A Linear Time Algorithm for Drawing a Graph in 3 Pages within its Isotopy Class in 3-Space

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Abstract. We consider undirected graphs up to an ambient isotopy in 3-space. Such a graph can be represented by a plane diagram or a Gauss code. We recognize in linear time if a Gauss code represents an actual graph in 3-space. We also design a linear time algorithm for drawing a topological 3-page embedding of a graph isotopic to a given graph.

Keywords: embedding, 3-page book, knot, link, spatial graph, isotopy

1 Introduction: Spatial Graphs and Book Embeddings

It is a well-known fact that any graph can be topologically embedded in 3 pages [1, Theorem 5.4]. However, an embedded graph may cross many times the spine of such 3-page book. It is only known that $O(|E|\log|V|)$ spine crossings suffice for a embedding graph with $|V|$ vertices and $|E|$ edges [3]. 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. Fig. 1 is a high-level illustration of our fast algorithm for a simple embedding $K_5 \subset \mathbb{R}^3$.

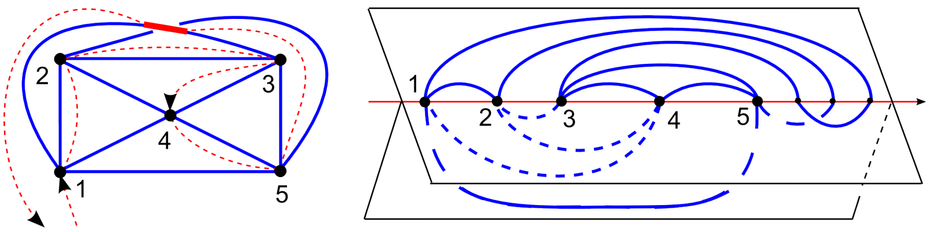

Fig. 1. A 3-page embedding of a spatial graph $K_5 \subset \mathbb{R}^3$ within its isotopy class

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 $f(X)$.

We study embeddings of undirected finite graphs, possibly disconnected and with loops or multiple edges. The concept of a spatial graph extends the classical theory of knots [9] to arbitrary graphs considered up to isotopy in 3-space $\mathbb{R}^3$.

Definition 1 *A* spatial graph *is an embedding $G \subset \mathbb{R}^3$ of a finite graph G. An ambient* isotopy *between spatial 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 $f_0 = \mathrm{id}_{\mathbb{R}^3}$ 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 spatial graph is a *knot*. A knot isotopic to a round circle is the *unknot* or *trivial*. The simplest non-trivial knot is the *trefoil* in Fig. 2. If G is a disjoint union of a few circles, then it is a *link*. The simplest non-trivial link is the *Hopf* link in Fig. 2.

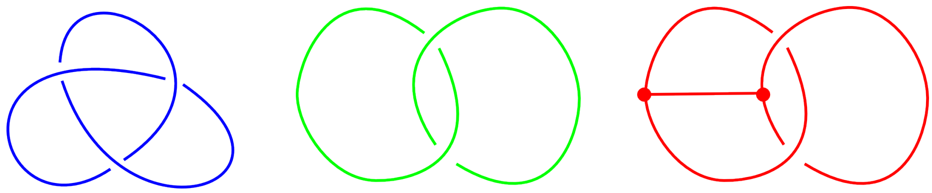

Fig. 2. Plane diagrams of the trefoil, the Hopf link and a spatial graph

If the ambient isotopy keeps a small neighborhood of each vertex of a spatial graph in one moving plane, the graph is called rigid. Rigid spatial 4-regular graphs are sometimes called *singular knots*, because they consist of one or several circles intersecting each other at singular points. The pictures in Fig. 2 show plane diagrams of spatial graphs, which are formally defined in section 2.

The input of our algorithm for drawing an embedding in 3 pages should be a spatial graph or its plane diagram, which is usually represented on a computer by a Gauss code. Even in the case of knots an abstract Gauss code may not represent a closed curve in 3-space. That is why we first solve the planarity problem for Gauss codes of spatial graphs in Theorem 8, see section 3.

If we know that a given Gauss code represents a plane diagram D of a spatial graph G, our next step in Theorem 9 from section 4 is to draw the diagram D in a 2-page book as defined below. In linear time we upgrade this topological 2-page embedding of D to a 3-page embedding of G, see Theorem 10 in section 4.

Definition 2 *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 a 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 an edge e such that $p \in \alpha$. If every edge of an embedded graph G is contained in a single page, then the k-page book embedding of G is called* combinatorial.

So we convert an abstract code of a spatial graph G into a 3-page embedding within the isotopy class of G. Section 4 highlights key advantages of 3-page embeddings over other representations of spatial graphs. Our fast drawing algorithm is applicable to huge spatial graphs. We anticipate applications of 3-page embeddings for Reeb graphs of shapes [2] and for knotted molecular structures.

2 Plane Diagrams and Gauss Codes of Spatial Graphs

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

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 spatial graphs can be realized by finitely many moves on plane diagrams. The following result extends Reidemeister's theorem for knots.

Theorem 4 (Reidemeister's moves) *[6] Two plane diagrams represent isotopic spatial graphs if and only if the diagrams can be obtained from each other by an isotopy in $\mathbb{R}^2$ and finitely many Reidemeister's moves in Fig. 3. (The move* R5 *is only for rigid graphs, the move* R5′ *is only for non-rigid graphs.)*

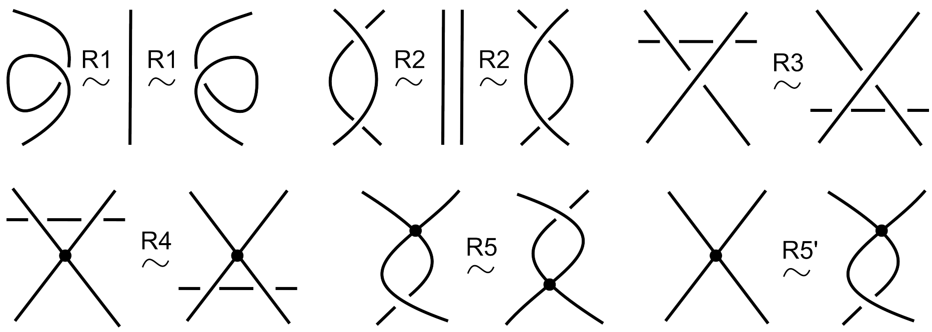

Fig. 3. Reidemeister moves on plane diagrams for any isotopy of spatial graphs

The move R4 is shown only for a degree 4 vertex, but also works for other degrees. The move R5 turns a small neighborhood of a vertex in the plane upside down, while the moves R5′ can arbitrarily reorder all edges at a vertex. Theorem 4 should formally include all symmetric images of moves in Fig. 3.

A standard way to encode a plane diagram of a knot is to use a Gauss code. The Gauss code of a link has several words and is sometimes called a Gauss paragraph [8]. We extend this classical concept to arbitrary spatial graphs.

Definition 5 *Let $D \subset \mathbb{R}^2$ be a plane diagram of a spatial graph G with vertices $A, B, C, \ldots$ We fix a direction on every edge of G and arbitrarily label all crossings of D by $1, 2, \ldots, n$. Then each crossing of D has the* sign *locally defined in Fig. 4. To get a* Gauss code *of D, we associate a single word W_{AB} to every directed edge (or a loop) of G from a vertex A to a vertex B as follows:*

• *the word W_{AB} starts with the letter A and finishes with the letter B;*

• *W_{AB} contains labels of all crossings in AB according to the direction of AB;*

• *if AB goes under another edge at a crossing i with a sign $\varepsilon \in \{\pm\}$ as in Fig. 4, we add the superscript ε to i and get the symbol i^ε with the sign ε in W_{AB}.*

The edges at each vertex A are clockwisely ordered in $\mathbb{R}^2$, so the code specifies a cyclic order of the words starting with A. The words might be written reversed.

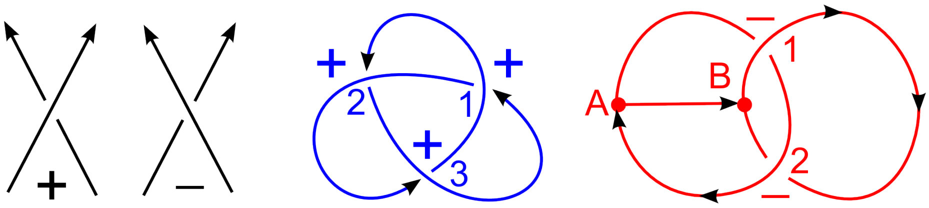

Fig. 4. Local rules for signs of crossings, signs in diagrams of directed graphs

If a graph G is a single circle as in the case of a knot, Definition 5 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 word *cyclically*. The plane diagram of the blue trefoil in Fig. 4 has the cyclic Gauss code $12^+31^+23^+$. The plane diagram of the red spatial graph in Fig. 4 has the Gauss code $\{AB,\, A1^-2A,\, B12^-B\}$ with the cyclic orders $AB \to A21^-A \to A1^-2A$, $B12^-B \to B2^-1B \to BA$. The edges $A1^-2A, B2^-1B, BA$ are reversed.

A Gauss code of any undirected graph depends on a choice of extra degree 2 vertices, directions of edges, an order of crossings. However, any Gauss code of G uniquely determines a plane diagram of G, hence the isotopy class of G.

The single cyclic word 12^+1^+2 does not encode any plane diagram. 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.

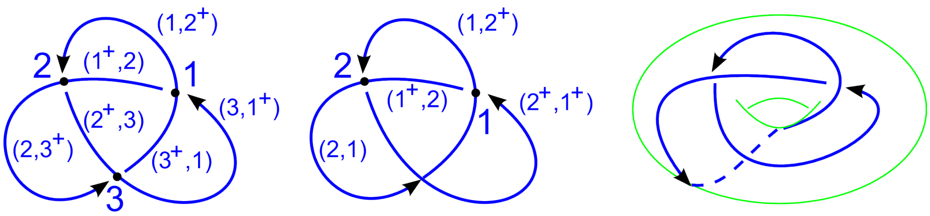

Fig. 5. Trefoil with 3 classical crossings, a diagram with 1 virtual, 2 classical crossings

This obstacle can be resolved if we draw a diagram on a surface as in Fig. 5, because we can hide a virtual crossing by adding a handle. A different approach is to embrace virtual crossings, which has led to the virtual knot theory.

3 Linear-Time Algorithm for Planarity of Gauss Codes

If we wish to study embedded graphs, not virtual, we need to recognize planarity of Gauss codes, namely determine if a Gauss code represents a plane diagram of a spatial graph. So we first introduce abstract Gauss codes in Definition 6 and then recognize their planarity in the general case of spatial graphs in Theorem 8.

Definition 6 *Let the alphabet consist of m letters $A, B, C, \ldots$ and $3n$ symbols i, i^+, i^-, $i = 1, \ldots, n$. An* abstract Gauss code *is a collection of words such that*

• *each word starts with a letter and finishes with a (possibly different) letter,*

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

Also each of the m letters defines a cyclic order of words that start or finish with this letter. The length $|W|$ *is the number of pairs of adjacent symbols in W, which equals the total number of symbols minus the number of words in W.*

The Gauss code of any plane diagram of a spatial graph G from Definition 5 satisfies the conditions above. Indeed, the letters $A, B, C, \ldots$ denote (projections of) vertices of G. Then an edge, say from A to B, contains crossings marked by i, i^+ or i^-. The clockwise order of edges around any vertex in the plane diagram of G defines the cyclic order of words (possibly reversed) starting with this vertex. If a component of G is a circle, we may remove its vertices of degree 2 and write only the remaining symbols as in the cyclic code $12^+31^+23^+$ of the trefoil.

Let us try to draw a plane diagram represented by an abstract Gauss code W. We can easily plot vertices $A, B, C, \ldots$ and crossings $1, 2, \ldots, n$. For any adjacent symbols in the code W, we should connect the corresponding vertices and crossings by a continuous arc in the plane. Since W also specifies the cyclic order of edges at each vertex, we may draw a diagram locally around each vertex, but arcs connecting vertices and crossings may intersect in the plane.

To avoid potential intersections, we shall draw a diagram not in the plane, but in the Carter surface defined below. We first introduce a combinatorial graph $G(W)$ describing the adjacency relations between symbols in W. Then we attach disks to $G(W)$ to get a surface containing a required diagram without self-intersections. The criterion of planarity will check if the resulting surface is S^2.

Definition 7 *Any abstract Gauss code W with m letters $A, B, C, \ldots$ and $2n$ symbols from $\{i, i^+, i^- \mid i = 1, \ldots, n\}$ gives rise to the combinatorial graph $G(W)$ with $m + n$ vertices labeled by $A, B, C, \ldots$ and $1, 2, \ldots, n$ (without signs).*

We connect vertices p, q by a single edge in $G(W)$ if p, q (possibly with signs) are adjacent symbols in the code 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, 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 Fig. 6:

• *at each of m vertices $A, B, C, \ldots$, say A, we turn to the next edge (in the graph $G(W)$ at A) from the (clockwise) order of words starting or finishing with A;*

• *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 $\varepsilon \in \{+, -\}$*

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

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

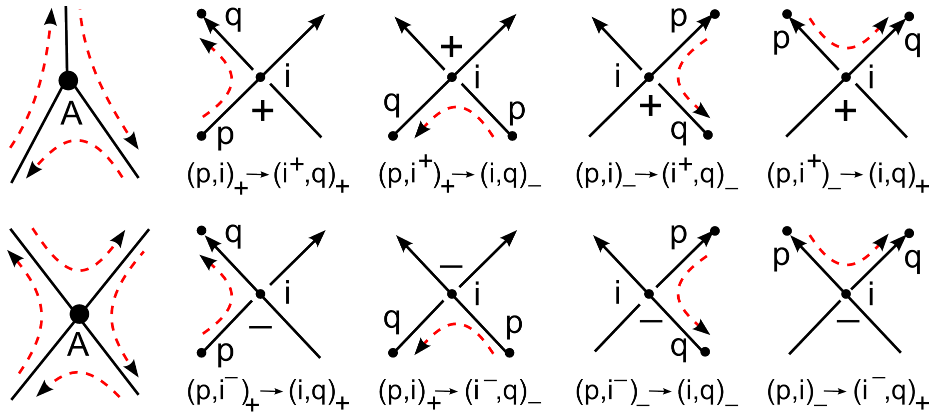

Fig. 6. A geometric interpretation of rules for turning left at crossings

The number of edges in the graph $G(W)$ equals the length $|W|$ of the code W. The rules for constructing cycles in Definition 7 geometrically mean that at each vertex or crossing we locally turn left to a unique edge. Hence the Carter surface is compact, orientable and has no boundary. If W is a Gauss code of a diagram $D \subset S^2$, then each disk is a face of D and the Carter surface is S^2.

For example, let us construct the Carter surface of the abstract Gauss code $W = 12^+1^+2$, whose plane diagram with one virtual crossing is in Fig. 7. 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 successive symbols in the Gauss 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 Fig. 7.

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 $(2, 1^+)_-$ we return to the first edge $(1, 2^+)_+$ by the same rule $(p, i^+)_\varepsilon \to (i, q)_{-\varepsilon}$ for $p = 2$, $i = 1$, $\varepsilon = -$, $q = 2^+$. So the first cycle consists of 2 edges $(12^+)_+$ and $(2, 1^+)_-$. The second cycle of 6 edges $(1^+, 2)_+ \to (2^+, 1^+)_+ \to (1, 2)_- \to (2^+, 1)_- \to (1^+, 2^+)_- \to (2, 1)_+$ is shown by a red dashed curve in Fig. 7. The resulting surface with 2 vertices, 4 edges, 2 faces has Euler characteristic $\chi = 2 - 4 + 2 = 0$ and should be a torus.

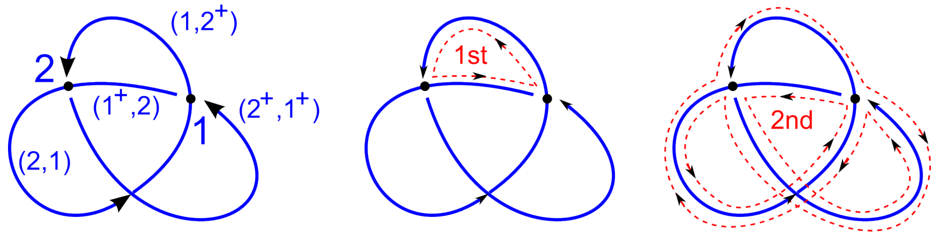

Fig. 7. Two red dashed cycles in the graph of the abstract Gauss code $W = 12^+1^+2$

In general, the *Euler characteristic* of a surface subdivided by a graph with $|V|$ vertices and $|E|$ edges into $|F|$ faces is defined by $\chi = |V| - |E| + |F|$ and is invariant up to homeomorphism. Any orientable connected compact surface of a genus g (the number of handles) with b boundary components has $\chi = 2-2g-b$. The following result extends [8, Algorithm 1.4] from links to spatial graphs.

Theorem 8 (planarity of Gauss codes of graphs) *Given an abstract Gauss code W of a length $|W|$, an algorithm of time complexity $O(|W|)$ can determine if the given code W represents a plane diagram of a spatial graph $G \subset \mathbb{R}^3$.*

Proof. The Carter surface of any abstract Gauss code W contains a diagram encoded by W due to the geometric interpretation of the rules in Fig. 6. This surface has the maximum Euler characteristic χ among all orientable connected compact surfaces S without boundary containing a diagram D encoded by W. 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 (with maximum $\chi = 1$) as in the Carter surface.

To decide the planarity of W, it remains to determine if the Carter surface of W is a sphere, 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 polygonal splitting from Definition 7. We have $m + n$ vertices, $|W|$ edges and the number of faces equal to the number of cycles. Hence we can compute $\chi = m + n - |W| + \#(\text{cycles})$ in linear time $O(|W|)$ by traversing the graph $G(W)$ according to the rules of Definition 7. □

4 Algorithm for Embedding a Spatial Graph in 3 Pages

In this section the prove main Theorem 10 using auxiliary Theorems 8 and 9.

Recall that a graph D is called *planar* if D can be embedded in $\mathbb{R}^2$. A *digraph* is a directed acyclic graph, possibly with undirected cycles, but without directed cycles. If we fix a vertical orientation on $\mathbb{R}^2$, then we can orient all edges of an embedded planar graph in the upward direction, which gives an *upward planar digraph*. Giordano et al. [4, Theorem 1] proves that there is a linear time algorithm to isotopically deform any upward planar diagraph into a 2-page topological embeddings with at most one bend per edge.

Theorem 9 *[4, 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.*

The planar graph D in the left hand side picture of Fig. 8 has no combinatorial 2-page embedding [1, section 5]. Two more pictures in Fig. 8 give an example how we can construct a path α that passes through each vertex once and intersects each edge at most once. By an isotopic deformation of $\mathbb{R}^2$ we can make the path α straight and get a required 2-page topological embedding of D.

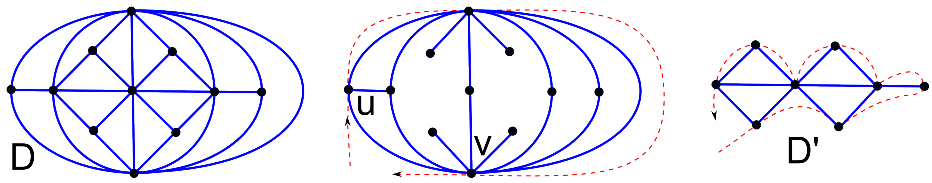

Fig. 8. A path α through vertices of the non-hamiltonian maximum planar graph

Theorem 10 *Given an abstract Gauss code W, an algorithm of time complexity $O(|W|)$ determines if W represents a plane diagram of a spatial 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 8 to determine if the code W represents a plane diagram D of a spatial graph G. If yes, we draw a 2-page embedding of the diagram $D \subset \mathbb{R}^2$ in linear time using Theorem 9.

We can upgrade the 2-page embedding of a small neighborhood of any crossing v in the diagram D to a 3-page embedding, where the 3rd page attached along α above the plane containing D. Fig. 9 shows these upgrades for 6 typical neighborhoods, other cases are symmetric. So we resolved the crossing v by pushing an arc into the 3rd page with at most 3 new points in the spine α.

After pushing short overcrossing arcs at all crossings of D into the 3rd page, we get a 3-page embedding of a spatial graph H with the same plane diagram D, hence H is isotopic to G. We need only a constant time per crossing, so $O(|W|)$ in total, for upgrading the 2-page embedding of D to a 3-page embedding of H.

Since the plane 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. The total number of intersections of the graph H with α is at most $8|W|$. □

5 Conclusion and Open Problems on Spatial Graphs

We have introduced new algorithmic problems of knot theory and spatial graphs to the computational topology community. The main results are the following.

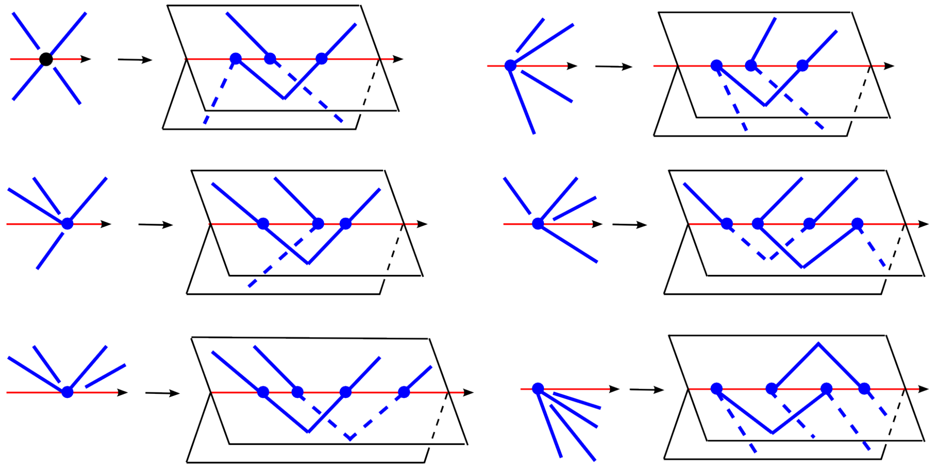

Fig. 9. Upgrading crossings to 3-page embeddings with at most 4 intersections

Theorem 8: a fast recognition of planarity for Gauss codes of spatial graphs.

Theorem 10: a practical linear time algorithm drawing a 3-page embedding of any spatial graph $G \subset \mathbb{R}^3$ starting from a Gauss code W of the graph G.

Here is the list of related open problems on spatial graphs for the future work.

• State and prove a criterion of planarity of Gauss codes of spatial graphs using combinatorial invariants like sums of signs similarly to [8, Theorem 3.6].

• Decide if the problem to find a 3-page embedding of a spatial graph $G \subset \mathbb{R}^3$ having the minimum number of intersections with the spine α is NP-hard.

• Design a polynomial time algorithm to solve the word problem for the semigroups RSG_n and NSG_n (equivalent to a classification of spatial graphs).

We are open to collaboration on the above problems and any related projects. The final version will be in the IEEE double-column style within 8 pages.

Acknowledgments. The author thanks any reviewers for helpful suggestions.

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Appendix: 3-page encoding of all spatial graphs

Finally, we highlight the following known advantages of 3-page embeddings over traditional representations such as plane diagrams or Gauss codes:

• Lemma 11 encodes a 3-page embedding by a single linear word, while plane diagrams are 2-dimensional, a Gauss code has a separate word for each edge;

• Theorem 12 decomposes any isotopy between 3-page embeddings of graphs into finitely many local relations between 3-page codes, while Reidemeister's moves or their analogs on Gauss codes involve distant parts of a graph or Gauss code.

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.

Lemma 11 *[7, Theorem 1.6a] Any 3-page embedding of a spatial graph G with vertices up to degree n can be encoded by a single 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 $i = 0, 1, 2$.*

Fig. 10 shows 12 local embeddings a_i, b_i, c_i, d_i, $i \in \{0, 1, 2\}$, that are sufficient for 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. Fig. 10 also has 3 embeddings for neighborhoods of degree 4 vertices denoted by x_i for simplicity.

To explain the 3-page encoding, we may 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.

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

Theorem 12 *[7, 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 spatial graphs with vertices of degree up to n. There is a linear time algorithm to determine if a given element belongs to the center of the semigroup.*

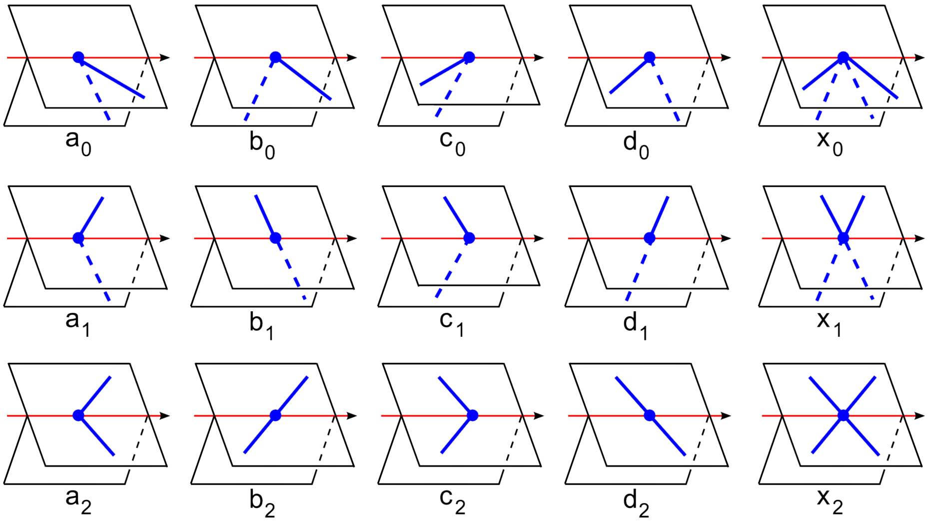

Fig. 10. Three-page embeddings of 15 generators for the semigroup in Theorem 10.

So two spatial 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. 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. 10. The empty word is the unit in the semigroups, but $a_i, c_i, x_{k,i}$ are not invertible. In the case of links for $n = 2$, the semigroup has only 48 relations below.

(1) $d_0 d_1 d_2 = 1$, $b_i d_i = 1 = d_i b_i$ for $i \in \{0,1,2\}$;

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

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

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

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.

The hard part of Theorem 12 says that any isotopy between spatial graphs decomposes into finitely many elementary isotopies. The 3-page encoding of all isotopy classes of spatial graphs has the crucial advantage over plane diagrams or Gauss codes. The Reidemeister moves on plane diagrams or Gauss codes are not local, while all elementary isotopies between 3-page embeddings are local.