On a complexity of a spatial graph (revised version)

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ABSTRACT

This note is a revised version of the research announcement [8] on a complexity of a spatial graph. In a research of proteins, molecules, or polymers, it is important to understand geometrically and topologically spatial graphs possibly with degree one vertices including knotted arcs. In this article, we introduce a concept of a complexity and related topological invariants for a spatial graph without degree one vertices, called the *warping degree* and related concepts of γ-, (γ, Γ)-*warping degrees* as well as the *unknotting number* and related concepts of γ-, Γ-, (γ, Γ)-*unknotting numbers* generalizing the usual unknotting number of a knot. These invariants are used to define geometric invariants for a spatial graph with degree one vertices, meaningful even for a knotted arc.

Keywords: Spatial graph, Unknotted graph, Warping degree, Complexity, Unknotting number

1. A spatial graph without degree one vertices and its diagram

For general references of knots, links and spatial graphs, we refer to [6]. First, we consider a finite graph Γ which does not have any vertices of degrees 0 and 1 and, for simplicity, has at most one component with vertices of degrees $\geqq 3$. A *spatial graph* of Γ is a topological embedding image G of Γ into $\mathbf{R}^3$ such that there is an orientation-preserving homeomorphism $h : \mathbf{R}^3 \to \mathbf{R}^3$ sending G to a polygonal graph in $\mathbf{R}^3$. We consider a spatial graph G by ignoring the degree two vertices which are useless in our argument. When Γ is a loop, G is called a *knot*, and it is *trivial* if it is the boundary of a disk in $\mathbf{R}^3$. When Γ is the disjoint union of finitely many loops, G is called a *link*, and it is *trivial* if it is the boundary of mutually disjoint disks. A spatial graph G is *equivalent* to a spatial graph G' if there is an orientation-preserving homeomorphism $h : \mathbf{R}^3 \to \mathbf{R}^3$ such that $h(G) = G'$. Let $[G]$ be the class of spatial graphs G' which are equivalent to G. It is well-known that two spatial graphs G and

G' are equivalent if and only if any diagram D_G of G is deformed into any diagram $D_{G'}$ of G' by a finite sequence of the *generalized Reidemeister moves*, where the moves necessary only for links are called the *Reidemeister moves* (cf. [6]). Let $[D_G]$ be the class of diagrams obtained from a diagram D_G of G by the generalized Reidemeister moves, which is identified with the class $[G]$.

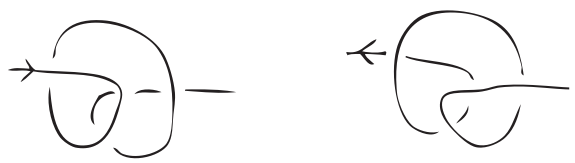

Figure 1: Monotone edge diagrams

2. Monotone diagram, warping degree and complexity

Our spatial graph G is obtained from a maximal tree T (containing all the vertices of degrees $\geqq 3$ of G) by adding the remaining edges or loops α_i $(i = 1, 2, \cdots, m)$. Clearly, $T = \emptyset$ if G is a link, and T is one vertex if G has just one vertex of degree $\geqq 3$. Let D be a diagram of G. Let DT and $D\alpha_i$ be the subdiagrams of D corresponding to T and α_i, respectively. The diagram D is a *based diagram* (on a *based tree* T) and denoted by $(D;T)$ if there are no crossing points of D belonging to DT. We can deform every diagram into a based diagram by a finite sequence of the generalized Reidemeister moves. Let $(D;T)$ be a based diagram of G with the remaining edges or loop diagrams $D\alpha_i$ $(i = 1, 2, \cdots, m)$. An edge diagram $D\alpha_i$ is *monotone* if there is an orientation on α_i such that a point going along the oriented diagram $D\alpha_i$ from the origin vertex meets first the upper crossing point at every crossing point (see Figure 1). A loop diagram $D\alpha_i$ is *monotone* if there is an orientation on α_i such that a point going along the oriented diagram $D\alpha_i$ from the vertex point (if α_i meets T) or a non-crossing point (if otherwise) meets first the upper crossing point at every crossing point. The based diagram $(D;T)$ is *monotone* if $D\alpha_i$ is monotone for every i and the diagram $D\alpha_i$ is upper than the diagram $D\alpha_j$ for any $j > i$ with respect to an oriented ordered sequence of $D\alpha_i$ $(i = 1, 2, \cdots, m)$. The *warping degree* $d(D;T)$ of a based diagram $(D;T)$ is the least number of crossing changes on the edge or loop diagrams $D\alpha_i (i = 1, 2, \cdots, m)$ needed to obtain a monotone diagram from $(D;T)$. For $T = \emptyset$, we denote $d(D;T)$ by $d(D)$. When the edges or loops α_i $(i = 1, 2, \cdots, m)$ are previpously oriented, we can also define the *oriented warping degree* $\vec{d}(D;T)$ (or $\vec{d}(D)$ for $T = \emptyset$) of D by considering only the crossing changes on the edge or loop diagrams $D\alpha_i$ $(i = 1, 2, \cdots, m)$ along the specified orientations. The *warping degree* $d(G)$ of G is the minimum of the warping degrees $d(D;T)$ for all based diagrams $(D;T) \in [D_G]$.

The *complexity* of a based diagram (D,T) is the pair $cd(D;T) = (c(D;T), d(D;T))$ together with the dictionary order. This notion was introduced in [7] for an oriented ordered link diagram. A. Shimizu also observed that the dictionary order on $cd(D;T)$ is equivalent to the numerical order on $c(D;T)^2 + d(D;T)$ by using the inequality

$d(D;T) \leqq c(D;T)$. The *complexity* $\gamma(G) = (c_\gamma(G), d_\gamma(G))$ of G is the minimum (in the dictionary order) of the complexities $cd(D;T)$ for all based diagrams $(D;T) \in [D_G]$, where the topological invariants $c_\gamma(G)$ and $d_\gamma(G)$ are called the *γ-crossing number* and the *γ-warping degree* of G, respectively. The minimal crossing number $c(G) = \min_{D\in[D_G]} c(D)$ of G has the inequality $c(G) \leqq c_\gamma(G)$. The following properties (1) and (2) on G give a reason why we call $\gamma(G)$ the complexity of G:

(1) *If* $d_\gamma(G) > 0$, *then there is a crossing change on* G *to obtain a spatial graph* G' *with* $\gamma(G') < \gamma(G)$. *The spatial graph* G *is equivalent to* G' *with a monotone diagram* $(D';T')$ *with* $c(D';T') = c_\gamma(G)$ *if and only if* $d_\gamma(G) = 0$.

(2) *If* $c_\gamma(G) > 0$, *then there is a spatial graph* G' *with* $c_\gamma(G') < c_\gamma(G)$ by any splice on G, *so that* $\gamma(G') < \gamma(G)$. *The crossing number* $c_\gamma(G) = 0$ *if and only if* $c(G) = 0$, *i.e.*, G *is equivalent to a graph in a plane.*

Similar notions around the complexity were earlier introduced by W. B. R. Lickorish and K. C. Millett in [9], S. Fujimura [3], T. S. Fung [4], M. Okuda [12] and M. Ozawa [13] as the ascending number of an oriented link, by the author in [7] as a notion of a complexity of an oriented link, and by A. Shimizu [14] as the minimum of the sum of two oriented warping degrees of a minimal crossing diagram of a knot. In particular, A. Shimizu characterized the alternating knot diagrams by establishing the inequality $\vec{d}(D) + \vec{d}(-D) \leqq c(D) - 1$ with $c(D)$ the crossing number of D where the equality holds if and only if D is an alternating diagram.

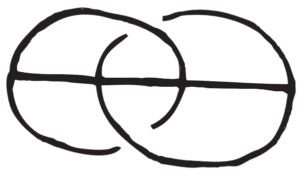

Figure 2: An unknotted plane graph with a Hopf constituent link

3. Uunknotting number

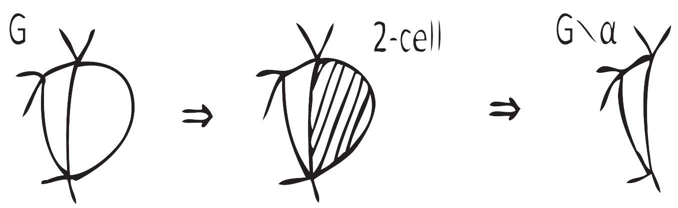

Figure 3: An edge reduction

A spatial graph G is *unknotted* if $d(G)=0$, and γ-*unknotted* if $d_\gamma(G)=0$. Let $\gamma(\Gamma)=(c_\gamma(\Gamma),d_\gamma(\Gamma))$ be the minimum of $\gamma(G)$ for all spatial graphs G of Γ. Then $d_\gamma(\Gamma)=0$. A spatial graph G is Γ-*unknotted* if G is a spatial graph of Γ with $\gamma(G)=\gamma(\Gamma)$. Then by definitions,

$$\text{“}\Gamma\text{-unknotted”} \Rightarrow \text{“}\gamma\text{-unknotted”} \Rightarrow \text{“unknotted”}.$$

A link L is unknotted if and only if L is a trivial link, and a spatial plane graph G is Γ-unknotted if and only if G is equivalent to a graph in a plane. A *constituent link* of G is a link contained in G. The spatial graph in Figure 2 is an unknotted but non-Γ-unknotted graph since it is a plane graph with a constituent Hopf link. In spite of the Conway-Gordon Theorem in [2] stating that every spatial 6-complete graph K_6 contains a non-trivial constituent link and every spatial 7-complete graph K_7 contains a non-trivial constituent knot, we have the following properties on unknotted graphs:

(1) *For every graph* Γ, *there are only finitely many unknotted graphs* G *of* Γ *up to equivalences.*

(2) *By a sequence of edge reductions illustrated in Figure 3, an unknotted connected graph* G *is deformed into a maximal tree.*

(3) *An unknotted connected graph* G *is equivalent to a trivial bouquet of circles after some edge contractions.*

As a corollary of (2), we see that *every edge of* G *is contained in a trivial constituent knot.* Let O be the set of unknotted graphs of Γ. Let O^G_γ be the set of unknotted graphs with monotone diagrams obtained by crossing changes from the based diagrams $(D;T)\in[D_G]$ with $cd(D)=\gamma(G)$. Let O_Γ be the set of Γ-unknotted spatial graphs. The sets O^G_γ and O_Γ may be disjoint in general. For example, the spatial graph G in Figure 2 has $O^G_\gamma\cap O_\Gamma=\emptyset$ since $\gamma(G)=(2,0)$, for G has a Hopf link as a constituent link, and O_Γ consists of only a graph G_0 in a plane with $\gamma(G_0)=(0,0)$, for the abstract graph Γ of G is a planar graph. This example motivates us to define the number

$$d^\Gamma_\gamma(G)=d_\gamma(G)+\rho(O^G_\gamma,O_\Gamma),$$

called the (γ,Γ)-*warping degree* of G, where $\rho(,)$ denotes the x-distance (i.e., Gordian distance) function on the spatial graphs of Γ. The *unknotting number* $u(G)$ and the Γ-*unknotting number* $u^\Gamma(G)$ of G are respectively defined by the identities:

$$u(G)=\rho(G,O), \text{and } u^\Gamma(G)=\rho(G,O_\Gamma).$$

Let $[D_G]_\gamma=\{(D;T)\in[D_G]\,|c(D;T)=c_\gamma(G)\}$. The γ-*unknotting number* $u_\gamma(G)$ and (γ,Γ)-*unknotting number* $u^\Gamma_\gamma(G)$ are defined by the identities:

$$u_\gamma(G)=\rho([D_G]_\gamma,O),$$
$$u^\Gamma_\gamma(G)=\rho([D_G]_\gamma,O_\Gamma).$$

We have the following theorem:

Theorem 2.1 The topological invariants $u(G)$, $u^{\Gamma}(G)$, $u^{\Gamma}_{\gamma}(G)$, $d(G)$, $u_{\gamma}(G)$ and $d^{\Gamma}_{\gamma}(G)$ satisfy the following inequalities and are mutually distinct topological invariants:

$$\begin{array}{ccccccc} u(G) & \leqq & u^{\Gamma}(G) & \leqq & u^{\Gamma}_{\gamma}(G) & \leqq & d^{\Gamma}_{\gamma}(G) \\ & & & & \vee\| & & \vee\| \\ & & & & u_{\gamma}(G) & \leqq & d_{\gamma}(G) \\ & & & & \vee\| & & \vee\| \\ & & & & u(G) & \leqq & d(G) \end{array}$$

For proof, the inequalities are easily obtained by definitions and the mutual distinctions of these invariants can be seen from several calculations on the concrete examples, which we suggest as follows:

The spatial graph G in Figure 2 has $u(G) = d(G) = u_{\gamma}(G) = d_{\gamma}(G) = 0$ and $u^{\Gamma}(G) = d^{\Gamma}_{\gamma}(G) = 1$. For the knot $K = 5_2$ which is a twist knot, we have $u(K) = u^{\Gamma}_{\gamma}(K) = d(K) = 1$ since T. S. Fung [4] and M. Ozawa [13] showed that a knot with $d = 1$ is characterized by a twist knot, and $d_{\gamma}(K) = d^{\Gamma}_{\gamma}(K) = 2$ by A. Shimizu [14]. For $K = 6_2$, we have $u(K) = u^{\Gamma}_{\gamma}(K) = 1$, but $d(K) = d^{\Gamma}_{\gamma}(K) = 2$ since K is not any twist knot. For $K = 10_8$, we have $u(K) = u^{\Gamma}(K) = 2 < u_{\gamma}(K) = u^{\Gamma}_{\gamma}(K) = 3$ by a result of S. A. Bleiler [1] and Y. Nakanishi [11]. The *Kinoshita θ-curve* in Figure 4 has $c_{\gamma}(G) = 7$ (cf. H. Moriuchi [10]) and $u(G) = u^{\Gamma}_{\gamma}(G) = 1 < d(G) = d^{\Gamma}_{\gamma}(G) = 2$. Also, we need the following result obtained by using a technique in [5]: *For every graph Γ and any integer $n \geqq 0$, there are infinitely many spatial graphs G of Γ such that*

$$u(G) = u^{\Gamma}(G) = u_{\gamma}(G) = u^{\Gamma}_{\gamma}(G) = d(G) = d_{\gamma}(G) = d^{\Gamma}_{\gamma}(G) = n.$$

Figure 4: Kinoshita's θ-curve

4. A spatial graph with degree one vertices

Let Γ be a finite graph with degree 1 vertices which has, for simplicity, just one connected component with vertices of degrees $\geqq 3$. Then spatial graphs of Γ are similarly considered. Let V be the set of degree one vertices of G. For the line segment $[a, b]$ between $a, b \in \mathbf{R}^3$ and $x \in G$, let $S_v(x) = [v, x] \cup (\bigcup_{v,v' \in V} [v, v'])$ be a star with origin v. Assume that $G_v(x) = G \cup S_v(x)$ is a spatial graph without degree one vertices for every $v \in V$ and $x \in G$. Then the *warping degree* $d(G,x)$ and the *unknotting number* $u(G,x)$ of (G,x) are defined by

$$d(G,x) = \max_{v \in V} d(G_v(x)) \text{ and } u(G,x) = \max_{v \in V} u(G_v(x)),$$

which are the *warping degree* and the *unknotting number* of G. When $x \in V$, we denote them by $d(G)$ and $u(G)$, respectively. An example is illustrated in Figure 5. In a similar way, the γ-*warping degrees* $d_\gamma(G,x)$, $d_\gamma(G)$, the (γ,Γ)-*warping degrees* $d_\gamma^\Gamma(G,x)$, $d_\Gamma(G)$, the γ-*unknotting numbers* $u_\gamma(G,x)$, $u_\gamma(G)$ and the Γ-*unknotting numbers* $u^\Gamma(G,x)$, $u^\Gamma(G)$ and the (γ,Γ)-*unknotting numbers* $u_\gamma^\Gamma(G,x)$, $u_\gamma^\Gamma(G)$ are defined. Different invariants taking the minimum or the average in place of the maximum are also defined.

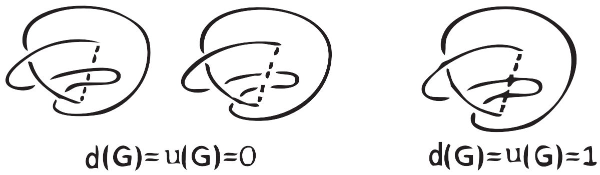

Figure 5: Knotted arcs

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