Enumeration of knot diagrams using constraint programming

Ciaran McCreesh, Alice Miller, Patrick Prosser, **Craig Reilly**, James Trimble

What is a knot?

- A *knot* is an embedding of the circle in $\mathbb{R}^3$.

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- A *knot* is an embedding of the circle in $\mathbb{R}^3$.
- An intuitive way to think about this is to consider a knot as a knotted piece of string with the ends glued together.

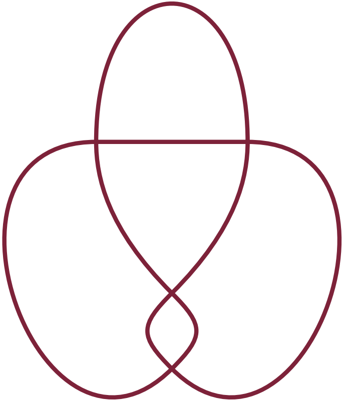
Drawing knots on paper

- A function $f : \mathbb{R}^3 \to \mathbb{R}^2$ where $f(x, y, z) = f(x, y)$, is called a *projection map*, and the image of a knot K under f is called the *projection* of K.
- Such a projection is often referred to as the *shadow* of K.

Drawing knots on paper

- Information regarding the orientation of arcs at crossings is given by leaving gaps in a knot's shadow.

Drawing knots on paper



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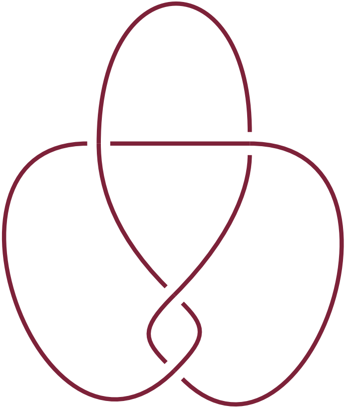
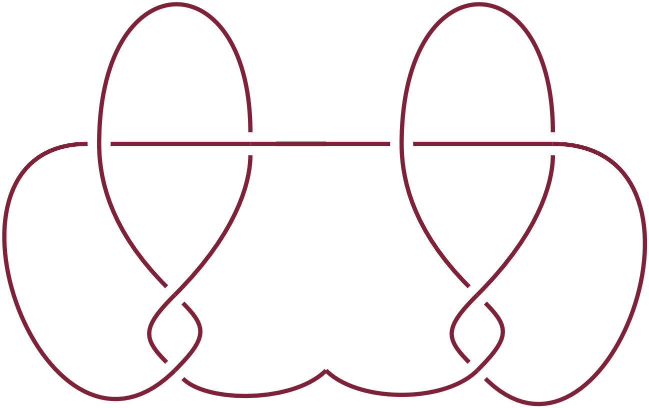


Prime knots

- *Prime knots* are knots which cannot be decomposed. For nontrivial knots this means that they cannot be written as the connect sum of two non-trivial knots.

Prime knots



Equivelent knots and Reidemeister Moves

- When enumerating prime knots it is convention to give each prime knot by a knot diagram which has as few as possible crossings.
- Two knots K and J are equivalent if K can be transformed into J by a series of elementary deformations.
- Showing that two knots are equivalent by elementary deformations is not practical.

Equivelent knots and Reidemeister Moves

- In the 1926 Reidermister proved that two knot diagrams k_0 and k_1 of the same knot K can be related by a sequence of the following three moves (called Reidermeister moves):[1]

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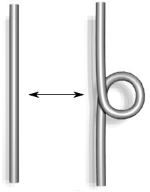

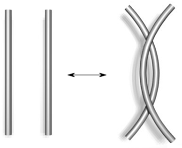

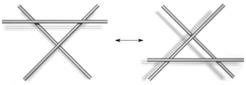

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Representations of knots

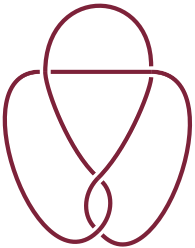
- Knot diagrams are really just 4-valent planar graphs.
  - The nodes in the graph correspond to the crossings in the knot diagram.
  - The edges between nodes correspond to arcs between crossings in the knot diagram.
  - The arcs are labelled with their orientation at their source and target crossings.
- Other structures familiar to computing scientists can be used, linked lists of crossings were popular in the 1950's.

Representations of knots

- The representations used by topologists are typically also used for representing knots in a computer.
- Examples are Dowker-Thistlethwait codes (DT codes), **Gauss codes**, braid representatives, Conway notation, and many more.

Representing knots with Gauss codes

- The strategy for representing a given knot (with n crossings) by a Gauss code is as follows.
  1. Label the crossings with the numbers 1 to n.
  2. Pick a point on the knot.
  3. Pick a direction and walk around the knot, writing out a list of the numbers you come to (with a negative sign indicating that a crossing was visited on an under strand). Stop when each number appears twice once with each sign.



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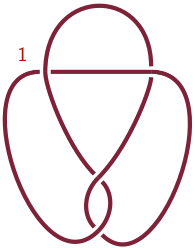

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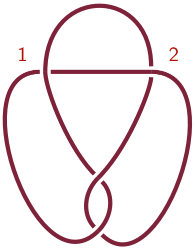

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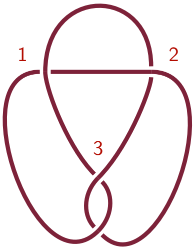

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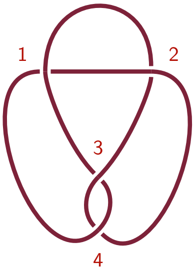

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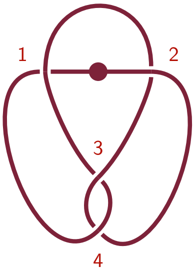

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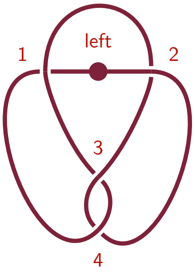

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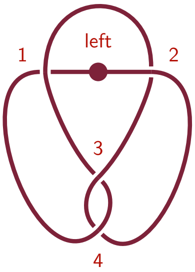
-1



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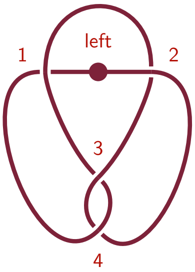
-1 , 4



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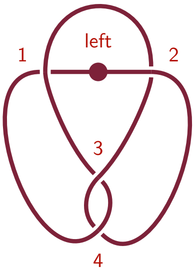

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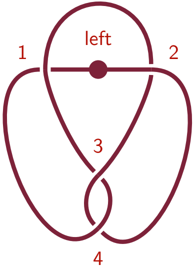
-1 , 4 , -3 , 1



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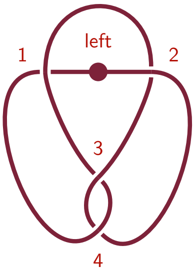
$-1\ ,\ 4\ ,\ -3\ ,\ 1\ ,\ -2$



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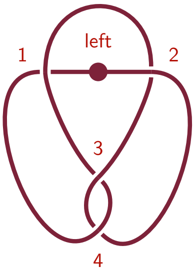

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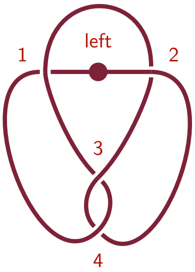

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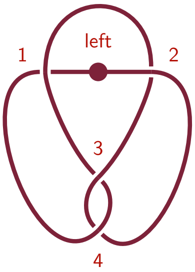
$-1 \; , 4 \; , -3 \; , 1 \; , -2 \; , 3 \; , -4 \; , 2$



Knot enumeration by Gauss codes

- There are three sensible questions to ask:
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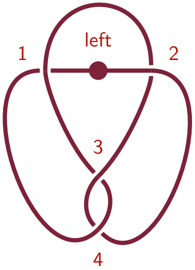
A candidate for a canonical Gauss code

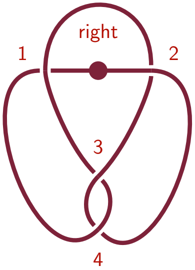
$-1, 4, -3, 1, -2, 3, -4, 2$



A candidate for a canonical Gauss code

$-1, 4, -3, 1, -2, 3, -4, 2$

$2, -4, 3, -2, 1, -3, 4, -1$



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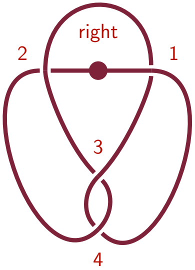

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$2, -4, 3, -2, 1, -3, 4, -1$

$1, -4, 3, -1, 2, -3, 4, -2$

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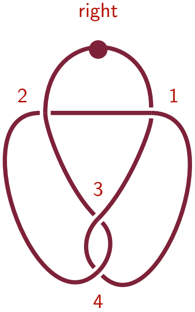
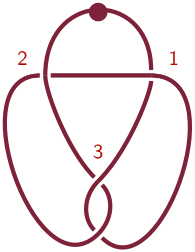


A candidate for a canonical Gauss code

- Our candidate is the lexicographically minimum unsigned code. For this knot we have:

  1, 2, 3, 1, 4, 3, 2, 4.



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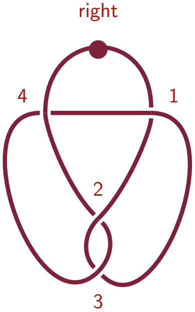
- For which the diagram now shows the labelling giving rise to the signed code:

  $-1, 2, -3, 1, -4, 3, -2, 4.$



A candidate for a canonical Gauss code

- Is this new?

A candidate for a canonical Gauss code

- Is this new? Kinda.

A candidate for a canonical Gauss code

- Is this new? Kinda.
- Topologists don't seem to care about labelling a knot in a canonical manner when determining a knot's Gauss code.
- But such a lexicographically minimum unsigned Gauss code is necessary input of an algorithm which follows.

A candidate for a canonical Gauss code

```
Name      Gauss  Notation
3_1       -1, 3, -2, 1, -3, 2
4_1        1, -4, 3, -1, 2, -3, 4, -2
5_1       -1, 4, -2, 5, -3, 1, -4, 2, -5, 3
5_2       -1, 5, -2, 1, -3, 4, -5, 2, -4, 3
6_1       -1, 4, -3, 1, -5, 6, -2, 3, -4, 2, -6, 5
6_2       -1, 4, -3, 1, -2, 6, -5, 3, -4, 2, -6, 5
6_3        1, -6, 2, -1, 4, -5, 6, -2, 3, -4, 5, -3
```

Symmetries involved in Gauss code enumeration

- The choices involved in each stage of obtaining a Gauss code from a given knot lead to rich symmetries in the problem of enumerating knots by Gauss codes.
- As we have seen many Gauss codes represent the same knot.

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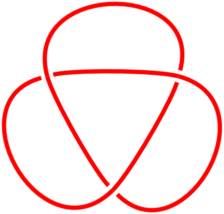

Symmetries involved in Gauss code enumeration

- The group of the symmetries of the problem is $S_{2n} \times \mathbb{Z}_{2n} \times \mathbb{Z}_2$ (over some quotient).
- Symmetry breaking on each of these groups is easy, but this is not the case for their product.

Virtual knots

Virtual knots

- The field of virtual knot theory arose from the question "do all Gauss codes represent knots?"
- Louis Kauffman lead the research into this new field and published his introduction to the subject in 1998.
- This introduction includes an algorithm for determining if a knot is classical or virtual.

Virtual knots

- It isn't hard to think of an example of a Gauss code which does not represent a classical knot.

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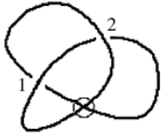
  1, −2, −1, 2



Evenly spaced Gauss codes

- Kauffman shows that a necessary condition for Gauss codes to give classical knots is that they are evenly spaced.

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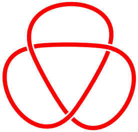
  1, 2, 3, 1, 2, 3



Evenly spaced Gauss codes

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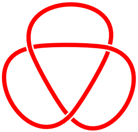
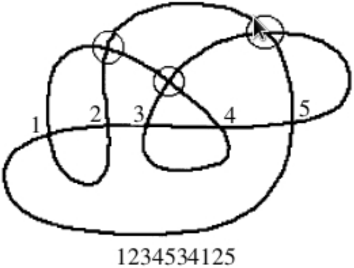
  1, 2, 3, 1, 2, 3

  1, 2, 3, 1, 4, 3, 2, 4



Evenly spaced Gauss codes

- However, he also provides an example where this condition is not sufficient.



The dually pairedness condition

- The other necessary condition, which when combined with the evenly spaced condition is sufficient, is that, for a Gauss code w its associated w^* must be dually paired.

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- The other necessary condition, which when combined with the evenly spaced condition is sufficient, is that, for a Gauss code w its associated w^* must be dually paired.
- For a Gauss code w, its associated w^* is obtained by the following algorithm: for each letter i in the code, reverse the order of all the letters between each instance of i in turn.

The dually pairedness condition

Original code 1, 2, 3, 1, 4, 3, 2, 4

Order between 1 reversed 1, 3, 2, 1, 4, 3, 2, 4

The dually pairedness condition

Original code 1, 2, 3, 1, 4, 3, 2, 4

Order between 1 reversed 1, 3, 2, 1, 4, 3, 2, 4

Order between 2 reversed 1, 3, 2, 3, 4, 1, 2, 4

The dually pairedness condition

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Order between 1 reversed 1, 3, 2, 1, 4, 3, 2, 4

Order between 2 reversed 1, 3, 2, 3, 4, 1, 2, 4

Order between 3 reversed 1, 3, 2, 3, 4, 1, 2, 4

The dually pairedness condition

Original code 1, 2, 3, 1, 4, 3, 2, 4

Order between 1 reversed 1, 3, 2, 1, 4, 3, 2, 4

Order between 2 reversed 1, 3, 2, 3, 4, 1, 2, 4

Order between 3 reversed 1, 3, 2, 3, 4, 1, 2, 4

Order between 4 reversed 1, 3, 2, 3, 4, 2, 1, 4

The dually pairedness condition

- For a shadow Gauss code w two labels i and j are called *interlaced* in w iff $w = w_1\ i\ w_2\ j\ w_3\ i\ w_4\ j\ w_5$ or $w = w_1\ j\ w_2\ i\ w_3\ j\ w_4\ i\ w_5$, where each w_n is a subcode (which is possibly empty).
- An unsigned Gauss code's w^* construction is *dually paired* iff each letter $i \in w^*$ can be placed into one of two sets, such that each i in both sets is not interlaced with another letter contained in the same set as i.

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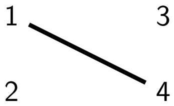
1 3

2 4

The dually pairedness condition

- For a shadow Gauss code w two labels i and j are called *interlaced* in w iff $w = w_1 \ i \ w_2 \ j \ w_3 \ i \ w_4 \ j \ w_5$ or $w = w_1 \ j \ w_2 \ i \ w_3 \ j \ w_4 \ i \ w_5$, where each w_n is a subcode (which is possibly empty).
- An unsigned Gauss code's w^* construction is *dually paired* iff each letter $i \in w^*$ can be placed into one of two sets, such that each i in both sets is not interlaced with another letter contained in the same set as i.



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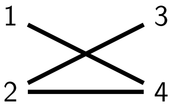

Kauffman's algorithm

Algorithm 1: Kauffman's algorithm for recognising planar unsigned Gauss codes

---

isPlanarUnsignedGaussCode (int[] *gc*) → Bool
begin
  if *gc is not evenly spaced* **then return false**
  else *gcStar* ← createWStar(*gc*)
  return whether *gcStar* is not dually paired

Implementation

- The aim of the project was to generate all knot diagrams of a given crossings number, up to some notion of equivalence.
- The project made use of both Constraint Programming and dedicated algorithms to efficently filter codes.

Implementation

- Constraint programming:
  - Generate Gauss codes which pass the evenly spaced condition.
  - Symmetry breaking on the S_n symmetry.
- Filtering:
  - Test that the code is dually paired.
  - Test that the code is the lexicographically minium code in its orbit in the group $\mathbb{Z}_{2n} \times \mathbb{Z}_2$.

A naive constraint model

For a knot with crossing number n:

$$\forall i \in \{0, 2n{-}1\} : \mathit{letter}[i] \in \{1, n\} \tag{V1}$$

$$\forall k \in \{1, n\} : \mathrm{occurrence}(\mathit{letter}[i] = k) = 2 \tag{C1}$$

$$\forall i, j \in \{0, 2n{-}1\}, i \neq j, \text{ with } i \text{ even } : \mathit{letter}[i] = k \implies \mathit{letter}[j] \neq k \text{ for } j \text{ even} \tag{C2}$$

$$\forall i, j \in \{0, 2n{-}1\}, i \neq j, \text{ with } i \text{ odd } : \mathit{letter}[i] = k \implies \mathit{letter}[j] \neq k \text{ for } j \text{ odd} \tag{C3}$$

$$\forall i \in \{0, 2n{-}1\} : \mathit{maxSoFar}[i] = \max(\mathit{letter}[0], \ldots, \mathit{letter}[i-1]) \tag{V2}$$

$$\forall i \in \{0, 2n{-}1\} : \mathit{letter}[i] \leq \mathit{maxSoFar}[i] + 1 \tag{C4}$$

$$\mathit{letter}[0] = 1 \tag{C5}$$

$$\forall i \in \{n, 2n-1\} : \mathit{letter}[i] \neq 1 \tag{C6}$$

Disallowing nonprime knots

- Given that during search we break the S_n symmetry we can use the following constraints to remove all nonprime knots from our solutions:
- A lexicographically minimum Gauss code representation of a prime alternating knot diagram satisfies the following constraints: $\forall i \in [2, n]$ the first instance of i occurs not later than the $2(n-1)-1$ (zero based) position in the Gauss code.

Disallowing nonprime knots

1, 2, 3, 1, 2,

Further work

- Add constraints to the model to determine if a partial assignment can never pass the dually paired condition.
- Parallelism: The problem is embarrassingly parallel

Thank you!