 & x_1 \end{pmatrix}} H_1(K) \longrightarrow 0$$

and thus

$$H_1(K) = \frac{x_1 S}{(x_1 x_2)} \oplus \frac{x_2 S}{(x_1 x_2)}.$$

CSV algorithm: example



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Conclusions

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- Need efficient implementation of algorithm by Chacholski, Scolamiero and Vaccarino.
- Computational algebra libraries are not efficient.
- How complex is the problem in practice?
- Insight from geometric invariant theory?