A Linear Time Algorithm for Visualizing Knotted Structures in 3 Pages

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Abstract: We introduce simple codes and fast visualization tools for knotted structures in molecules and neural networks. Knots, links and more general knotted graphs are studied up to an ambient isotopy in Euclidean 3-space. A knotted graph can be represented by a plane diagram or by an abstract Gauss code. First we recognize in linear time if an abstract Gauss code represents an actual graph embedded in 3-space. Second we design a fast algorithm for drawing any knotted graph in the 3-page book, which is a union of 3 half-planes along their common boundary line. The running time of our drawing algorithm is linear in the length of a Gauss code of a given graph. Three-page embeddings provide simple linear codes of knotted graphs so that the isotopy problem for all graphs in 3-space completely reduces to a word problem in finitely presented semigroups.

1 MOTIVATION AND PROBLEMS

Knotted structures are common in nature. For example, microscopic lines in liquid-crystals (Tkalec et al., 2011) or Reeb graphs of complex shapes (Biasotti et al., 2008) can be knotted. Figure 1 shows a neuron and a microscopic scan of a chemical. These structures are usually huge and more complicated than simple closed curves studied in classical knot theory.

Pictures of knots can be attractive for humans, but robots would prefer a smaller form or codes representing the same knotted object. Such codes are needed for automatic analysis, however a final output is important to visualize. We summarize our requirements for processing knotted structures in 3 problems.

• **Modeling:** find a suitable mathematical model for analyzing all possible knotted structures in 3-space.

• **Encoding:** represent any knotted structure by its simple and small code in a computer's memory.

• **Visualization:** design a fast algorithm to visualize knotted structures represented by their abstract codes.

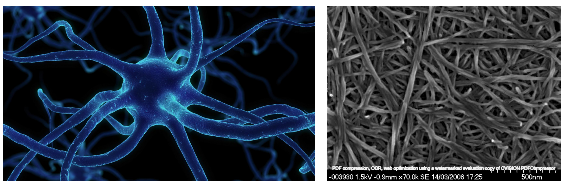

Figure 1: Neurons and molecules have branching points.

Our suggested model for knotted structures is a possibly disconnected graph with branching vertices and multiple edges that might be knotted in 3-space, see Definition 1. For instance, any knot in 3-space is a non-self-intersecting closed curve, which is a topological circle without any branching points.

Knots live in 3-space, but it is easier to draw their planar projections with double crossings. Such plane diagrams are usually represented by Gauss codes that specify the order of overcrossings and undercrossings along a knot. We extend classical Gauss codes of knots to arbitrary knotted graphs in Definition 4.

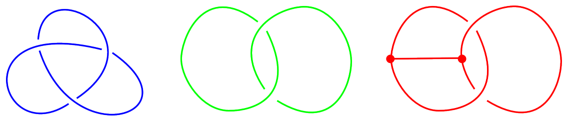

Figure 2: Diagrams of the trefoil, Hopf link, knotted graph.

A random code (of a required form) may not represent a real knotted graph, because a planar drawing may need extra crossings. We solve this planarity problem for Gauss codes of knotted graphs in Theorem 9. Namely, our algorithm checks if a Gauss code is realized by an actual graph in 3-space with a linear time complexity in the length of the given code.

Starting from any realizable Gauss code, we draw a corresponding graph in the *3-page book*, see Theorem 12. This book consists of 3 half-planes attached along their common boundary α called the *spine*.

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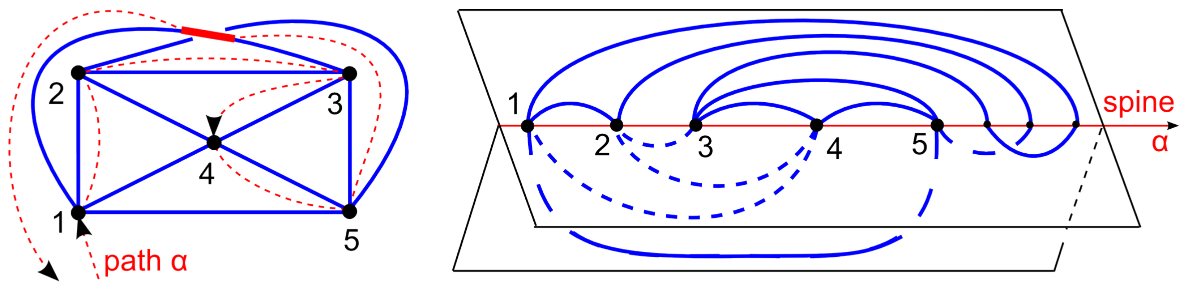

Figure 3: Straighten a red path α to build a 3-page embedding of a knotted graph $K_5 \subset \mathbb{R}^3$ from its plane diagram.

It is well-known that any graph can be topologically embedded in the 3-page book (Bernhart and Kainen, 1979, Theorem 5.4). However, an embedded graph may cross many times the spine of the book. It is only known that $O(|E|\log|V|)$ spine crossings suffice for embedding a graph with $|V|$ vertices and $|E|$ edges (Enomoto and Miyauchi, 1999).

We largely strengthen the former result by designing a linear time algorithm to continuously move any graph embedded in 3-space to a graph within 3 pages. We review other related work throughout the paper. Figure 3 is a high-level illustration of our fast algorithm for a knotted graph $K_5 \subset \mathbb{R}^3$. Appendix contains more details on the following advantages of 3-page embeddings over traditional plane diagrams.

• Theorem 13 encodes 3-page embeddings of all knotted graphs by easy codes that form a semigroup.

• Theorem 14 decomposes any topological equivalence between 3-page embeddings of graphs into finitely many local relations between 3-page codes.

2 KEY CONCEPTS ON GRAPHS

A *homeomorphism* between spaces is a bijection that is continuous in both directions. An *embedding* of one space into another is a continuous function $f : X \to Y$ that induces a homeomorphism between X and its image $f(X) \subset Y$. We study embeddings of undirected finite graphs, possibly disconnected and with loops or multiple edges. The concept of a knotted graph extends the classical theory of knots to arbitrary graphs considered up to isotopy in 3-space $\mathbb{R}^3$.

Definition 1. *A* knotted graph $G \subset \mathbb{R}^3$ *is an embedding of a finite graph G. An ambient* isotopy *between knotted graphs $G, H \subset \mathbb{R}^3$ is a continuous family of homeomorphisms $f_t : \mathbb{R}^3 \to \mathbb{R}^3$, $t \in [0,1]$ such that $f_0 = \mathrm{id}$ is the identity map on $\mathbb{R}^3$ and $f_1(G) = H$.*

An isotopy between directed graphs is similarly defined and should respect directions of edges. If the underlying graph G is a circle S^1, then a knotted graph is a *knot*. If G is a disjoint union of several circles, then $G \subset \mathbb{R}^3$ is a *link*. A link isotopic to a union of disjoint circles in $\mathbb{R}^2$ is called *trivial*. The simplest non-trivial knot is the *trefoil* in Figure 2. The simplest non-trivial link is the *Hopf* link in Figure 2.

If an ambient isotopy keeps a small neighborhood of each vertex of a knotted graph in one moving plane, the graph is called *rigid*. Rigid knotted graphs with vertices of only degree 4 are sometimes called *singular knots*, because they consist of one or several circles intersecting each other at singular points.

Definition 2. *A* plane diagram *D of a knotted graph $G \subset \mathbb{R}^3$ is the image of G under a projection $\mathbb{R}^3 \to \mathbb{R}^2$ from 3-space $\mathbb{R}^3$ to a horizontal plane $\mathbb{R}^2$. In a general position we assume that all intersections of a plane diagram D are double* crossings *so that the crossings and the projections of all vertices of G are distinct. For each crossing of D, we specify one of two intersecting arcs that* crosses over *another arc.*

The key problem in knot theory is to efficiently classify knots and graphs up to ambient isotopy. The first natural step is to reduce the dimension from 3 to 2. Any isotopy of knotted graphs can be realized by finitely many moves on plane diagrams. The following result extends Reidemeister's theorem for knots.

Theorem 3. *(Kauffman, 1989) Two plane diagrams represent isotopic knotted graphs in 3-space $\mathbb{R}^3$ if and only if the diagrams can be obtained from each other by an isotopy in $\mathbb{R}^2$ and finitely many Reidemeister moves in Figure 4. (The move* R5 *is only for rigid graphs, the move* R5$'$ *is only for non-rigid graphs.)*

The move R4 is shown only for a degree 4 vertex, moves for other degrees are similar. The move R5 turns a small neighborhood of a vertex in the plane upside down. So a cyclic order of edges at vertices is preserved in rigid graphs. The move R5$'$ can arbitrarily reorder all edges at a vertex. Theorem 3 formally includes all symmetric images of moves in Figure 4.

The Reidemeister moves or their analogs on Gauss codes are not local as they involve distant parts of a

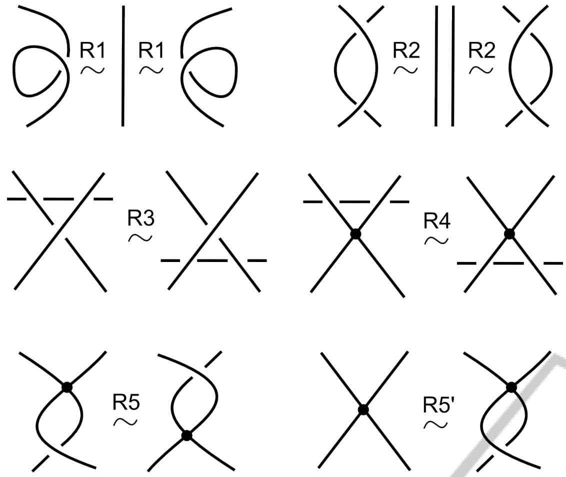

Figure 4: Reidemeister moves on diagrams of graphs.

graph or a Gauss code. This non-locality is a key obstacle for simplifying codes of knots. That is why we later consider 3-page embeddings that allow only finitely many local moves, see Theorem 12.

3 CODES OF KNOTTED GRAPHS

A standard way to encode a plane diagram of a knot is to write down labels of crossings in a Gauss code. The Gauss code of a link has several words corresponding to all link components. We extend this classical concept to arbitrary knotted graphs $G \subset \mathbb{R}^3$. If a component of G is a circle without vertices, we add a *base point* (a degree 2 vertex) to this circle.

Definition 4. *Let $D \subset \mathbb{R}^2$ be a plane diagram of a knotted graph G with vertices $A, B, C, \dots$ We fix directions of all edges of G and arbitrarily label all crossings of D by $1, 2, \dots, n$. Then each crossing of D has the* sign *locally defined in Figure 5. The* Gauss code *of D consists of all words W_{AB} associated to directed edges from a vertex A to a vertex B as follows:*

• *the word W_{AB} starts with A, finishes with B and has the labels of all crossings in the directed edge AB;*

• *if AB goes under another edge at a crossing i with a sign $\varepsilon \in \{\pm\}$ as in Figure 5, we add the superscript ε to i and get the symbol i^ε with the sign ε in W_{AB}.*

The neighbors (vertices or crossings) of each vertex A are clockwisely ordered in $\mathbb{R}^2$, so the code also specifies a cyclic order of all symbols adjacent to A.

If a graph G is a knot, Definition 4 requires at least one degree 2 vertex (a base point) on G. For simplicity, we may ignore degree 2 vertices in this case and consider the corresponding single word *cyclically*.

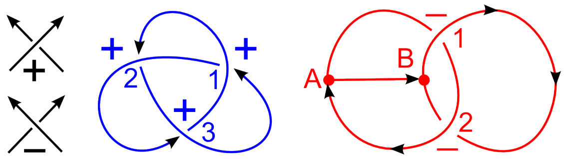

Figure 5: Local rules for signs of crossings with examples.

In Figure 5 the diagram of the blue trefoil has the cyclic Gauss code $12^+31^+23^+$. The diagram of the red knotted graph has the Gauss code $W = \{AB, A1^-2A, B12^-B\}$ with the cyclic orders of neighbors at both vertices $A : (B, 2, 1^-)$, $B : (A, 1, 2^-)$.

A Gauss code of any undirected graph depends on a choice of extra degree 2 vertices, directions of edges, an order of crossings. If a plane diagram of a knotted graph corresponds to a Gauss code, then this diagram is unique up to isotopy in the plane. We give an explicit construction in the proof of Theorem 9.

Here is a naive approach to drawing a plane diagram represented by a Gauss-like code W. We can put vertices $A, B, C, \dots$ and crossings $1, 2, \dots, n$ at arbitrary points in $\mathbb{R}^2$. Since the code W specifies the cyclic order of edges at each vertex A in Definition 4, we may draw short arcs around A in a correct cyclic order. Now we should connect all vertices and crossings that have adjacent positions in the code W by continuous non-intersecting arcs in the plane.

The last step fails for the word 12^+1^+2 that does not encode any plane diagram. Indeed, if we try to draw a closed curve with 2 self-intersections as required by 12^+1^+2, we have to add a 3rd intersection (a virtual crossing) to make the curve closed. This obstacle can be resolved if we draw a diagram on a torus as in Figure 6, because we can hide a virtual crossing by adding a handle. Another approach is to embrace virtual crossings, which has led to virtual knots.

If we study properly embedded graphs, we need to recognize planarity of Gauss codes, namely determine if a Gauss code represents a plane diagram of a knotted graph. So we first introduce abstract Gauss codes in Definition 5 and then recognize their planarity in the general case of knotted graphs in Theorem 9.

Definition 5. *Let the alphabet consist of m letters $A, B, C, \dots$ and $3n$ symbols i, i^+, i^- for $i = 1, \dots, n$. An* abstract Gauss code *is a set of words such that*

• *the first and last symbols of each word are letters,*

• *the set of symbols in all words (apart from the initial and final letters) contains, for each $i = 1, \dots, n$, the symbol i and exactly one symbol from the pair i^+, i^-.*

Each of the m letters defines a cyclic order of all symbols adjacent to this letter. The length *$|W|$ is the total* *length of all words minus the number of words.*

The Gauss code of any plane diagram of a knotted graph G from Definition 4 satisfies the conditions above. Indeed, the letters $A,B,C,\dots$ denote (projections of) vertices of G. Then every edge contains crossings labeled by i, i^+ or i^- for $i = 1,\dots,n$.

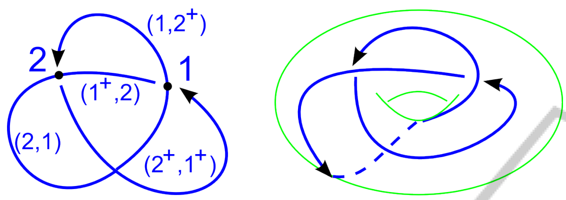

Figure 6: A diagram with 1 virtual, 2 usual crossings.

The clockwise order of edges around any vertex A in the plane diagram of G in $\mathbb{R}^2$ defines the cyclic order of vertices and crossings adjacent to A. If a component of G is a circle, we may remove its vertices of degree 2 and write the remaining symbols as in the cyclic code $12^+31^+23^+$ of the trefoil in Figure 5. The total number of these symbols equals the doubled number of crossings.

4 PLANARITY OF GAUSS CODES

The planarity problem is to determine whether it is possible to draw a plane diagram represented by an abstract Gauss code W. To avoid potential self-intersections, we shall draw a diagram not in the plane, but in the Gauss surface $S(W)$ defined below.

First we introduce the abstract graph $G(W)$ describing the adjacency relations between symbols in a Gauss code W. Then we attach disks to $G(W)$ to get the surface $S(W)$ containing a required diagram without self-intersections. The criterion of planarity will check if the surface $S(W)$ is a topological sphere S^2.

Definition 6. *Any abstract Gauss code W with m letters $A,B,\dots$ and $2n$ symbols from $\{i,i^+,i^- \mid i = 1,\dots,n\}$ gives rise to the Gauss graph $G(W)$ with $m+n$ vertices labeled by $A,B,\dots$ and $1,2,\dots,n$.*

We connect vertices p,q by a single edge in $G(W)$ if p,q (possibly with signs) are adjacent symbols in W. Below when we travel along an edge from p to q, we record our path by $(p,q)_+$ if q follows p in the code W (in the cyclic order), otherwise by $(p,q)_-$.

We define unoriented cycles in the graph $G(W)$ by going along edges and turning at vertices according to the following rules illustrated in Figure 7:

- *if we came to one of the vertices $A,B,C,\dots$ from its neighbor, then we turn to the next neighbor in the clockwise order specified in the Gauss code W;*

- *at each vertex labeled by $i \in \{1,\dots,n\}$ we turn to the next edge by one of the rules below for a unique possible choice of $\delta \in \{+,-\}$ and both $\varepsilon \in \{+,-\}$*

$$(p,i)_+ \to (i^\delta,q)_\delta, \quad (p,i)_- \to (i^\delta,q)_{-\delta},$$
$$(p,i^+)_\varepsilon \to (i,q)_{-\varepsilon}, \quad (p,i^-)_\varepsilon \to (i,q)_\varepsilon.$$

We stop traversing cycles when every edge was passed once in each direction. The Gauss surface *$S(W)$ is obtained from $G(W)$ by gluing a disk to each cycle.*

The number of edges in the graph $G(W)$ equals the length $|W|$ of the code W. The rules for traversing cycles in Definition 6 geometrically mean that at each vertex or crossing we turn left to a unique edge and can pass every edge exactly once in each direction. Hence the Gauss surface of any abstract Gauss code is a compact orientable surface without boundary.

Lemma 7. *For the Gauss code W of any plane diagram of a knotted graph $G \subset \mathbb{R}^3$, the Gauss surface $S(W)$ is homeomorphic to a topological sphere S^2.*

Proof. We assume that the given diagram D is contained in a sphere S^2 instead of a plane $\mathbb{R}^2$. Then the Gauss graph $G(W)$ can be identified with the diagram D, though $G(W)$ was introduced as an abstract graph not embedded into any space. When we traverse the cycles in $D = G(W)$ from Definition 6, we pass over the boundaries of all connected components of $S^2 - D$. Indeed, each time we turn left in the diagram $D \subset S^2$ according to the geometric rules in Figure 7. Hence the Gauss surface $S(W)$ can be identified with the sphere S^2 containing the diagram $D = G(W)$. $\square$

Example 8. *We construct the Gauss surface of the abstract Gauss code $W = 12^+1^+2$, whose diagram with one virtual crossing is in Figure 8. For simplicity, we removed the degree 2 vertex from the circle and consider the word 12^+1^+2 in the cyclic order.*

Then 4 pairs 12^+, 2^+1^+, 1^+2, 21 of adjacent symbols in the code W lead to the graph $G(W)$ whose 2 vertices with labels $1,2$ are connected by 4 edges with labels $(1,2^+)$, $(2^+,1^+)$, $(1^+,2)$, $(2,1)$ in Figure 8. Recall that the edges labeled by $(2,1)$ and $(2^+,1^+)$ meet at a non-avoidable virtual crossing in the plane, but the abstract graph $G(W)$ has only 2 vertices.

If we start traveling from the edge $(1,2^+)_+$ in the same direction as in W, the next edge should be $(2,1^+)_-$ by the rule $(p,i^+)_\varepsilon \to (i,q)_{-\varepsilon}$, where $p = 1$, $i = 2$, $\varepsilon = +$ uniquely determine the next symbol $q = 1^+$ from the code W (going from 2 in the opposite direction). After the second edge $(2,1^+)_-$

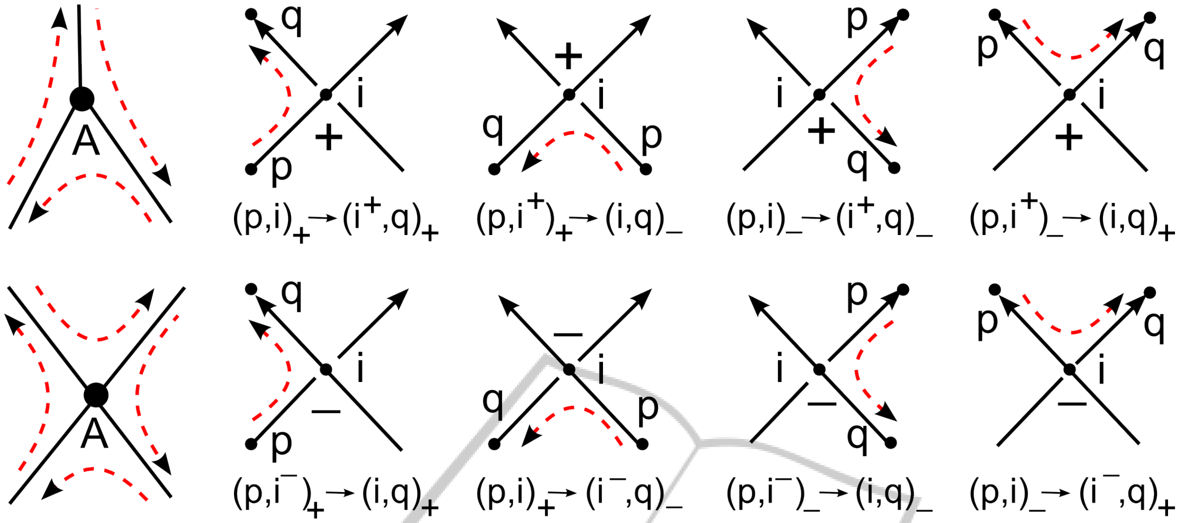

Figure 7: A geometric interpretation of the 'turning-left' rules for traversing cycles in the Gauss graph $G(W)$.

we return to the first edge $(1,2^+)_+$ *by the same rule* $(p,i^+)_\varepsilon \to (i,q)_{-\varepsilon}$ *for* $p=2$, $i=1$, $\varepsilon=-$, $q=2^+$.

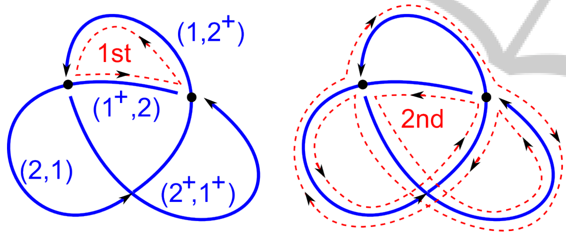

Figure 8: Two red dashed cycles in $G(W)$ for $W = 12^+1^+2$.

So the 1st cycle consists of 2 edges $(12^+)_+$ *and* $(2,1^+)_-$. *The 2nd cycle consists of 6 edges* $(1^+,2)_+ \to (2^+,1^+)_+ \to (1,2)_- \to (2^+,1)_- \to (1^+,2^+)_- \to (2,1)_+$. *Both cycles of* $G(W)$ *are shown by red dashed closed curves in Figure 8. The resulting Gauss surface* $S(W)$ *with 2 vertices, 4 edges, 2 faces has the Euler characteristic* $\chi = 2-4+2 = 0$ *and should be a torus as expected from Figure 6.*

The *Euler characteristic* of a surface subdivided by a graph with $|V|$ vertices and $|E|$ edges into $|F|$ faces (topological disks) is defined as $\chi = |V| - |E| + |F|$ and is invariant up to a *homeomorphism* (a bijection continuous in both directions).

Any orientable connected compact surface of a genus g (the number of handles) and b boundary components (circles) has $\chi = 2-2g-b \le 2$. Hence a sphere S^2 with $\chi(S^2) = 2$ is detectable by the Euler characteristic among connected compact surfaces.

Theorem 9 extends (Kurlin, 2008, Algorithm 1.4) from links to arbitrary knotted graphs.

Theorem 9. *Given an abstract Gauss code* W *of a length* $|W|$, *an algorithm of time complexity* $O(|W|)$ *can determine if the given Gauss code* W *represents a plane diagram of a knotted graph* $G \subset \mathbb{R}^3$.

Proof. The Gauss surface $S(W)$ of any abstract Gauss code W contains the diagram D encoded by W due to the geometric interpretation of the rules in Figure 7. This surface has the maximum Euler characteristic χ among all orientable connected compact surfaces S that contain the diagram D and have no boundary.

Indeed, after cutting the underlying graph of the diagram $D \subset S$, the surface S splits into several components. The Euler characteristic of S is maximal when all these components are disks as in the Gauss surface. The disk has $\chi = 1$, which is maximal among all compact surfaces whose boundary is a circle.

To decide the planarity of W, it remains to determine if the Gauss surface $S(W)$ is a sphere S^2, which is detectable by the Euler characteristic $\chi = 2$ in the class of all orientable connected compact surfaces S without boundary. For computing the Euler characteristic χ, we use the Gauss graph $G(W)$, which splits $S(W)$ into topological disks by Definition 6.

Namely, $S(W)$ has $m+n$ vertices, $|W|$ edges and the number of faces equal to the number of cycles. We count all cycles in $G(W)$ in time $O(|W|)$ by a double traversal of W according to the rules in Figure 7. Hence in time $O(|W|)$ we compute $\chi = m+n-|W| + \#(\text{cycles})$ and determine if the Gauss surface $S(W)$ is homeomorphic to a topological sphere S^2. □

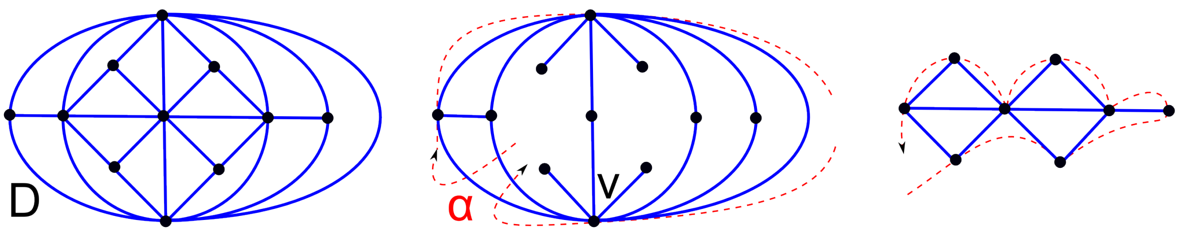

Figure 9: A path α through vertices of the non-hamiltonian maximum planar graph meets any edge at most once.

5 EMBEDDING A GRAPH IN 3 PAGES

The input of our algorithm for drawing an embedding in 3 pages should be a knotted graph or its plane diagram, which is usually represented on a computer by a Gauss code. Even for knots an abstract Gauss code may not represent a closed curve in 3-space. That is why we first solved the planarity problem for Gauss codes of knotted graphs in Theorem 9.

If we know that a given Gauss code represents a plane diagram D of a knotted graph G, our next step in Theorem 11 is to draw the diagram D in a 2-page book as defined below. After that we upgrade this topological 2-page embedding of D to a 3-page embedding of G in linear time, see Theorem 12.

Definition 10. *The* k-page book *consists of* k *half-planes with a common boundary line* α *called the* spine *of the book. An embedding of an undirected graph* G *into the* k*-page book is* topological *if the intersection of* G *with the spine* α *is finite and includes all vertices of* G*. A* bend *of an edge* $e \subset G$ *is any interior point* p *of* e *such that* $p \in \alpha$*. If every edge of an embedded graph* G *is contained in a single page, the* k*-page book embedding of* G *is* combinatorial.

A graph D is *planar* if D can be embedded in $\mathbb{R}^2$. Any undirected planar graph has a combinatorial 4-page embedding (Yannakakis, 1989). Figure 9 shows a planar graph that can not be combinatorially embedded into 2 pages (Bernhart and Kainen, 1979, section 5). Any topological 2-page embedding of this graph will have extra bends where edges intersect the spine. The linear time algorithm below guarantees at most one bend per edge for any planar graph.

Theorem 11. *(Di Giacomo et al., 2005, Theorem 1) Given a planar undirected graph* $D \subset \mathbb{R}^2$ *with* $|V|$ *vertices, an algorithm of linear time complexity* $O(|V|)$ *can draw a topological embedding of the graph* D *in the 2-page book with at most one bend per edge.*

Two more pictures in Figure 9 illustrate the key idea how we can construct a non-self-intersecting path α that passes through each vertex once and intersects each edge at most once. By an isotopic deformation of $\mathbb{R}^2$, the path α can be converted into a straight spine, which splits the plane into 2 pages. Since all vertices and crossings of D are in the spine α, we get a required topological 2-page embedding of D.

We are not going to minimize the number of bends of edges in a 2-page embedding of a plane diagram D, because we shall construct 3-page embeddings of original knotted graphs with a linear number $O(|W|)$ of total bends in the length of a Gauss code W.

Theorem 12. *Given an abstract Gauss code* W*, an algorithm of time complexity* $O(|W|)$ *determines if* W *represents a plane diagram of a knotted graph* $G \subset \mathbb{R}^3$ *and then draws a topological 3-page embedding of a graph* H *isotopic to* G*. Moreover, the graph* H *has at most* $8|W|$ *intersections with the spine of the book.*

Proof. We first apply the linear time algorithm from Theorem 9 to determine if the code W represents a plane diagram D of a knotted graph G. If yes, we draw a 2-page embedding of the diagram $D \subset \mathbb{R}^2$ in linear time using the algorithm from Theorem 11.

At every crossing in the diagram D, we mark a short red arc that crosses over another arc in D. The centers of all these marked arcs are all crossings of D, which are already in the straight spine α of the 2-page book. We may slightly deform the embedding of D by pushing the marked red arcs into the spine α, see typical cases in the first 5 pictures of Figure 10 where a crossing of D leads to 3 intersections with α.

If the undercrossing arc was in only one page, we first make an additional intersection so that the deformed undercrossing arc goes from one page to another and back, see the last 5 pictures of Figure 10 where a crossing leads to 4 intersections with α.

Now we push all marked red arcs into the extra 3rd page attached along α above the diagram D. So we have upgraded the 2-page embedding of D to a 3-page embedding of a knotted graph H isotopic to the original graph G, see Fig. 12, 13.

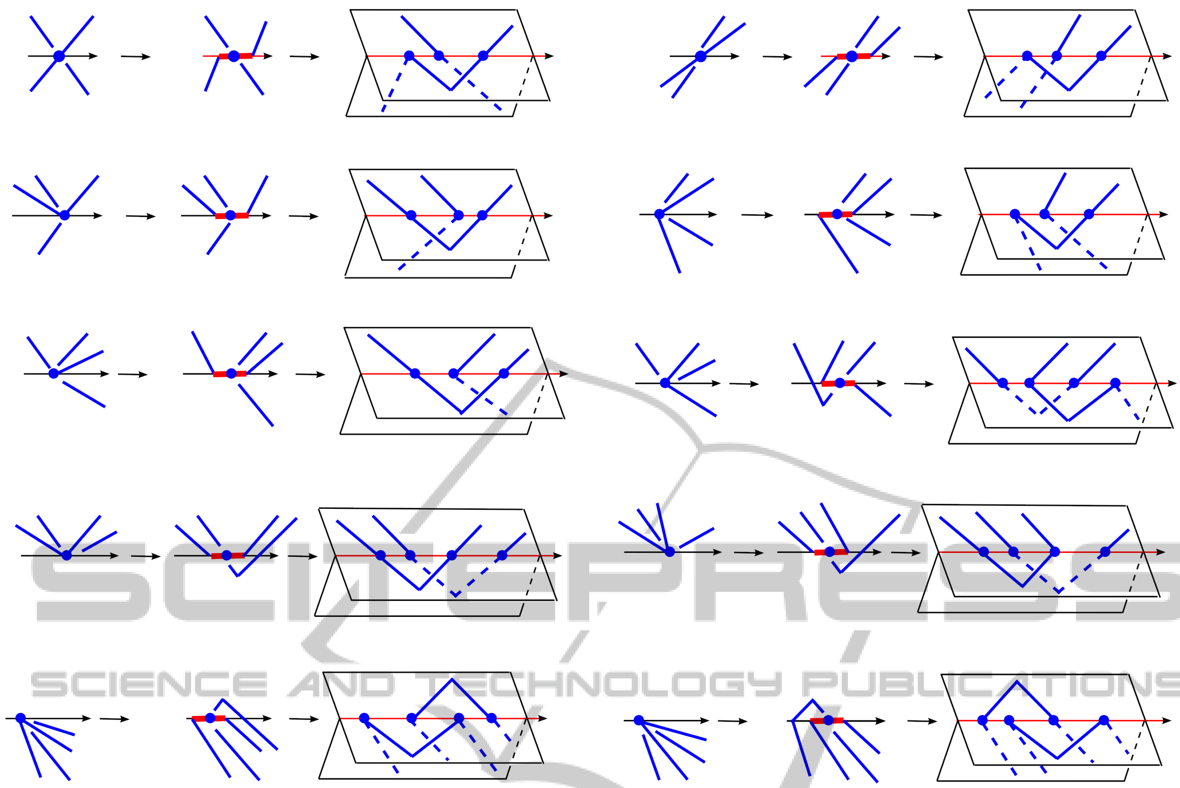

Figure 10: Upgrading crossings to 3-page embeddings.

We need a constant time per crossing, so $O(|W|)$ in total, for a 3-page embedding of H. Since the diagram D has $|W|$ edges, the 2-page embedding of D with at most one bend per edge has at most $2|W|$ points in the spine α. Each crossing of D is replaced by at most 4 intersections with the spine α in a 3-page embedding of H. The total number of points in the intersection of H and the spine α is at most $8|W|$. □

We remind how to encode 3-page embeddings of all knotted graphs by words in a simple alphabet. Since edges with vertices of degree 1 can be easily unknotted by isotopy in 3-space, for simplicity we consider below only graphs without degree 1 vertices.

To explain the 3-page encoding, let us deform any 3-page embedding so that all arcs are monotonically projected to the spine α. Then the whole embedding can be uniquely reconstructed by its thin neighborhood around the spine α. Namely, if we know only directions of arcs going from points in the spine, we can uniquely join these arcs in each of 3 pages. Hence we can encode any 3-page embedding by the list of local embeddings at all intersections in the spine α.

Theorem 13. *(Kurlin, 2007, Theorem 1.6a) Any 3-page embedding of a knotted graph G with vertices up to degree n can be encoded by a word in the alphabet consisting of the letters a_i, b_i, c_i, d_i and $x_{k,i}$ for each degree $k = 3, \ldots, n$, where $i = 0, 1, 2$, see Fig. 11.*

Fig. 11 shows 12 local embeddings a_i, b_i, c_i, d_i, $i \in \mathbb{Z}_3 = \{0, 1, 2\}$, that are sufficient for encoding any 3-page embeddings of knots and links. The notation a_i emphasizes that the embeddings a_i can be obtained from each other by a rotation around the spine α.

For encoding graphs in Theorem 13, we can make sure that at each vertex the spine separates one or two arcs from others.Then only 3 local embeddings are enough for each degree, see 3 neighborhoods $x_{3,0}$, $x_{3,1}$, $x_{3,2}$ of a degree 3 vertex in Fig. 11.

The 3-page embedding $K_5 \subset \mathbb{R}^3$ in Fig. 3 can be represented by the code $w = a_1 d_1 (a_1 b_1 x_{4,1})^2 (a_1 d_1 x_{4,1}) d_1 (x_{4,1} d_1 c_1)(x_{4,1} b_1 c_1) d_2 c_1 c_2$.

6 DISCUSSION AND PROBLEMS

We now discuss our results in the light of a huge gap between real-life experiments and pure mathematics. Experimental data are usually given in the form of unstructured and noisy clouds of points. If we have only 2D images as in Figure 1, then we also need to extract a knotted structure in a suitable form.

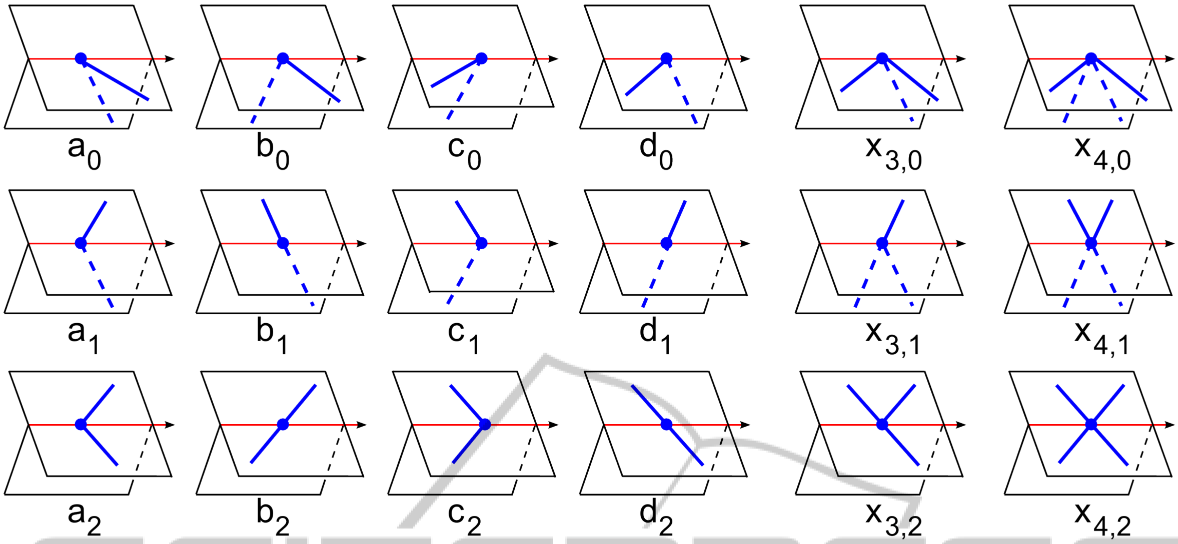

Figure 11: Local 3-page embeddings for the generators of the semigroups from Theorem 14.

Pure mathematicians have developed deep theories how to classify complicated geometric objects including knots. However, all mathematical algorithms start from ideal models, say a closed curve given by continuous functions or a polygonal curve given by a sequence of points connected by straight edges.

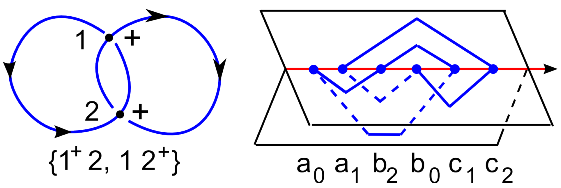

Figure 12: Hopf link, its Gauss code, a 3-page embedding.

The key open challenge is to convert any unstructured experimental data into an ideal theoretical model that can be rigorously analyzed by existing mathematical methods. The first advance in this direction is computing the fundamental group of a knot complement from a point cloud in (Brendel et al., 2015). We state open problems relating practice and theory for knotted graphs. We are open to collaboration on these problems and related projects.

1. Algorithmically produce a Gauss diagram of a knot given by a sequence of discrete points in 3-space $\mathbb{R}^3$.

2. Let a link of n components be given as an unordered union of $m \geq 2n$ open arcs (or sequences of points). How can we 'correctly' join corresponding endpoints of the arcs to form n closed curves in $\mathbb{R}^3$?

3. When drawing pictures on a tablet, a few intersecting curves can be represented by several sequences of 2D points sampled along the curves. Under what conditions on the curves and sample, can we quickly reconstruct the curves using only the sample?

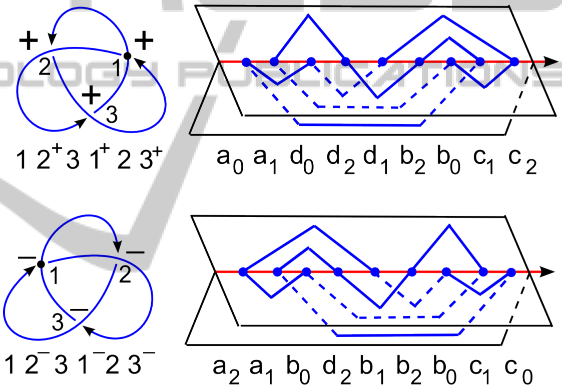

Figure 13: Trefoils, Gauss codes, 3-page embeddings.

4. Design a fast algorithm to convert an unstructured 3D point cloud sampled around an unknown knotted structure into a Gauss code W of a knotted graph.

5. Design a robust algorithm to convert a 2D image of an unknown knotted graph into a Gauss code W.

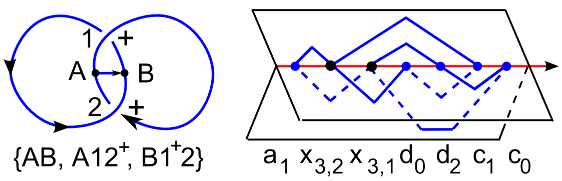

Figure 14: Hopf graph, its Gauss code, a 3-page embedding.

Our current work on visualizing Gauss codes is an important step in the hard problems above. First we may try to recognize small patches of vertices and crossings in a 2D image of a knotted graph, but after that we should combine them in a Gauss codes whose planarity can be quickly checked by Theorem 9.

Second if we need to visualize any noisy cloud sampled from an unknown knot $K \subset \mathbb{R}^3$, we may draw a knot isotopic to K using its Gauss code and Theorem 12. Even more importantly we often wish to get a simplified (minimal) version of a knot.

The state-of-the-art simplification algorithm for recognizing trivial knots available at http://www.javaview.de/services/knots is based on 3-page embeddings. We remind theoretical arguments for extending this 3-page approach to graphs in Appendix and state more problems below.

6. Design a simplification algorithm to untangle diagrams of 3D graphs isotopic to planar graphs.

7. Extend our algorithm for drawing graphs in 3 pages to drawing 2-dimensional surfaces in a universal 3D polyhedron from (Kearton and Kurlin, 2008).

8. Compute topological invariants of a knotted graph $G \subset \mathbb{R}^3$ starting from its Gauss code, say the fundamental group of the graph complement $\mathbb{R}^3 - G$.

9. Use the computed invariants to build a database of isotopy classes of knotted graphs similarly to the Knot Atlas at http://katlas.math.toronto.edu.

10. Define a kernel (Schölkopf and Smola, 2002) on point clouds representing knotted graphs so that one can use tools of machine learning for automatic recognition of real-life knotted structures in 3D.

Algorithms from Theorems 9 and 12 will be available on author's webpage http://kurlin.org. We thank all reviewers for their helpful suggestions and EPSRC for funding the author's secondment at Microsoft.

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APPENDIX

3-page Semigroups

The following result completely reduces the topological classification of spatial graphs up to isotopy in 3-space to a word problem in some semigroups.

Theorem 14. *(Kurlin, 2007, Theorems 1.6 and 1.7) There is a finitely presented semigroup whose all central elements are in a 1-1 correspondence with all isotopy classes of knotted graphs with vertices of degree up to n. There is a linear time algorithm to determine if an element belongs to the center of the semigroup.*

So two knotted graphs $G, H \subset \mathbb{R}^3$ are isotopic in 3-space if and only if their corresponding central elements w_G, w_H are equal in the semigroup. A stronger result in (Kearton and Kurlin, 2008) says that all isotopies between 3-page embeddings are realizable in a 3-dimensional polyhedron (a *hexabasic book*).

More formally, there are two slightly different semigroups: RSG_n for rigid spatial graphs with vertices up to degree n and NSG_n for non-rigid graphs. Both semigroups have 12 generators a_i, b_i, c_i, d_i, $i \in$

$\{0,1,2\}$, and $3(n-2)$ generators for vertices up to degree n, namely 3 generators for each degree from 3 to n, see Fig. 11. The empty word is the unit and $a_i, c_i, x_{k,i}$ are not invertible. In the case of links for $n=2$, the semigroup has 48 relations (1)–(4) below, where $i \in \mathbb{Z}_3 = \{0,1,2\}$ is considered modulo 3.

(1) $d_0 d_1 d_2 = 1$ and $b_i d_i = 1 = d_i b_i$;

(2) $a_i = a_{i+1} d_{i-1}, \quad b_i = a_{i-1} c_{i+1}$,
$c_i = b_{i-1} c_{i+1}, \quad d_i = a_{i+1} c_{i-1}$;

(3) $w(d_i c_i) = (d_i c_i) w$ for $w \in \{\, c_{i+1},\ b_i d_{i+1} d_i \,\}$;

(4) $uv = vu$, where $u \in \{\, a_i b_i, \quad b_{i-1} d_i d_{i-1} b_i \,\}$ and $v \in \{\, a_{i+1}, \quad b_{i+1}, \quad c_{i+1}, \quad b_i d_{i+1} d_i \,\}$.

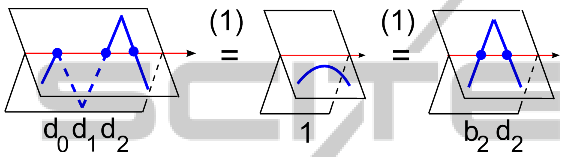

Figure 15: Relations (1) in the semigroup of Theorem 14.

One of the 7 relations in (1) is superfluous as it follows from the remaining 6. The generators a_i, b_i, c_i, d_2 can be expressed only in terms of d_0, d_1, but the resulting relations between d_0, d_1 will be longer. All defining relations of the semigroups represent elementary isotopies between 3-page embeddings, see typical examples for relations (1)–(4) in Figures 15–18.

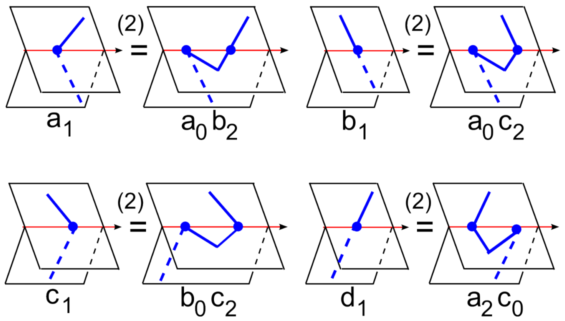

Figure 16: Relations (2) in the semigroup of Theorem 14.

For knotted graphs with vertices of only degree 3, any non-rigid isotopy can be made rigid, because we can keep 3 short arcs at any vertex in a moving plane. Hence both semigroups for rigid and non-rigid isotopies from Theorem 14 are the same for $n=3$. In this case the extra relations in addition to (1)-(4) are (5)–(9), see (Kurlin, 2001) and (Kurlin, 2007):

(5) $x_{3,i-1} = d_{i-1} x_{3,i} d_{i+1}$;

(6) $x_{3,i} b_i (d_i^2 d_{i+1}^2 d_{i-1}^2) = (d_i d_{i+1} d_{i-1}) x_{3,i} b_i$;

(7) $x_{3,i} d_i = a_i (x_{3,i} d_i) c_i, \quad b_i x_{3,i} b_i = a_i (b_i x_{3,i} b_i) c_i$;

(8) $u x_{3,i+1} = x_{3,i+1} u$ for any word u from the set $\{\, a_i b_i, \quad d_i c_i, \quad x_{3,i} b_i, \quad b_{i-1} d_i d_{i-1} b_i \,\}$;

(9) $(x_{3,i} b_i) v = v (x_{3,i} b_i) v$ for any word v from the set $\{\, a_{i+1}, \quad b_{i+1}, \quad c_{i+1}, \quad b_i d_{i+1} d_i \,\}$.

Knotted graphs that have only vertices of degree 4 and are considered up to rigid isotopy are often called *singular knots*. Each singular point remains a transversal intersection of two arcs during a rigid isotopy, so the cyclic order of all arcs at any degree 4 vertex is invariant. The semigroup of Theorem 14 for singular knots has 15 generators $a_i, b_i, c_i, d_i, x_{4,i}$, relations (1)–(4) above and relations (10)–(14) below, see (Kurlin and Vershinin, 2004) and (Kurlin, 2007):

(10) $x_{4,i-1} = b_{i+1} x_{4,i} d_{i+1}$;
(11) $(d_i x_{4,i} b_i)(d_i^2 d_{i+1}^2 d_{i-1}^2) = (d_i^2 d_{i+1}^2 d_{i-1}^2)(d_i x_{4,i} b_i)$;
(12) $d_i x_{4,i} d_i = a_i (d_i x_{4,i} d_i) c_i, \ b_i x_{4,i} b_i = a_i (b_i x_{4,i} b_i) c_i$;
(13) $w x_{4,i+1} = x_{4,i+1} w$ for any word w from the set $\{\, a_i b_i, \quad d_i c_i, \quad d_i x_{4,i} b_i, \quad b_{i-1} d_i d_{i-1} b_i \,\}$;

(14) $(d_i x_{4,i} b_i) v = v (d_i x_{4,i} b_i) v$ for any word v from the set $\{\, a_{i+1}, \quad b_{i+1}, \quad c_{i+1}, \quad b_i d_{i+1} d_i \,\}$.

The hard part of Theorem 14 says that any isotopy between graphs decomposes into finitely many elementary isotopies involving *a small part* of a 3-page code. This is the main advantage of the 3-page encoding over plane diagrams and Gauss codes. Indeed, Reidemeister moves on plane diagrams in Fig. 4 and their analogues on Gauss codes are not local.

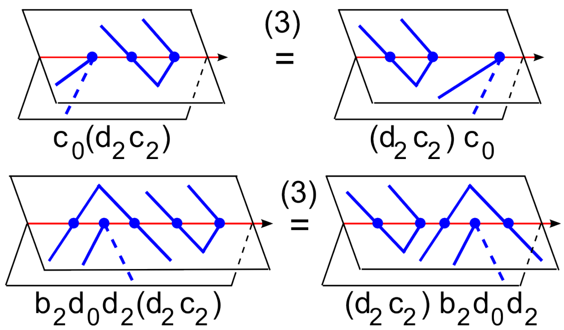

Figure 17: Relations (3) in the semigroup of Theorem 14.

The linear time algorithm for detecting a central element w checks if the arcs corresponding to all letters of w properly meet each other in every page to form an embedding of a graph without hanging edges. For example, the letter a_2 doesn't encode any knotted graph, but $a_2 c_2$ does, because the arcs of a_2 and c_2 meet and form a closed curve in pages 0 and 1.

The 3-page code of a knotted graph commutes with any other element w in the semigroups from Theorem 14. For instance, a trivial knot has the code $a_2 c_2$ and can be isotopically moved in $\mathbb{R}^3$ to another side of the 3-page embedding represented by the word w.

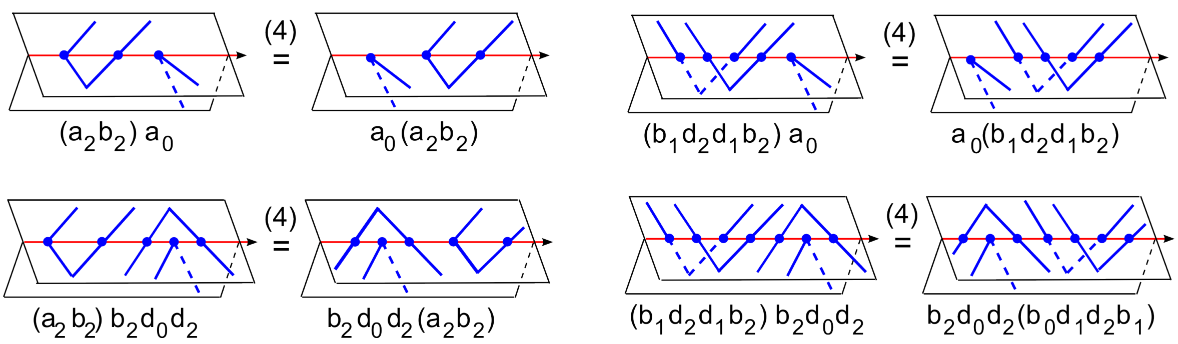

Figure 18: Relations (4) in the semigroup of Theorem 14.

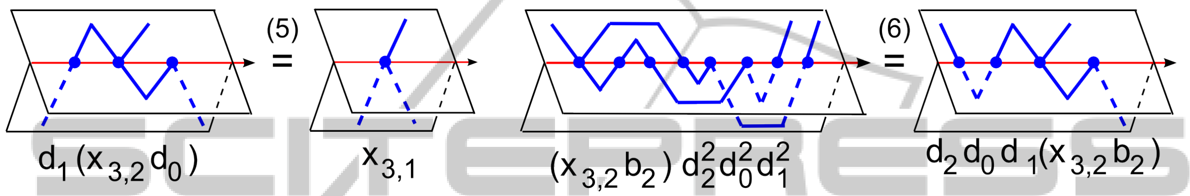

Figure 19: Relations (5)-(6) in the semigroup of Theorem 14.

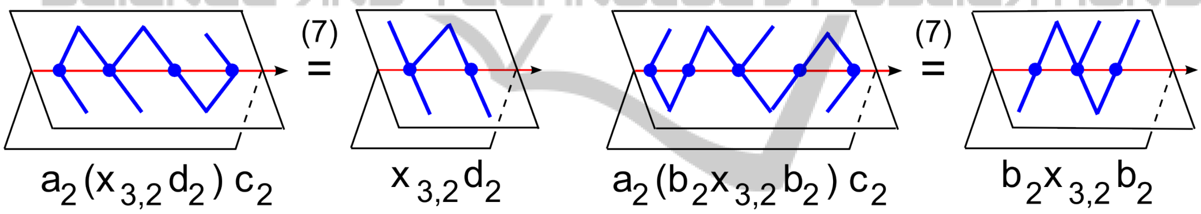

Figure 20: Relations (7) in the semigroup of Theorem 14.

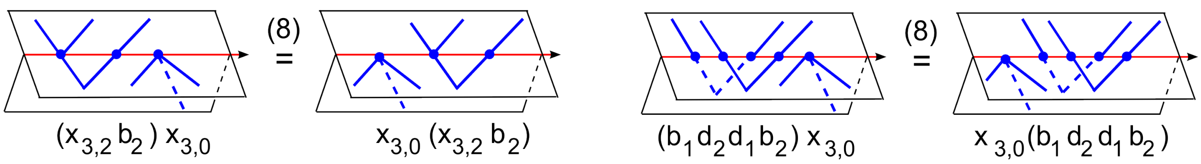

Figure 21: Relations (8) in the semigroup of Theorem 14.

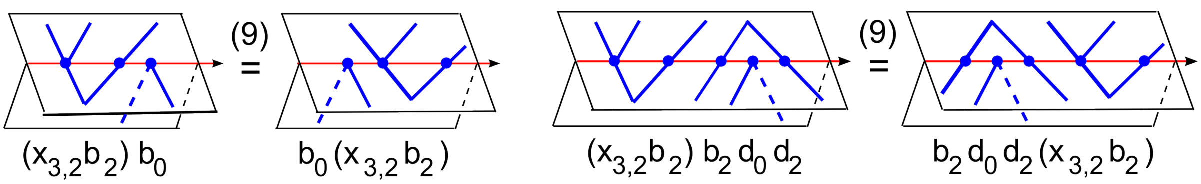

Figure 22: Relations (9) in the semigroup of Theorem 14.

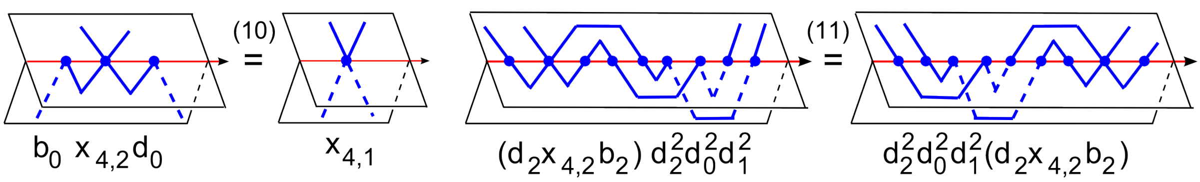

Figure 23: Relations (10)-(11) in the semigroup of Theorem 14.

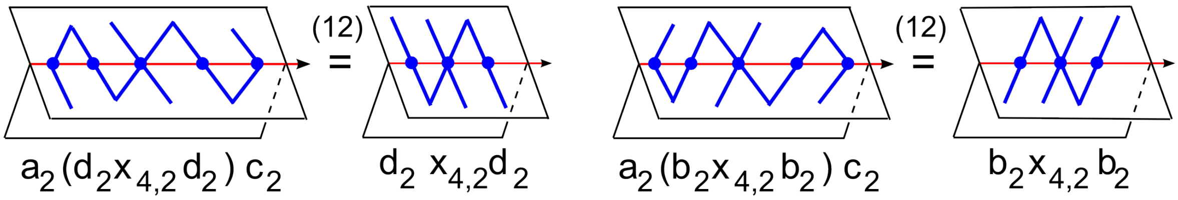

Figure 24: Relations (12) in the semigroup of Theorem 14.

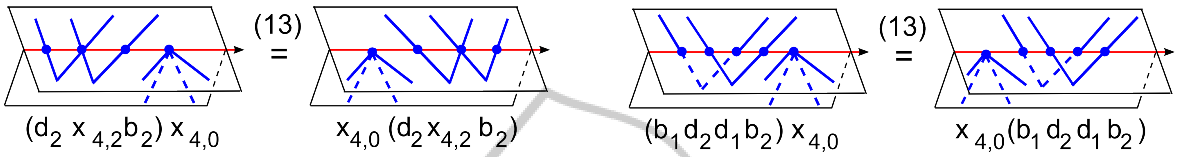

Figure 25: Relations (13) in the semigroup of Theorem 14.

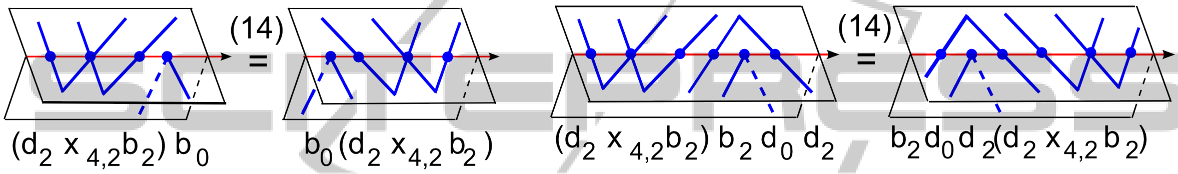

Figure 26: Relations (14) in the semigroup of Theorem 14.