Applied Computational Group Theory?

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Are $\pi_1 X$ and $\pi_2 X$ practical tools for computational topology?

Part I: The Fundamental Group
(with P. Dlotko, M. Mrozek)

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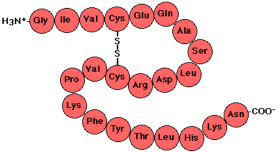
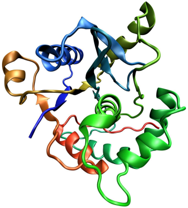
Every protein has a representation as an amino acid chain.

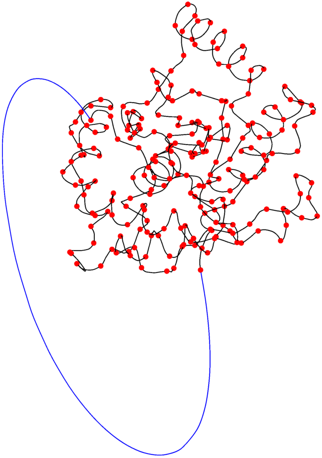


Anfinsen's Dogma

This representation determines the 3-D structure of the protein.

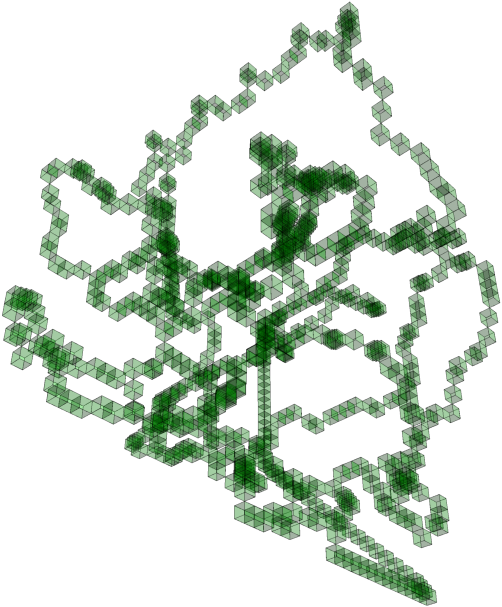


Protein Data Base: image of *H. Sapiens 1xd3* data



Protein ends joined to form an embedding $K\colon S^1 \longrightarrow \mathbb{R}^3$.

Pure cubical complex representation of *H. Sapiens 1xd3*



GAP system for computatiponal algebra

$$G := \pi_1(\mathbb{R}^3 \setminus K) \cong \langle x, y \mid y^{-1}x^{-1}yxyx^{-1}y^{-3}x^{-1}yxyx^{-1}y^{-1}x \rangle$$

```
gap> K:=ReadPDBfileAsPureCubicalComplex("1XD3.pdb");;

gap> G:=KnotGroup(K);;
#I there are 2 generators and 1 relator of length 14

gap> RelatorsOfFpGroup(G);
[ f2^-1*f1^-1*f2*f1*f2*f1^-1*f2^-3*f1^-1*f2*f1*f2*
  f1^-1*f2^-1*f1 ]
```

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EXAMPLE

For $N \lhd G$, $G/N \cong C_5$ and $Q = N/[[N,N],N]$ we could compute

$$H_3(BQ, \mathbb{Z}) = (\mathbb{Z}_3)^6 \oplus \mathbb{Z}_{192}$$

```
gap> N:=LowIndexSubgroupsFpGroup(G,5)[4];;

gap> Q:=NilpotentQuotient(N,2);;

gap> GroupHomology(Q,3);
[ 3, 3, 3, 3, 3, 3, 192 ]
```

$$Inv(K) = \{\ H_1(N, \mathbb{Z})\ :\ N \leq G := \pi_1(\mathbb{R}^3 \setminus K),\ |G : N| \leq 5\ \}$$

distinguishes between all prime knots with ≤ 10 crossings.

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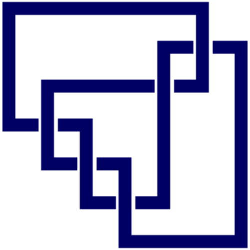
This invariant shows that the *H. Sapiens 1xd3* knot is



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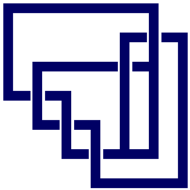
K'= 

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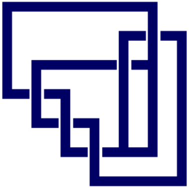
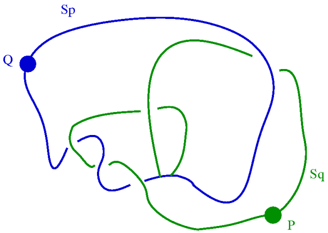
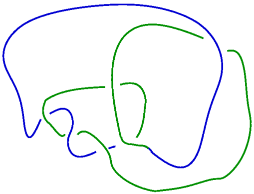
K'=  

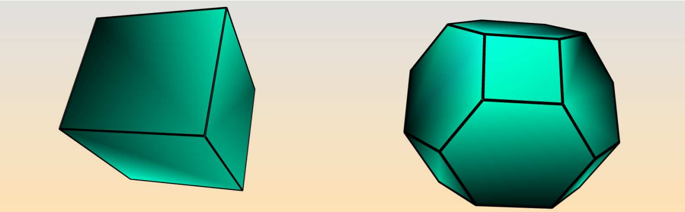
A few extra thickenings contribute no further isotopy changes. So perhaps the 1XD3 knot is actually a trefoil.

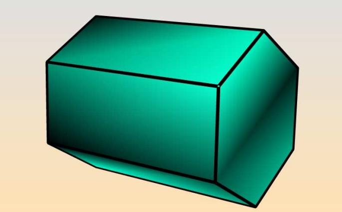


A representation of proteins (and other Euclidean data)

Choose a lattice $L \subseteq \mathbb{R}^n$ and determine

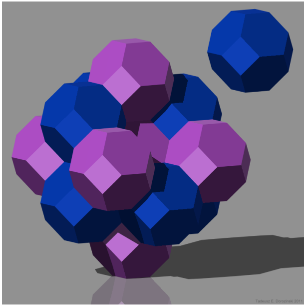
$$D_L = \{x \in \mathbb{R}^n \ : \ ||x|| \leq ||x - v|| \ \forall v \in L\} \ .$$





Any finite set $\Lambda \subset L$ determines an *L-complex*

$$X = \bigcup_{\lambda \in \Lambda} D_L + \lambda$$



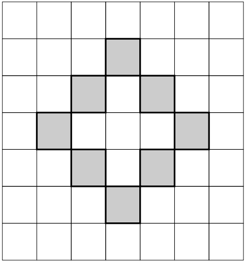
which we represent as a binary array

$$(a_\lambda)_{\lambda \in \Lambda}$$

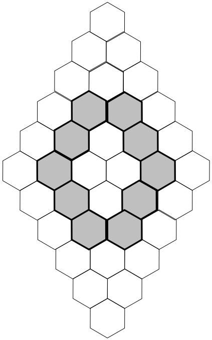
$a_\lambda = 1$ if $\lambda \in \Lambda$, $a_\lambda = 0$ otherwise.

One advantage to permutahedral complexes

They are always topological manifolds, and so their complements behaves nicely.



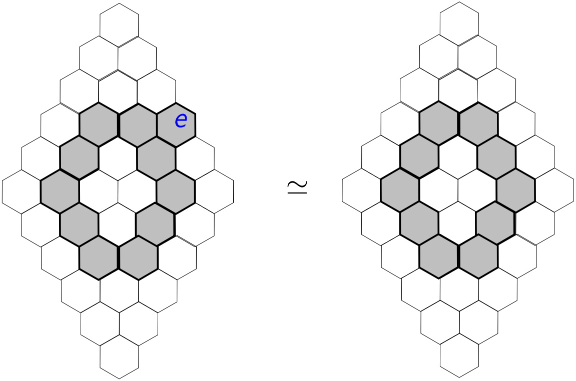
a



b

Second advantage to permutahedral complexes

Permutahedron has at most $2^{n+1}-2$ neighbours (compared to $3^n - 1$ for the cube) so for $n \leq 4$ we cheaply compute retracts



because $e \in S$ with $|S| < 2^{2^{n+1}-2}$.

A zig-zag homotopy retract

$$X \overset{\simeq}{\hookrightarrow} X_1 \overset{\simeq}{\hookleftarrow} X_2 \overset{\simeq}{\hookrightarrow} X_3 \cdots \overset{\simeq}{\hookleftarrow} Y$$

```
gap> K:=ReadPDBfileAsPureCubicalComplex("1XD3.pdb");;

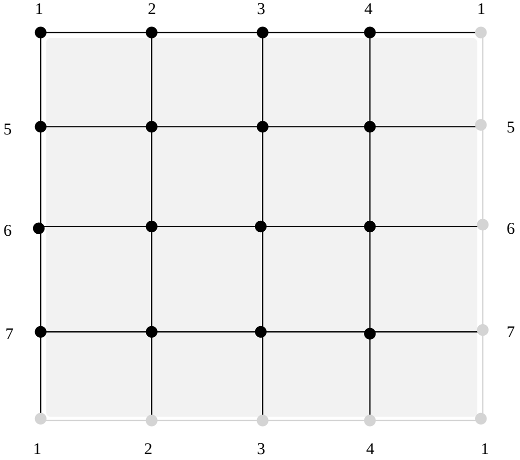
gap> X:=ComplementOfPureCubicalComplex(K);;

gap> Size(X);
14692851

gap> Y:=ZigZagContractedPureCubicalComplex(X);;

gap> Size(Y);
74649
```

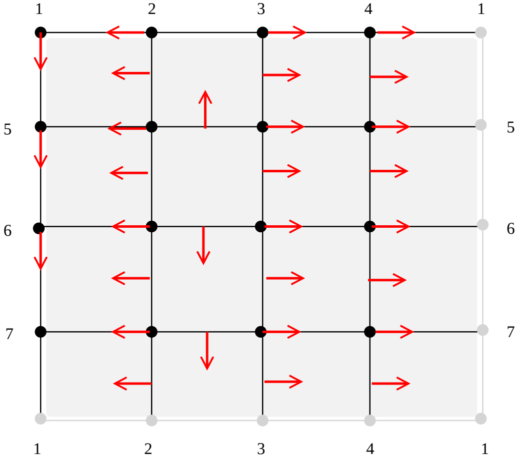
Computing fundamental groups of finite regular CW-spaces



Torus:
16 vertices
32 edges
16 faces

A discrete vector field on a regular CW-space X is a collection of arrows $s \to t$ where

> s, t are cells and any cell is involved in at most one arrow
>
> $\dim(t) = \dim(s) + 1$ and s lies in the boundary of t



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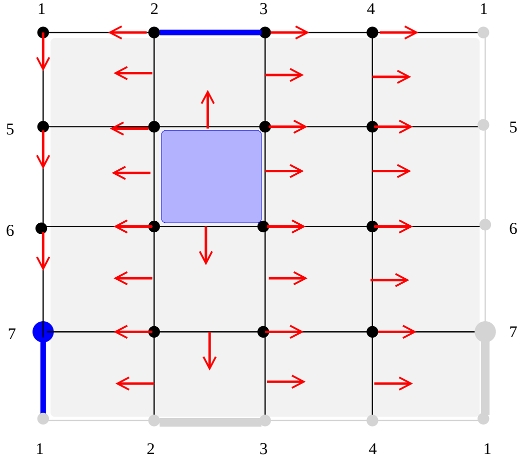

Torus:
1 critical vertex
2 critical edges
1 critical face

The critical cells are those not involved in arrows.

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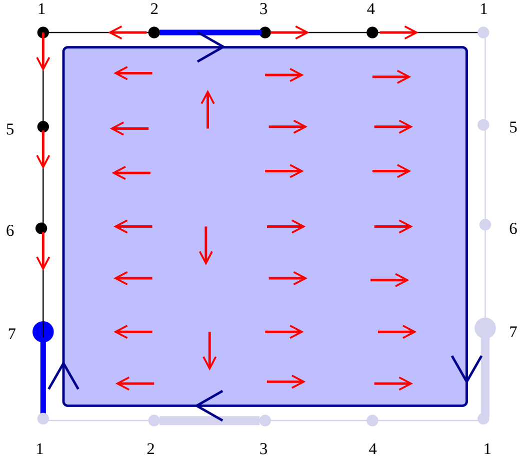

$\pi_1(\text{Torus}) =$

$\langle x, y \mid xyx^{-1}y^{-1} \rangle$

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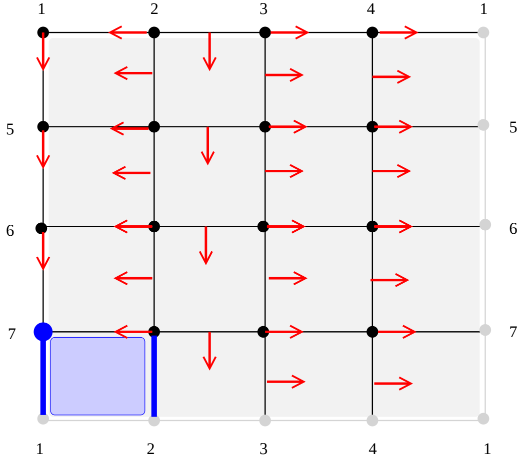
Algorithm produces a presentation for the fundamental group of a regular CW-space with admissible discrete vector field.



Torus:
1 critical vertex
2 critical edges
1 critical face
non-admissible vector field

Computing low-index groups of a finitely presented group G

Index n subgroup $H \leq G$ corresponds to a homomorphism

$$G \to S_n$$

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Index n subgroups $H \leq G$ are finitely presented (Reidemeister-Schreier).

Multiplication in a nilpotent group G

Use power-commutator presentations

$$\langle x, y, z \mid x^2 = 1, y^2 = z, z^2 = 1, x^{-1}yxy^{-1} = z\rangle$$

and GAP or Magma's fast rewrite rules for such presentations.

Computing homology $H_n(BG,\mathbb{Z})$ of a nilpotent group G

Implement theoretical descriptions of BG for abelian G.

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For G of class 2

$$[G, G] \to G \to G/[G, G]$$

construct BG from spaces $B([G, G])$ and $B(G/[G, G])$ by homological perturbation techniques involving contracting discrete vector fields on universal covers.

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For G of nilpotency class c use recursion on

$$\gamma_c G \to G \to G/\gamma_c G \ .$$

An application

$$H_4(B\mathbb{M}_{24}, \mathbb{Z}) = 0$$

```
gap> GroupHomology(MathieuGroup(24),4);
[ ]
```

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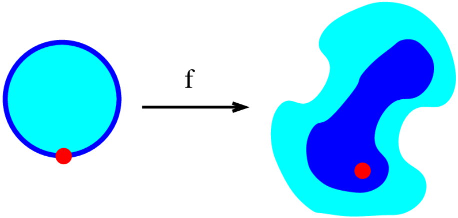
$$H^3(B\mathbb{M}_{24}, \mathbb{U}(1)) = \mathbb{Z}_{12}$$

Part II: The Second Homotopy Group
(joint work with Le Van Luyen)

For spaces $Y \subset X$ and $D^2 = \{x \in \mathbb{R}^2 : ||x|| \leq 1\}$ define

$$\pi_2(X, Y) = \{f : D^2 \to X \ : \ f(S^1) \subset Y\}/homotopy$$



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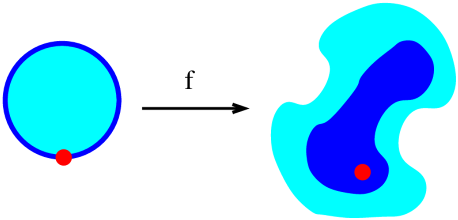
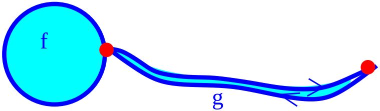


There is a “restriction” homomorphism

$$\partial\colon \pi_2(X, Y) \to \pi_1(Y)$$

and $g \in \pi_1(Y)$ acts canonically on $f \in \pi_2(X, Y)$.



Theorem (JHC Whitehead): There is an exact sequence of groups

$$\pi_2(Y) \to \pi_2(X) \to \pi_2(X,Y) \xrightarrow{\partial} \pi_1(Y) \to \pi_1(X)$$

in which ∂ is a *crossed module*:

A crossed module is a group homomorphism $\partial\colon M \to G$ with action $(g,m) \mapsto^{g} m$ statisfying

- $\partial({}^{g}m) = g\,\partial(m)\,g^{-1}$
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We define

$$\pi_1(\partial) = G/\mathrm{image}\,\partial \qquad \pi_2(\partial) = \ker\partial\ .$$

Taking $Y = X^1$ we get Whitehead's functor

$$Ho(\text{regular CW} - \text{spaces}) \longrightarrow \Sigma^{-1}(\text{crossed modules})$$

which is faithful on homotopy types X with $\pi_n X = 0$ for $n \neq 1, 2$.

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Let

$$B(M \xrightarrow{\partial} G)$$

denote a CW-space with $\pi_n X = 0$ for $n \neq 1, 2$ that maps to ∂.

Two algebraic examples of crossed modules

$$\partial\colon M \to Aut(M), m \mapsto \{x \mapsto mxm^{-1}\}$$

for any group M. $\pi_1(\partial) = Out(M)$, $\pi_2(\partial) = Z(M)$.

$$\partial\colon M \hookrightarrow G$$

for any normal subgroup $M \leq G$. $\pi_1(\partial) = G/M$, $\pi_2(\partial) = 0$.

Computing $H_n(\ B(M \xrightarrow{\partial} G)\ ,\ \mathbb{Z})$ in GAP

$$H_5(\ B(D_{32} \to Aut(D_{32}))\ ,\ \mathbb{Z}) \cong (\mathbb{Z}_2)^5 \oplus \mathbb{Z}_8$$

```
gap> M:=DihedralGroup(64);;
gap> C:=AutomorphismGroupAsCatOneGroup(M);;
gap> Size(C); #Size(M) * Size(Aut(M))
32768

gap> Homology(C,5);
[ 2, 2, 2, 2, 2, 8 ]
gap>
```

A morphism of crossed modules is a commutative diagram

$$\begin{tikzcd} M \arrow[r, "\phi_2"] \arrow[d, "\partial"] & M' \arrow[d, "\partial'"] \\ G \arrow[r, "\phi_1"] & G' \end{tikzcd}$$

with ϕ_1, ϕ_2 group homomorphisms satisfying

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Two crossed modules ∂, ∂'' are quasi-isomorphic if there exists a sequence of quasi-isomorphisms:

$$\partial \to \partial_1 \leftarrow \partial_2 \to \cdots \leftarrow \partial_k \to \partial''$$

Application of homology computation

There are 49487365422 different groups (i.e. homotopy 1-types) of order 1024.

Question: Define the order of $\partial\colon M \to G$ to be $|M||G|$. How many quasi-isomorphism types of crossed module of order 16 are there?

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$$\pi_1(\partial),\ \pi_2(\partial),\ H_2(\partial,\mathbb{Z}),\ H_3(\partial,\mathbb{Z})$$

establish at least 49 quasi-isomorphism types of crossed modules of order 16.

Computing the homology of $M \xrightarrow{\partial} G$

1. The cellular chain complex $C_*(B(\partial))$ has an algebraic description using the language of simplicial sets.

2. By the Homological Perturbation Lemma and discrete vector fields we need only compute a much smaller homotopic chain complex $C_* \simeq C_*(B(\partial))$.

3. Coreduction can be applied to obtain an even smaller chain complex $D_* \simeq C_*$.

The crossed module

$$\partial \colon \mathbb{Z}_2 \to 0$$

yields a homotopy 2-type $B = B(\partial)$ with

$$\pi_2(B) = \mathbb{Z}_2, \quad \pi_k(B) = 0 \text{ for } k \neq 2.$$

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```
gap> B:=EilenbergMacLaneComplex(CyclicGroup(2),2,11);;
gap> C:=ChainComplex(B);;
gap> List([0..11],CK!.dimension);
[ 1, 1, 2, 4, 8, 16, 32, 64, 128, 256, 512, 1024 ]
```

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gap> List([0..11],CK!.dimension);
[ 1, 1, 2, 4, 8, 16, 32, 64, 128, 256, 512, 1024 ]
```

```
gap> D:=CoreducedChainComplex(C);;
gap> List([0..10],D!.dimension);
[ 1, 0, 1, 1, 2, 3, 5, 8, 13, 21, 34 ]
```

$$\mathcal{N} : \text{(crossed modules)} \longrightarrow \text{(simplicial groups)}$$

Given $\partial\colon M \to G$ we consider the category

$$\begin{array}{ll} A = M \ltimes G & \\ s\colon A \to A, & (m,g) \mapsto (1,g) \\ t\colon A \to A, & (m,g) \mapsto (1,\partial(m)\,g) \\ \circ\colon A \times_G A \to A, & ((m,g),(m',g') \mapsto (m,(\partial m)^{-1}g') \end{array}$$

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\end{array}
$$

s, t, $\circ$ are group homomorphisms and A is a category internal to the category of groups.

The nerve $\mathcal{N}(A)$ is thus a simplicial group.

$$\begin{tikzcd} B\colon \text{(crossed modules)} \arrow[r, "\mathcal{N}"] & \text{(simplicial groups)} \arrow[d, "\mathcal{N}"] & \\ & \text{(bisimplicial sets)} \arrow[r, "\Delta"] & \text{(simplicial sets)} \end{tikzcd}$$

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\end{tikzcd}$$

$$F\colon (\text{sets}) \longrightarrow (\text{free abelian groups})$$

$C_*(B(\partial\colon M \to G))$ is the total complex of the bicomplex:

$$\begin{tikzcd}
& \arrow[d] & \arrow[d] & \arrow[d] \\
\arrow[r] & F\mathcal{N}_2\mathcal{N}_2(A) \arrow[r] \arrow[d] & F\mathcal{N}_2\mathcal{N}_1(A) \arrow[r] \arrow[d] & F\mathcal{N}_2\mathcal{N}_0(A) \arrow[d] \\
\arrow[r] & F\mathcal{N}_1\mathcal{N}_2(A) \arrow[r] \arrow[d] & F\mathcal{N}_1\mathcal{N}_1(A) \arrow[r] \arrow[d] & F\mathcal{N}_1\mathcal{N}_0(A) \arrow[d] \\
\arrow[r] & F\mathcal{N}_0\mathcal{N}_2(A) \arrow[r] & F\mathcal{N}_0\mathcal{N}_1(A) \arrow[r] & F\mathcal{N}_0\mathcal{N}_0(A)
\end{tikzcd}$$

The jth column $F\mathcal{N}_*(\mathcal{N}_j(A))$ is the bar complex for the group $\mathcal{N}_j(A)$.

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We could replace each column by

$$R_*^{\mathcal{N}_j(A)} \otimes_{\mathbb{Z}\mathcal{N}_j(A)} \mathbb{Z}$$

where $R_*^{\mathcal{N}_j(A)}$ is an arbitrary free $\mathbb{Z}\mathcal{N}_j(A)$-resolution of $\mathbb{Z}$.

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Homological Perturbation Lemma solves this problem by providing a filtered complex

$$R_*^{\mathcal{N}_*(A)} \otimes_{\mathbb{Z}\mathcal{N}_*(A)} \mathbb{Z}$$

A homotopy equivalence data

$$(L, d) \underset{\xrightarrow{i}}{\xleftarrow{p}} (M, d),\ \ h \qquad (*)$$

consists of chain complexes L, M, quasi-isomorphisms i, p and a homotopy $ip - 1 = dh + hd$. A perturbation on $(*)$ is a homomorphism $\epsilon\colon M \to M$ of degree -1 such that $(d+\epsilon)^2 = 0$.

PERTURBATION LEMMA: If $A = (1 - \epsilon h)^{-1}\epsilon$ exists then

$$(L, d') \underset{\xrightarrow{i'}}{\xleftarrow{p'}} (M, d+\epsilon),\ \ h' \qquad (**)$$

is a homotopy equivalence data where

$$i' = i + hAi, \quad p' = p + pAh, \quad h' = h + hAh, \quad d' = d + pAi \quad .$$

M. Crainic, "On the perturbation lemma, and deformations", 2004

$$
\begin{tikzcd}
 & {} \arrow[d] & {} \arrow[d] & {} \arrow[d] & \\
{} \arrow[r, "0"] & F\mathcal{N}_2\mathcal{N}_2(A) \arrow[r, "0"] \arrow[d] & F\mathcal{N}_2\mathcal{N}_1(A) \arrow[r, "0"] \arrow[d] & F\mathcal{N}_2\mathcal{N}_0(A) \arrow[d] & \\
{} \arrow[r, "0"] & F\mathcal{N}_1\mathcal{N}_2(A) \arrow[r, "0"] \arrow[d] & F\mathcal{N}_1\mathcal{N}_1(A) \arrow[r, "0"] \arrow[d] & F\mathcal{N}_1\mathcal{N}_0(A) \arrow[d] & (M, d) \\
{} \arrow[r, "0"] & F\mathcal{N}_0\mathcal{N}_2(A) \arrow[r, "0"] & F\mathcal{N}_0\mathcal{N}_1(A) \arrow[r, "0"] & F\mathcal{N}_0\mathcal{N}_0(A) &
\end{tikzcd}
$$

$$
\begin{tikzcd}
 & {} \arrow[d] & {} \arrow[d] & {} \arrow[d] & \\
{} \arrow[r, "0"] & R_2^{\mathcal{N}_2(A)} \otimes \mathbb{Z} \arrow[r, "0"] \arrow[d] & R_2^{\mathcal{N}_1(A)} \otimes \mathbb{Z} \arrow[r, "0"] \arrow[d] & R_2^{\mathcal{N}_0(A)} \otimes \mathbb{Z} \arrow[d] & \\
{} \arrow[r, "0"] & R_1^{\mathcal{N}_2(A)} \otimes \mathbb{Z} \arrow[r, "0"] \arrow[d] & R_1^{\mathcal{N}_1(A)} \otimes \mathbb{Z} \arrow[r, "0"] \arrow[d] & R_1^{\mathcal{N}_0(A)} \otimes \mathbb{Z} \arrow[d] & (L, d) \\
{} \arrow[r, "0"] & R_0^{\mathcal{N}_2(A)} \otimes \mathbb{Z} \arrow[r, "0"] & R_0^{\mathcal{N}_1(A)} \otimes \mathbb{Z} \arrow[r, "0"] & R_0^{\mathcal{N}_0(A)} \otimes \mathbb{Z} &
\end{tikzcd}
$$

$$
\begin{tikzcd}
{} & {} \arrow[d] & {} \arrow[d] & {} \arrow[d] & \\
{} \arrow[r] & F\mathcal{N}_2\mathcal{N}_2(A) \arrow[r] \arrow[d] & F\mathcal{N}_2\mathcal{N}_1(A) \arrow[r] \arrow[d] & F\mathcal{N}_2\mathcal{N}_0(A) \arrow[d] & \\
{} \arrow[r] & F\mathcal{N}_1\mathcal{N}_2(A) \arrow[r] \arrow[d] & F\mathcal{N}_1\mathcal{N}_1(A) \arrow[r] \arrow[d] & F\mathcal{N}_1\mathcal{N}_0(A) \arrow[d] & (M, d+\epsilon) \\
{} \arrow[r] & F\mathcal{N}_0\mathcal{N}_2(A) \arrow[r] & F\mathcal{N}_0\mathcal{N}_1(A) \arrow[r] & F\mathcal{N}_0\mathcal{N}_0(A) &
\end{tikzcd}
$$

$$
\begin{tikzcd}
{} & {} \arrow[d] & {} \arrow[d] & {} \arrow[d] & \\
{} \arrow[r] \arrow[urr] & R_2^{\mathcal{N}_2(A)} \otimes \mathbb{Z} \arrow[r] \arrow[d] \arrow[urr] & R_2^{\mathcal{N}_1(A)} \otimes \mathbb{Z} \arrow[r] \arrow[d] & R_2^{\mathcal{N}_0(A)} \otimes \mathbb{Z} \arrow[d] & \\
{} \arrow[r] \arrow[urr] & R_1^{\mathcal{N}_2(A)} \otimes \mathbb{Z} \arrow[r] \arrow[d] \arrow[urr] & R_1^{\mathcal{N}_1(A)} \otimes \mathbb{Z} \arrow[r] \arrow[d] & R_1^{\mathcal{N}_0(A)} \otimes \mathbb{Z} \arrow[d] & (L, d') \\
{} \arrow[r] \arrow[urr] & R_0^{\mathcal{N}_2(A)} \otimes \mathbb{Z} \arrow[r] \arrow[urr] & R_0^{\mathcal{N}_1(A)} \otimes \mathbb{Z} \arrow[r] & R_0^{\mathcal{N}_0(A)} \otimes \mathbb{Z} &
\end{tikzcd}
$$

Persistent homology of crossed modules

$B = B(\partial\colon M \to G)$
$\pi_i = \pi_i B$

$$\cdots \hookrightarrow [[\pi_2, \pi_1], \pi_1] \hookrightarrow [\pi_2, \pi_1] \hookrightarrow \pi_2$$

$$\to \cdots \pi_1/[[[\pi_1, \pi_1], \pi_1] \to \pi_1/[\pi_1, \pi_1]$$

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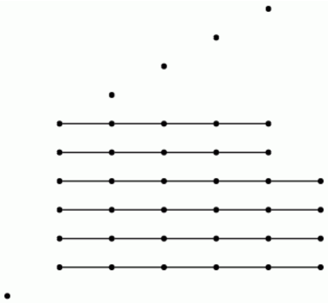
induce a sequence of homotopy 2-types

$$\to B_{-2} \to B_{-1} \to B \to B_1 \to B_2 \to \cdots$$

whose degree k homology is a homotopy invariant bar code for B.

$H_3(B_*, \mathbb{Z}_2)$ barcode for $B = B(C_{32} \to Aut(C_{32}))$



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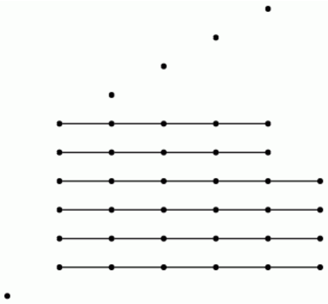

THANK YOU