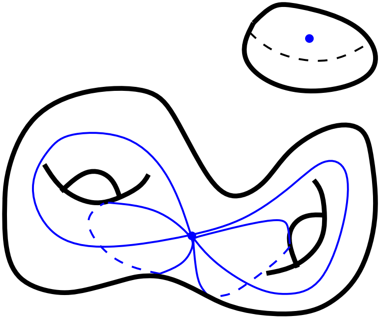
Multi-Field Persistent Homology

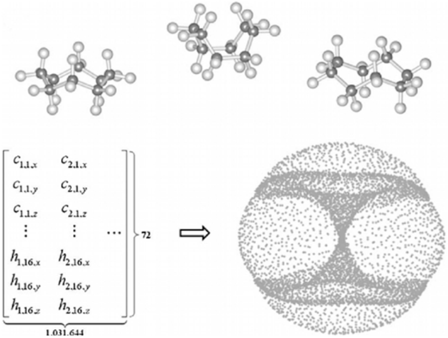
Jean-Daniel Boissonnat & Clément Maria

1
Introduction

Motivation

Homology features:
components, **holes**, **voids**, etc.





Conformation Space of the Cyclo-octane Molecule

Image: **[Martin, Thompson, Coutsias, Watson]**

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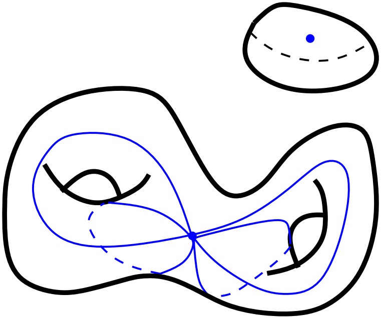
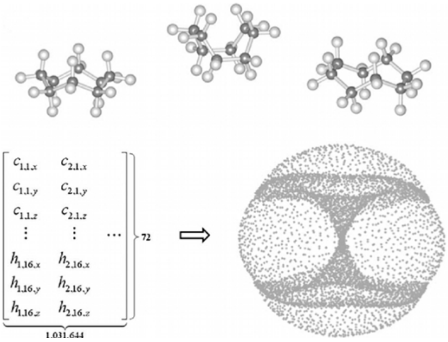


but... that guy on the right is **"twisting"**!



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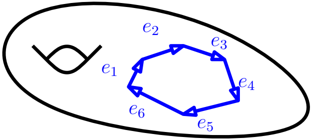
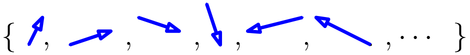
Homology with $\mathbb{Z}$-coefficients

$e_1 + e_2 + e_3 + e_4 + e_5 + e_6$



$\{e_1, e_2, e_3, e_4, e_5, e_6, \cdots\}$

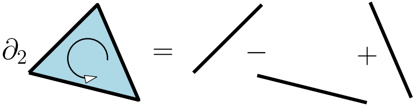
$\mathbf{K}^p$: set of p-simplices of $\mathbf{K}$



$\mathbf{C}_p$: Abelian group of formal sums of p-simplices with $\mathbb{Z}$-coefficients

$$\mathbf{C}_1 = (\{\sum_i k_i e_i\}, +)$$

$\partial_p : \mathbf{C}_p \to \mathbf{C}_{p-1}$: Boundary operator



$\mathbf{H}_p = \ker \partial_p / \operatorname{im} \partial_{p+1}$

$$\partial_2 \, [a, b, c] = [ab] - [bc] + [ca]$$

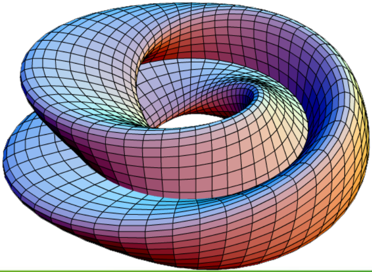
Homology and Torsion

Fundamental theorem of finitely generated abelian groups:

$$\mathbf{H}_p(\mathbb{Z}) \cong \mathbb{Z}^{\beta_p(\mathbb{Z})} \bigoplus_{q \text{ prime}} \left(\mathbb{Z}_{q^{k_1}} \oplus \cdots \oplus \mathbb{Z}_{q^{k_{t(p,q)}}} \right) \text{ vs } \mathbf{H}_p(\mathbb{F}) = \mathbb{F}^{\beta_p(\mathbb{F})}$$

- $\beta_p(\mathbb{Z})$ and $\beta_p(\mathbb{F})$ are *Betti numbers*: $\beta_p(\mathbb{Z}) \neq \beta_p(\mathbb{F})$ in general
- $k_i > 0$ and $t(p,q) \geq 0$ over all prime numbers q
- if $t(p,q) \neq 0$, $q^{k_1} \cdots q^{k_{t(p,q)}}$ are *torsion coefficients*

Klein bottle:



Homology and Torsion

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$$\begin{array}{lcll}
\mathbf{H}_0(\mathbb{Z}) & = & \mathbb{Z} & \beta_0(\mathbb{Z}) = 1 \\
\mathbf{H}_1(\mathbb{Z}) & = & \mathbb{Z} \oplus \mathbb{Z}_2 & \beta_1(\mathbb{Z}) = 1 \\
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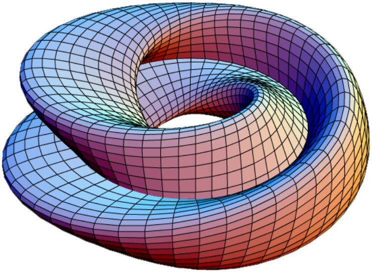

Homology and Torsion

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Klein bottle???

o_O ???

Homology and Torsion

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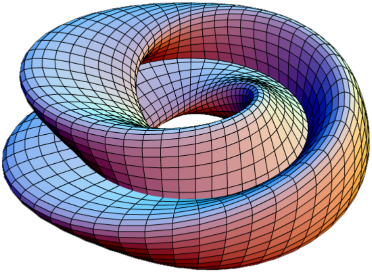
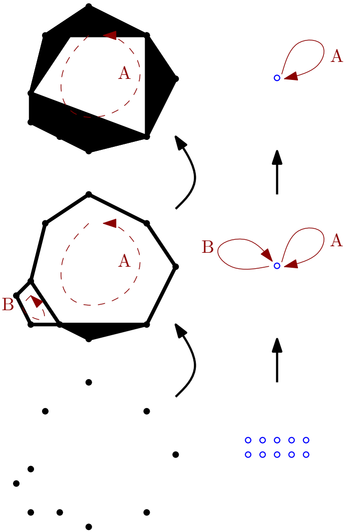


Remember Persistence?



Very useful!

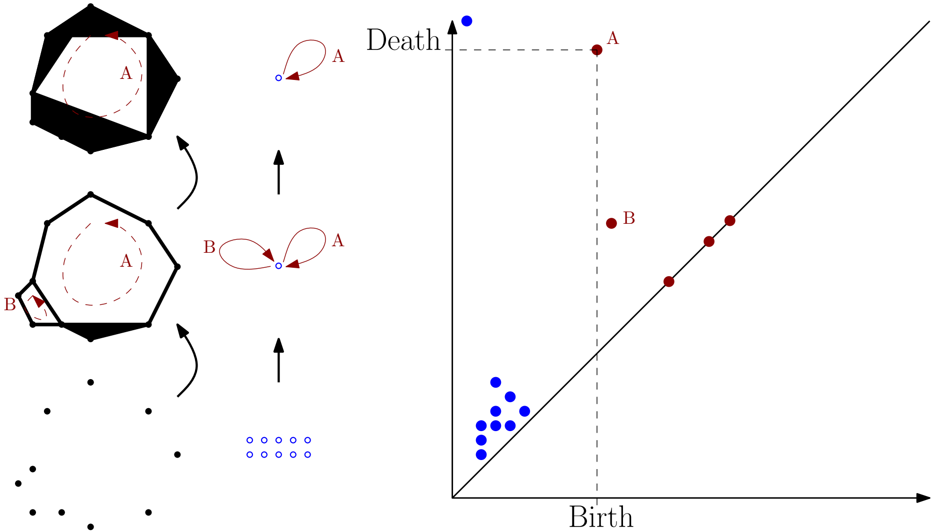
- General
- Stable w.r.t noise
- Efficient Algorithm

BUT

Strictly restricted to FIELD coefficients!

(algebraic reason)

Remember Persistence?



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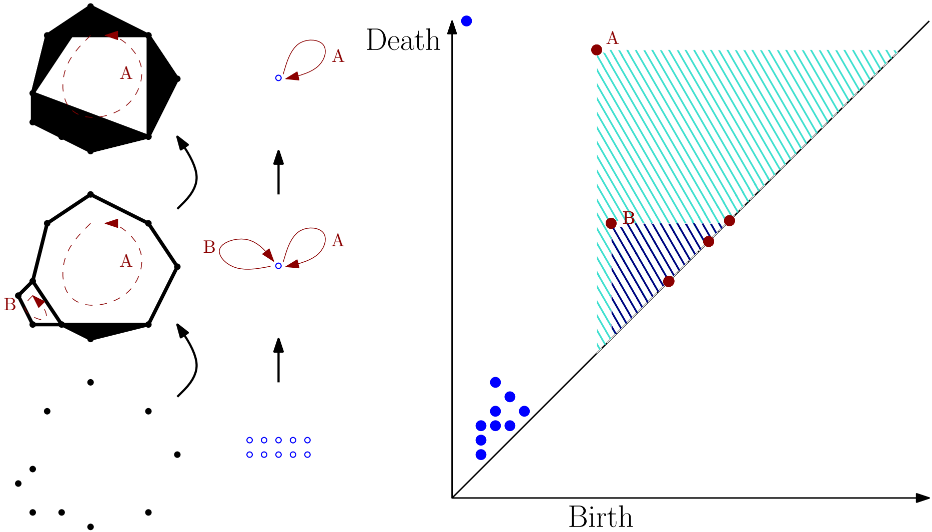

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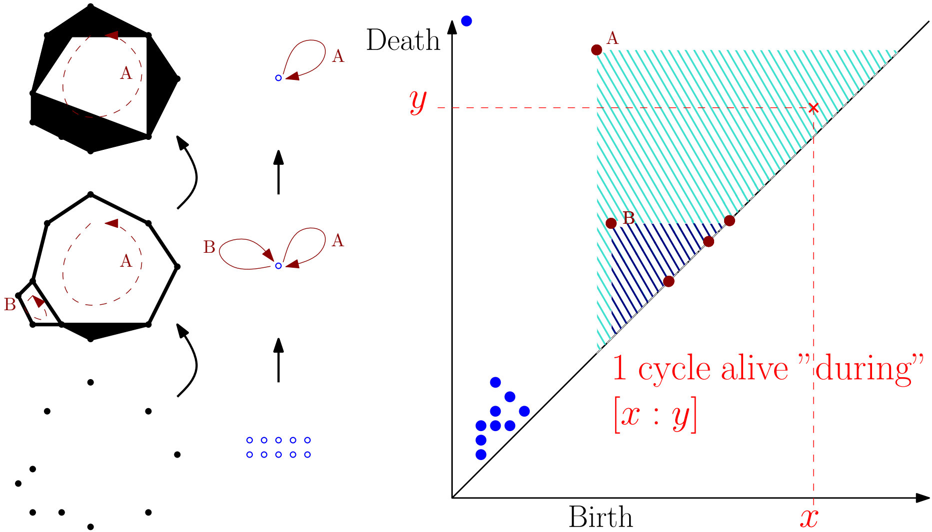

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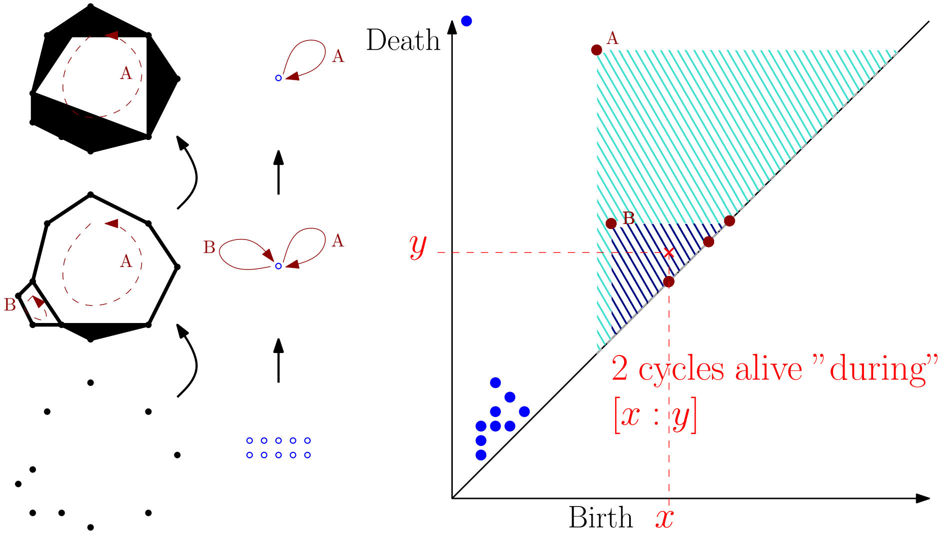

2
Multi-Field Persistence Diagram

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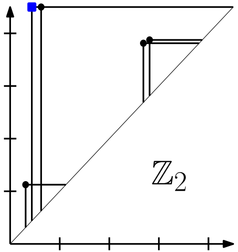

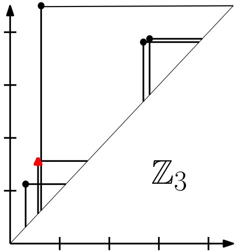

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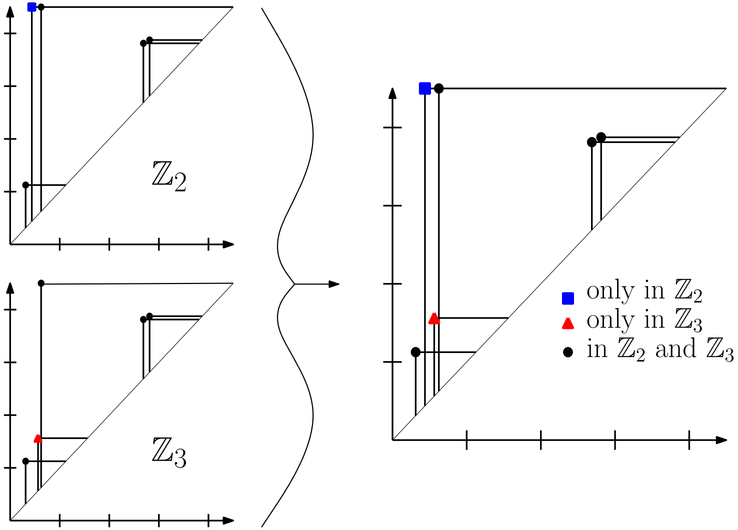

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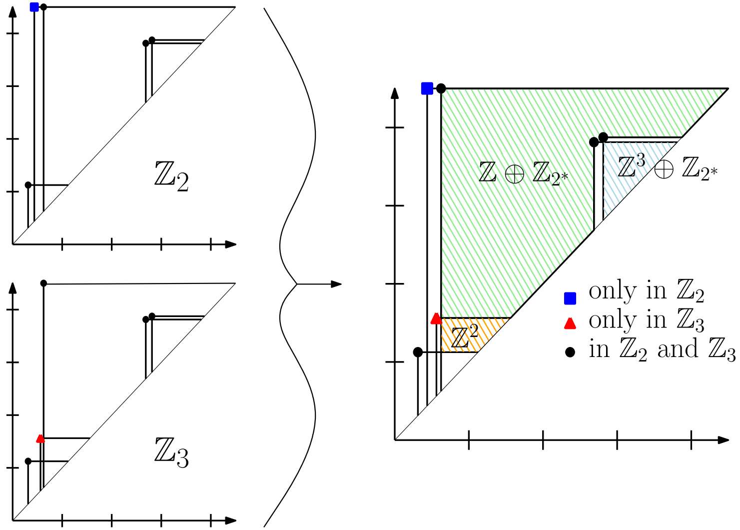

Homology Group Reconstruction

We compute the **Multi-Field Persistence Diagram** for the fields:
$\{\mathbb{Z}_{q_1}, \cdots, \mathbb{Z}_{q_r}\}$ for the family of first r distinct primes $q_1, \cdots, q_r$

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Suppose we know $\beta_p(\mathbb{Z}_{q_s}), \forall 1 \leq s \leq r$ (with $\mathbf{H}_p(\mathbb{Z}_{q_s}) \cong \mathbb{Z}_{q_s}^{\beta_p(\mathbb{Z}_{q_s})}$).

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The **Universal Coefficient Theorem of Homology** allows to compute $\mathbf{H}_p(\mathbf{K}, \mathbb{F})$ from $\mathbf{H}_p(\mathbf{K}, \mathbb{Z})$ and $\mathbf{H}_{p-1}(\mathbf{K}, \mathbb{Z})$.

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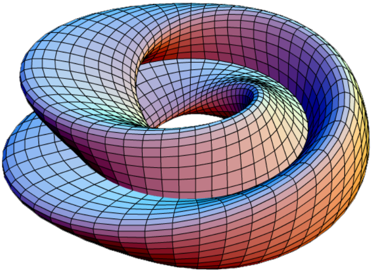
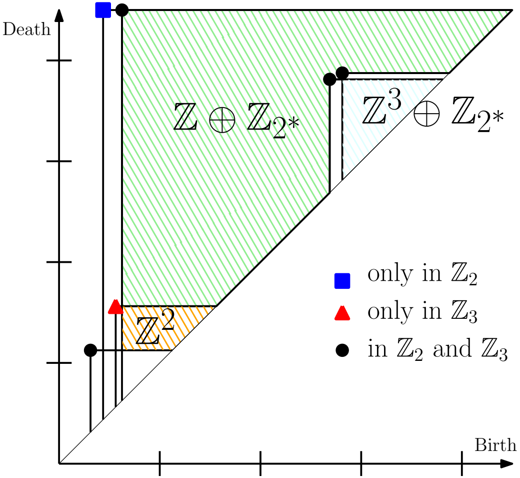
With q_r "big enough", we partially reverse the computation:

$$t(p, q_s) = \beta_p(\mathbb{Z}_{q_s}) - \beta_p(\mathbb{Z}_{q_r}) - t(p-1, q_s)$$

Homology Group Reconstruction



$$\begin{aligned} \mathbf{H}_0(\mathbb{Z}) &= \mathbb{Z} \\ \mathbf{H}_1(\mathbb{Z}) &= \mathbb{Z} \oplus \mathbb{Z}_2 \\ \mathbf{H}_2(\mathbb{Z}) &= 0 \end{aligned}$$



Multi-Field Persistence Diagram

We compute the **Multi-Field Persistence Diagram** for the fields: $\{\mathbb{Z}_{q_1}, \cdots \mathbb{Z}_{q_r}\}$ for a family of distinct primes $q_1, \cdots, q_r$,

with q_r **strict upper bound** on the *primary divisors of torsion coefficients*.

$$\mathbf{H}_p(\mathbb{Z}) \cong \mathbb{Z}^{\beta_p(\mathbb{Z})} \bigoplus_{q \text{ prime}} \left(\mathbb{Z}_{q^{k_1}} \oplus \cdots \oplus \mathbb{Z}_{q^{k_{t(p,q)}}} \right)$$

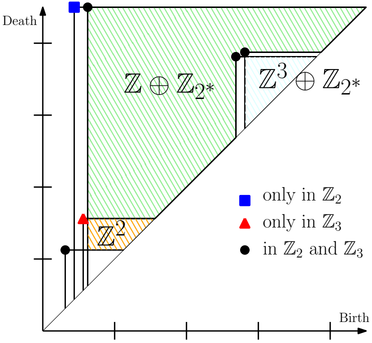
Let:

- $\mathbf{K}$ be a filtered simplicial complex with m simplices
- $|\mathrm{D}(\mathbf{K}, \mathbb{F})| = \Theta(m)$ be the number of points in the persistence diagram for any $\mathbb{F}$ (field) coefficients
- $|\mathrm{D}(\mathbf{K}, \mathbb{Z}_{q_1} \cdots \mathbb{Z}_{q_r})|$ be the number of distinct points in the **superimposition** of diagrams $\mathrm{D}(\mathbf{K}, \mathbb{Z}_{q_1}), \cdots \mathrm{D}(\mathbf{K}, \mathbb{Z}_{q_r})$

Multi-Field Persistence Diagram

Usually:

- $q_1, \cdots, q_r$ are the first r prime numbers, and $r \leq 100$
- m is huge!
- $m \simeq |\mathrm{D}(\mathbf{K}, \mathbb{F})| \simeq$ $|\mathrm{D}(\mathbf{K}, \mathbb{Z}_{q_1} \cdots \mathbb{Z}_{q_r})| \ll r \times m$



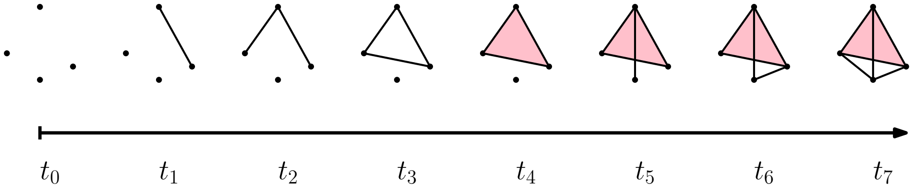
We design algorithms such that:

$$O(f(|\mathrm{D}(\mathbf{K}, \mathbb{F})|)) \quad \text{becomes} \quad O(f(|\mathrm{D}(\mathbf{K}, \mathbb{Z}_{q_1} \cdots \mathbb{Z}_{q_r})|) \times \mathrm{A})$$

for some small A.

3
Modular Reconstruction for Gaussian Elimination

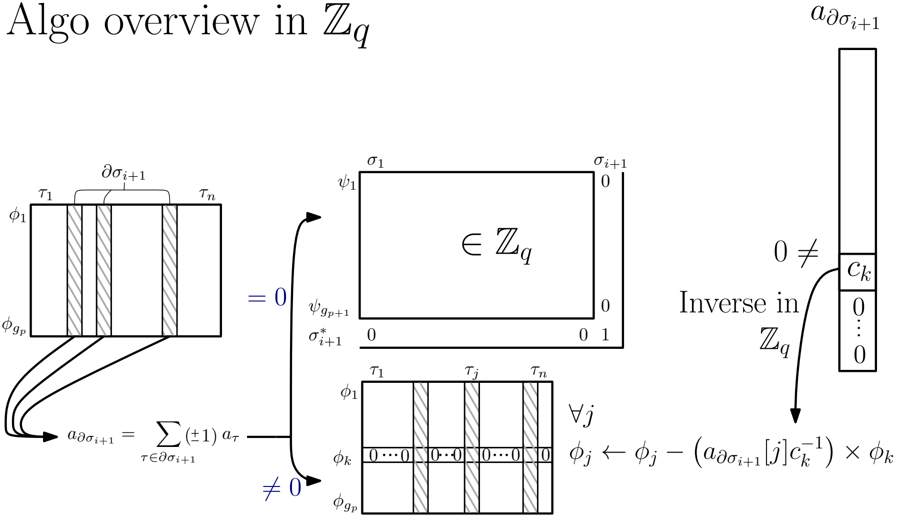
Remember the Persistent Cohomology Algorithm?



$$\mathcal{K}_0 \subseteq \mathcal{K}_1 \subseteq \mathcal{K}_2 \subseteq \mathcal{K}_3 \subseteq \mathcal{K}_4 \subseteq \mathcal{K}_5 \subseteq \mathcal{K}_6 \subseteq \mathcal{K}_7$$

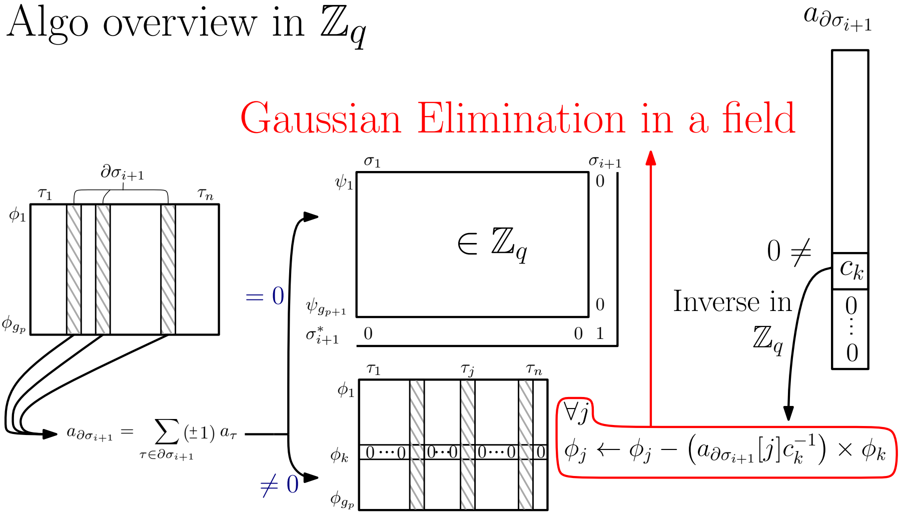
- Insert the simplices in the order of the filtration
- Update the cohomology groups accordingly

Algo overview in $\mathbb{Z}_q$



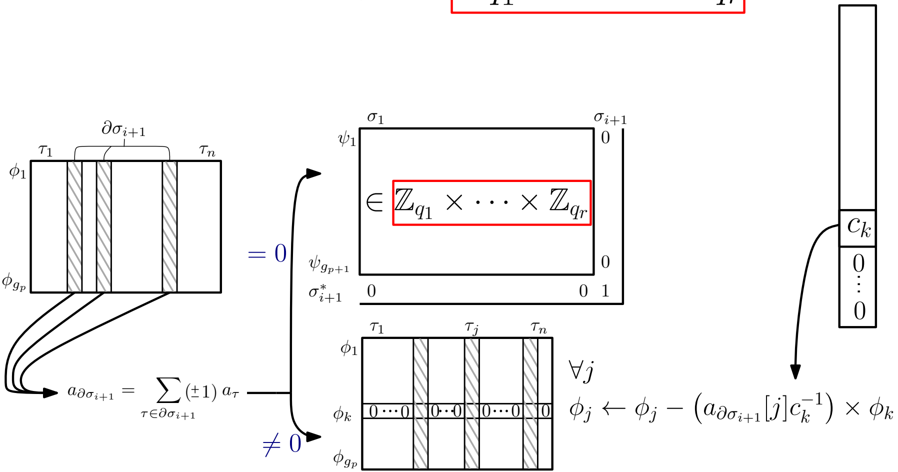
Multi-Field Persistent Cohomology

Algo overview in $\mathbb{Z}_q$



Multi-Field Persistent Cohomology

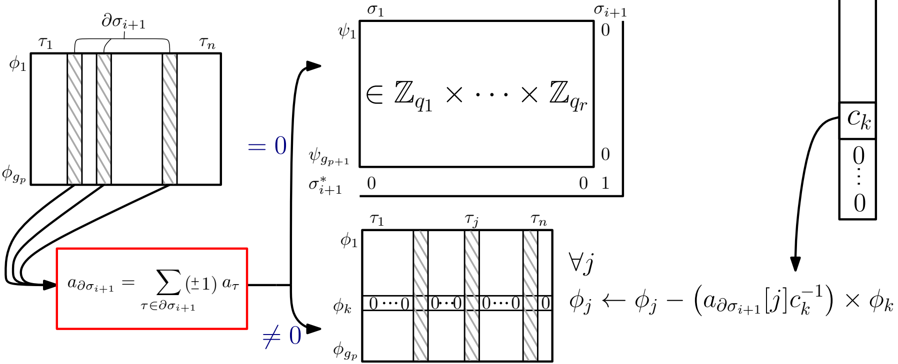
Multi-Field? $\leftarrow$ Algo in $\mathbb{Z}_{q_1} \times \cdots \times \mathbb{Z}_{q_r}$



Multi-Field Persistent Cohomology

Multi-Field? $\leftarrow$ Algo in $\mathbb{Z}_{q_1} \times \cdots \times \mathbb{Z}_{q_r}$

$$(u_1, \cdots, u_r) \times (v_1, \cdots, v_r) + (w_1, \cdots, w_r)$$
$$= \ (u_1 \times v_1 + w_1, \cdots, u_r \times v_r + w_r)$$



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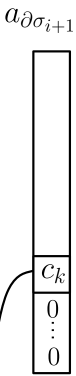

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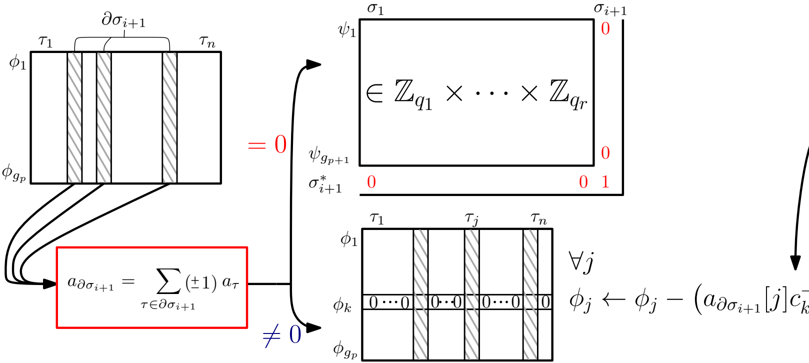

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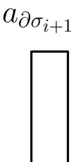
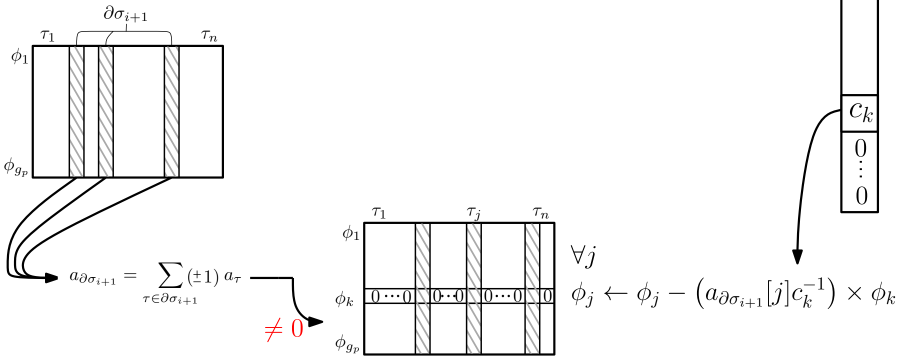
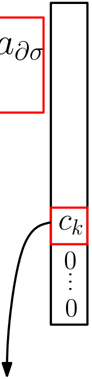


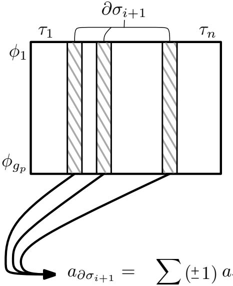


Multi-Field Persistent Cohomology

Multi-Field? $\leftarrow$ Algo in $\mathbb{Z}_{q_1} \times \cdots \times \mathbb{Z}_{q_r}$

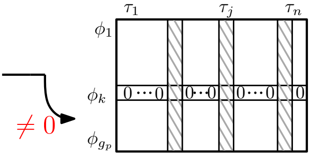
$c_k = (u_1, \cdots, u_r)$ with u_s lowest $\neq 0$ of $a_{\partial\sigma}$ in $\mathbb{Z}_{q_s}$ for $s \in S \subseteq [r]$





$$a_{\partial\sigma_{i+1}} = \sum_{\tau\in\partial\sigma_{i+1}} (\pm 1)\, a_\tau$$

$\neq 0$



$\forall j$

$$\phi_j \leftarrow \phi_j - \left(a_{\partial\sigma_{i+1}}[j]\, c_k^{-1}\right) \times \phi_k$$

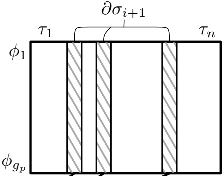
Multi-Field Persistent Cohomology

Multi-Field? $\leftarrow$ Algo in $\mathbb{Z}_{q_1} \times \cdots \times \mathbb{Z}_{q_r}$

$c_k = (u_1, \cdots, u_r)$ with u_s lowest $\neq 0$ of $a_{\partial\sigma}$ in $\mathbb{Z}_{q_s}$ for $s \in S \subseteq [r]$

$(\overline{u_1}^S, \cdots, \overline{u_r}^S) = c_k^{-1}$ partial inverse w.r.t. S

$$\overline{u_s}^S = \begin{cases} u_s^{-1} & \text{if } s \in S \\ 0 & \text{o.w.} \end{cases}$$



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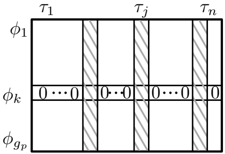

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$\mathbb{Z}_{q_1} \times \cdots \times \mathbb{Z}_{q_r} \cong \mathbb{Z}_{q_1 \times \cdots \times q_r}$

Theorem (Chinese Remainder Theorem)

For a family $q_1, \cdots, q_r$ of r distinct prime numbers, there is a ring isomorphism

$$\begin{array}{llll} \psi : & \mathbb{Z}_{q_1} \times \cdots \times \mathbb{Z}_{q_r} & \rightarrow & \mathbb{Z}_{q_1 \times \cdots \times q_r} \\ \psi^{\times} : & \mathbb{Z}_{q_1}^{\times} \times \cdots \times \mathbb{Z}_{q_r}^{\times} & \rightarrow & \mathbb{Z}_{q_1 \times \cdots \times q_r}^{\times} \end{array}$$

s.t. the restriction is a group isomorphism.

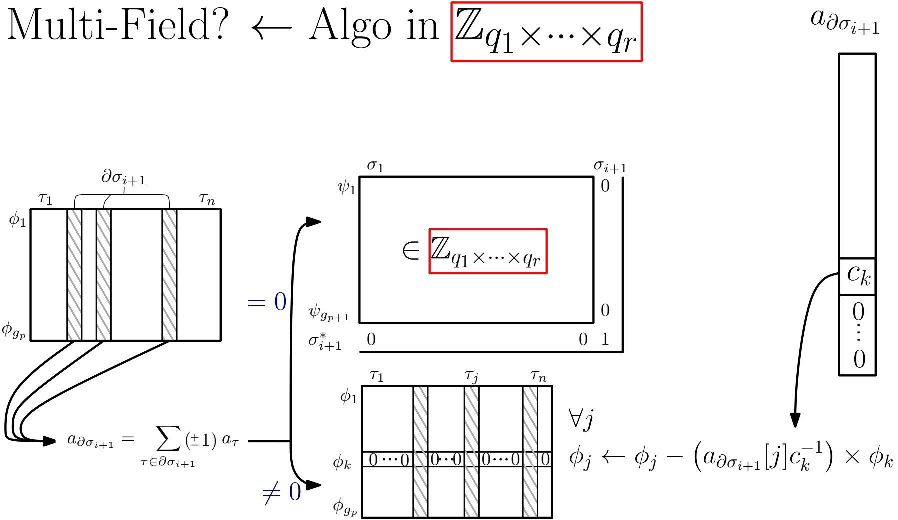
for

- $\mathbb{Z}_{q_1 \times \cdots \times q_r}$ *with pointwise addition/multiplication*
- $\mathcal{R}^{\times}$ *the multiplicative group of invertible elements of ring* $\mathcal{R}$

Moreover, ψ is easily constructible.

Multi-Field Persistent Cohomology

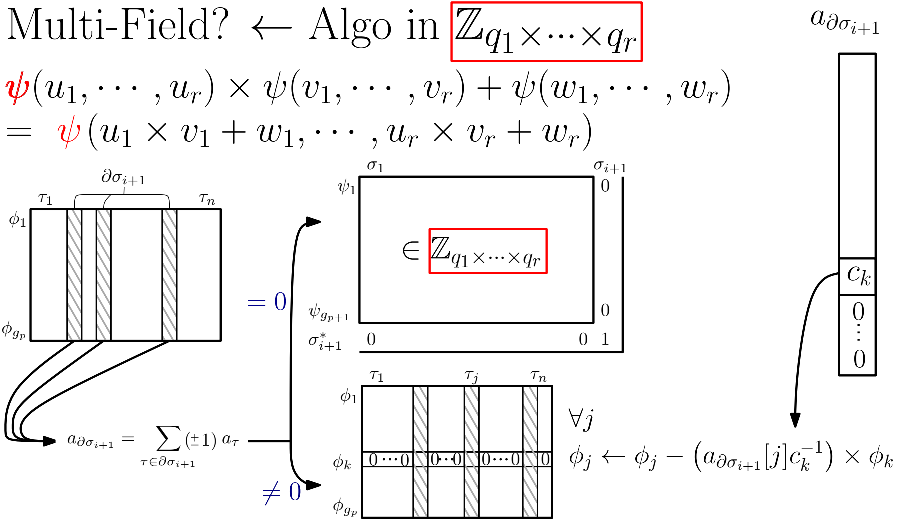
Multi-Field? ← Algo in $\mathbb{Z}_{q_1 \times \cdots \times q_r}$



Multi-Field Persistent Cohomology

$$\text{Multi-Field?} \leftarrow \text{Algo in } \boxed{\mathbb{Z}_{q_1 \times \cdots \times q_r}}$$

$$\psi(u_1, \cdots, u_r) \times \psi(v_1, \cdots, v_r) + \psi(w_1, \cdots, w_r)$$
$$= \psi(u_1 \times v_1 + w_1, \cdots, u_r \times v_r + w_r)$$



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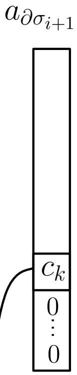

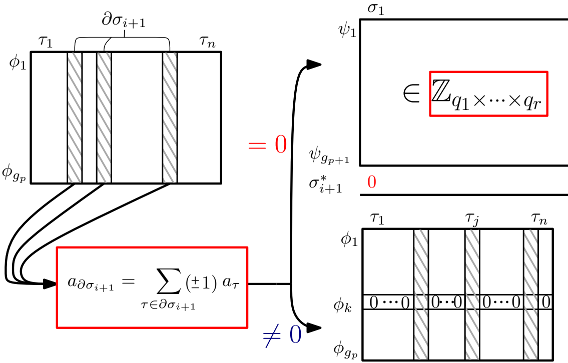

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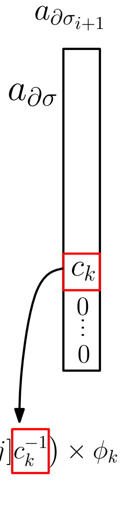

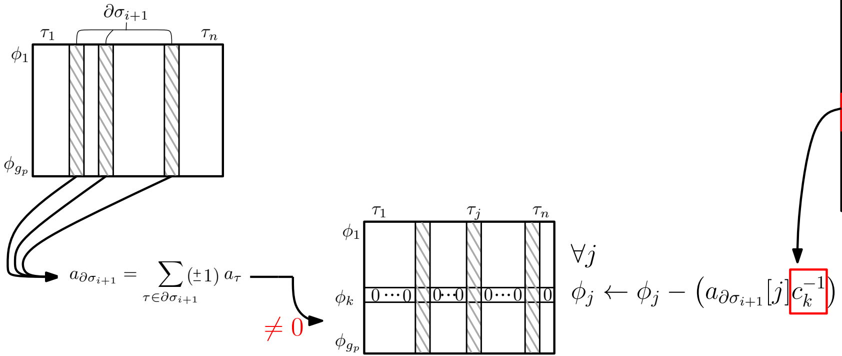

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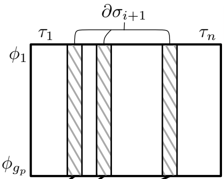

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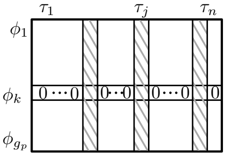

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Partial Inverse Construction

Define $Q_S = \sum_{s \in S} q_s$ for $S \subseteq [r]$. We prove that:

Data: x, Q_S
$Q_R \leftarrow \gcd(x, Q_S)$; **via the euclidean algorithm:** $O(\mathsf{A}_\div(Q))$;
$Q_T \leftarrow Q_S / Q_R$;
$v \leftarrow \textsc{Extended-Euclidean-Algorithm}(x, Q_T)$; **such that**; $vx + wQ_T = 1$;
$v \leftarrow v \bmod Q_T$;
$L_T \leftarrow D(Q_T)$; **some preprocessed constant**;
$\overline{x}^S \leftarrow (v \times L_T) \bmod Q$;
return $\overline{x}^S$;

computes the partial inverse of x w.r.t. S.

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computes the partial inverse of x w.r.t. S. Cost: $O(\mathrm{A})$ in $\mathbb{Z}_{q_1 \cdots q_r}$

3
Complexity Analysis and Experiments

Arithmetic Complexity

- For an integer z, let $\lambda(z) = \lfloor \log_2 z/\mathrm{w} \rfloor + 1$ the number of w-bits memory words to store z.
- Let $Q = q_1 \times \cdots \times q_r$ be the product of the first r primes
- For $\mathrm{B} = \lambda(z)$, we have:
  - **Addition** $\mathrm{A}_+(z) = O(\mathrm{B})$
  - **Multiplication** $\mathrm{A}_\times(z) = O(M(\mathrm{B}))$
  - **Division** $\mathrm{A}_\div(z) = O(M(\mathrm{B}) \log \mathrm{B})$

  with $M(\mathrm{B}) = O(\mathrm{B} \log \mathrm{B}\ 2^{O(\log^* \mathrm{B})})$

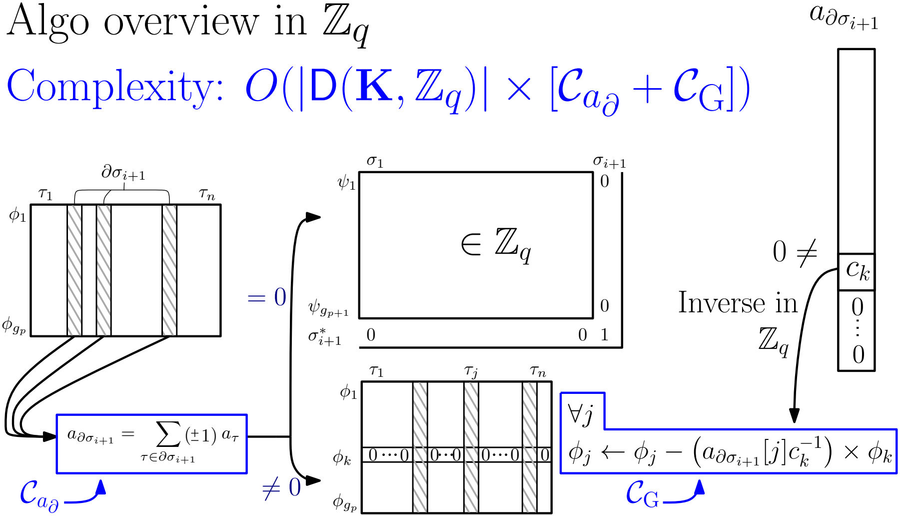
Moreover:

$$\lambda(Q) < \left\lfloor \frac{1.46613 r \ln(r \ln r)}{\mathrm{w}} \right\rfloor + 1$$

Complexity Analysis

Algo overview in $\mathbb{Z}_q$

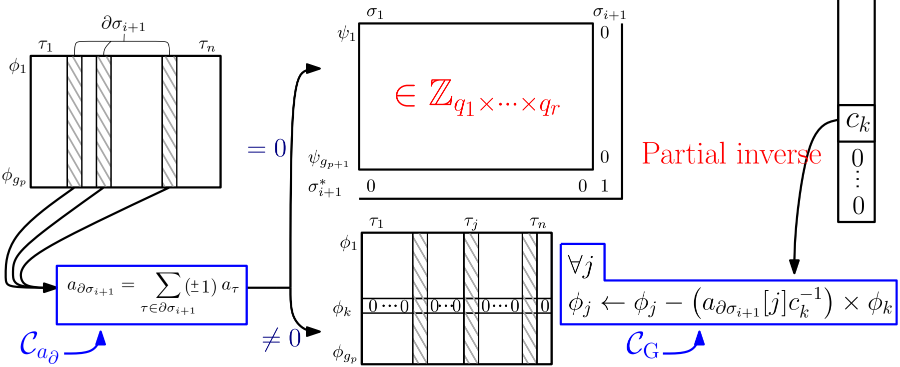
Complexity: $O(|\mathsf{D}(\mathbf{K}, \mathbb{Z}_q)| \times [\mathcal{C}_{a_\partial} + \mathcal{C}_{\mathrm{G}}])$



Complexity Analysis

Algo overview in $\mathbb{Z}_{q_1 \times \cdots \times q_r}$

$$O(|\mathsf{D}(\mathbf{K}, \mathbb{Z}_{q_1} \cdots \mathbb{Z}_{q_r})| \times [\mathcal{C}_{a_\partial} + \mathcal{C}_{\mathrm{G}}] \times \mathsf{A})$$



Experiments

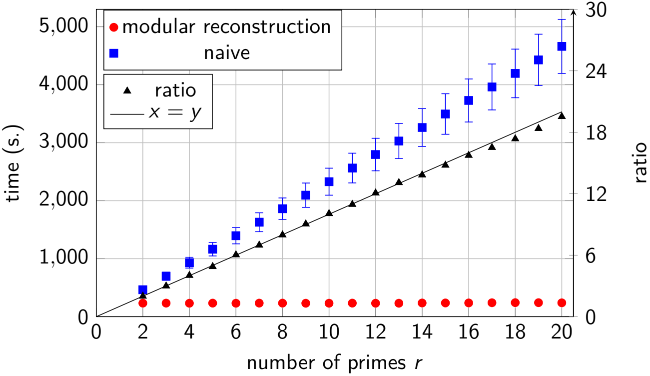


Figure: Timings for the modular reconstruction algo vs naive.

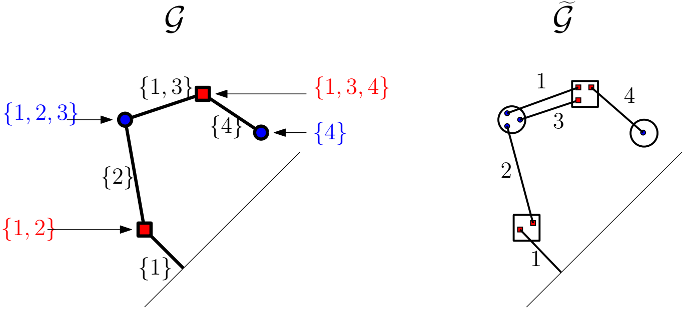
$$O(|\mathrm{D}(\mathbf{K}, \mathbb{Z}_{q_1} \cdots \mathbb{Z}_{q_r})| \times [\mathcal{C}_{\mathsf{a}_\partial} + \mathcal{C}_{\mathsf{G}}] \times \mathsf{A}) \quad \text{vs} \quad O(r \times |\mathrm{D}(\mathbf{K}, \mathbb{Z}_q)| \times [\mathcal{C}_{\mathsf{a}_\partial} + \mathcal{C}_{\mathsf{G}}])$$

Conclusion

Why Multi-Field Persistence?

Not for today but: we also have

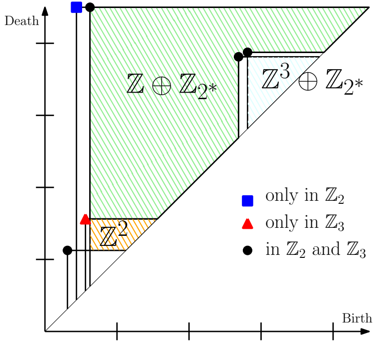
- **Multi-Field Bottleneck Distance** between diagrams
- Generalized algorithm for maximal point set matching
- Efficient algorithm in $O(m'^{3/2} \log m' \sqrt{t}A)$ (instead of $O(m^{3/2} \log m)$)



Why Multi-Field Persistence?

The Multi-Field Persistence Diagram

- is **more accurate**: characterizes torsion
- admits a **fast construction algorithm**
- admits a **generalized bottleneck distance** with a fast algorithm



Code available soon.

Thank you!

Question?