# COMPUTING FUNDAMENTAL GROUP VIA FORMAN'S DISCRETE MORSE THEORY (EXTENDED ABSTRACT)

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Abstract. We present research in progress on the algorithmic computation of the fundamental group of a CW complex. We use the algorithm to compute certain algebraic invariants of the fundamental group of the complement of a knot. We show that the invariants classify the prime knots up to 13 crossings. The long term goal is an automated classification of knots in 3D images, in particular images of proteins.

## 1. Fundamental group of a CW complex

Let $K$ be an *oriented CW complex*, i.e. a CW complex with a fixed orientation for every its cell. Then, for a 2-cell $\sigma$ there is a closed path $\tau_1, \tau_2, \ldots, \tau_n$ of oriented 1-cells and a map $\theta : S^1 \to K^1$ in the homotopy class of $\varphi_{\sigma|S^1}$ such that $S^1 = \bigcup_{j=1}^{n} I_j$ and $\theta_{|I_j}$ is the characteristic map of the edge $\tau_j$. The path $\tau_1, \tau_2, \ldots, \tau_n$ is called the *homotopical boundary* of $\sigma$ and denoted $d(\sigma)$.

We propose an algorithm computing a presentation of the fundamental group of a CW complex based on the following theorem of Whitehead [6]

**Theorem 1.1.** *Assume $K$ is a connected CW complex with precisely one vertex. Then, the fundamental group of $K$ depends only on the 2-skeleton of $K$. Moreover, up to an isomorphism it is the group generated by the edges of $K$ with arbitrarily selected orientation of $K$ and homotopical boundaries of all 2 cells as relators.*

In order to reduce the computations for an arbitrary CW complex $K$ to the setting of the Whitehead Theorem, we apply the Discrete Morse Theory proposed by R. Forman [3]. More precisely, we use the algorithm presented in [4, 5] to construct a discrete vector field on $K$. Then, the fundamental theorem of Forman reduces the computations of a presentation of the fundamental group of $K$ to the setting of the Whitehead theorem. In order to further speed up the computations we

precede them by two special cases of the Forman theorem: reductions by shaving and the construction of a collapsible subset. The intermediate results are stored in a special data structure for CW complexes, called C-structure. The details will be presented in [1, 2]).

This leads to the following fundamental group presentation algorithm:

fundGroup(`collection of top dimensional cells of a CW complex` $K$)
$K :=$ shaving($K$);
$A :=$ collapsibleSubset($K$);
$C :=$ C-structure of $K/A$;
$V :=$ discreteVectorField($C$);
**for each** $\alpha \in V$ **do**
  assign to $C$ the $\alpha$-collapse of $C$;
**endfor**;
**return** $(C_1, d(C_2))$;

**Theorem 1.2.** *The algorithm always stops and returns a presentation, up to an isomorphism, of the fundamental group of $K$.*

An implementation of this algorithm will be available via the RedHoms software library [9].

## 2. Knot invariants

Let $G$ be a finitely generated group. Recall that for $g, h \in G$ the group element $[g, h] := ghg^{-1}h^{-1}$ is called the *commutator* of $g, h$. For any normal subgroup $H \subset G$ let

$$[H, G] := \langle [h, g] \mid h \in H, g \in G \rangle$$

and define the *lower central series* of $G$ recursively by given by $\gamma_1 G := G$, $\gamma_{n+1} G = [\gamma_n G, G]$.

Set

$$I^{[n,c,m]}(G) := \{\, H_m(S/\gamma_{c+1}S, \mathbb{Z}) \mid S \subset G,\ |G : S| \leq n \,\}$$

We prove the following theorem

**Theorem 2.1.** *For a prime knot $K\colon S^1 \to \mathbb{R}^3$ set $G(K) := \pi_1(\mathbb{R}^3 \setminus K(S^1))$ and define the knot invariant $I_n(K) := I^{[n,1,1]}(G(K))$. Then, $I_n(K)$ distinguishes between all prime knots (modulo mirror image) with $N$ or fewer crossings with $n$ given by the following table:*

| $N$ | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $i_N$ | 2 | 2 | 3 | 3 | 3 | 3 | 5 | 5 | 6 | **6** | **7** | **7-?** |

The proof is computer assisted, based on our fundamental group algorithm and computations of group invariants provided by the GAP [8] and HAP [7] packages. The complexity of computations depends obviously on $N$ and on the number of prime knots with up to $N$ crossings. For $N$ up to 11 the cost is small and the computations may be completed withim minutes using only one CPU core. For $N \geq 12$ the number of knots is huge and also the time needed to compute the relevant algebraic invariants grows rapidly. Therefore, we used a cluster of 352 CPU cores for $N \geq 12$. In the case of $N = 12$ and $N = 13$ we obtained the result using only a few hours of cluster time. For $N = 14$ we are done for all but one knot. In this case the computations for many knots take days of cluster time. Nevertheless, we have reasons to expect that we will manage to complete the computations for the remaining case.

Whatever is the outcome of these computations, we expect that the classification we have obtained so far will turn out very useful in the automated recognition of knots in 3D images of proteins.

## References


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