

On a complexity of a spatial graph

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Abstract: 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 γ -warping and warping degrees as well as the γ -unknotting and unknotting numbers generalizing the usual unknotting number of a knot. These invariants define geometric invariants for a spatial graph with degree one vertices, meaningful even for a knotted arc.

1 A spatial graph without degree one vertices and its diagram

For general references of knots, links and spatial graphs, we refer to [3]. First, we consider a compact polygonal 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 ≥ 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 $h : \mathbf{R}^3 \rightarrow \mathbf{R}^3$ 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 $h : \mathbf{R}^3 \rightarrow \mathbf{R}^3$ 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 we call the moves necessary for links the *Reidemeister moves* (cf. [3]). 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 $[G]$.

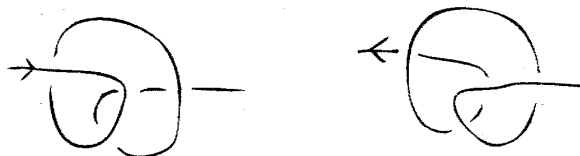


Figure 1: Monotone edge diagrams

2 A monotone diagram and complexity

Our spatial graph G is obtained from a maximal tree T (containing all the vertices of degrees ≥ 3 of G) by adding edges or loops α_i ($i = 1, 2, \dots, m$). Clearly, $T = \emptyset$ if G is a link, and T is

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one vertex if G has just one vertex of degree ≥ 3 . Let D be a diagram of G . The subdiagrams of D corresponding to T and α_i are called the *maximal tree diagram* DT and the *edge or loop diagram* $D\alpha_i$, respectively. Let $c_D(DT)$ be the number of crossing points of D belonging to DT . The diagram D is a *based diagram* (on T) and denoted by $(D; T)$ if $c_D(DT) = 0$. 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 , obtained from T by adding the edges or loops α_i ($i = 1, 2, \dots, m$). The 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). The 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 a non-crossing point always meets every upper crossing point first. The based diagram $(D; T)$ on T is *monotone* if $D\alpha_i$ is monotone for every i and contains the upper crossing point on every crossing point between $D\alpha_i$ and $D\alpha_j$ for any $j > i$ with respect to an oriented ordered sequence of $D\alpha_i$ ($i = 1, 2, \dots, m$). A similar notion of a monotone diagram was used by W. B. R. Lickorish and K. C. Millett in [5] for an oriented ordered link diagram. 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 $D\alpha_i$ ($i = 1, 2, \dots, m$) needed to obtain a monotone diagram from D . For $T = \emptyset$, we denote $d(D; T)$ by $d(D)$. When the edges or loops α_i ($i = 1, 2, \dots, m$) are preivously oriented, we can also define the *oriented warping degree* $d^+(D; T)$ (or $d^+(D)$ for $T = \emptyset$) of D by considering only the crossing changes on the oriented edge or loop diagrams $D\alpha_i$ ($i = 1, 2, \dots, m$). For an oriented knot diagram D , A. Shimizu in [7] established the inequality $d^+(D) + d^+(-D) \leq c(D) - 1$ with $c(D)$ the crossing number of D , where the equality holds if and only if D is an alternating diagram. 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 [4] 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 $d(D; T) \leq c(D; T)$. The *complexity* $\gamma(G)$ of G is the minimum (in the dictionary order) of the complexities $cd(D; T)$ for all based diagrams $(D; T) \in [D_G]$. This topological invariant $\gamma(G)$ is also denoted by $(c_\gamma(G), \delta_\gamma(G))$ where $c_\gamma(G)$ and $\delta_\gamma(G)$ 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 $c(G) \leq c_\gamma(G)$. The following properties (1) and (2) on G gives a reason why we call $\gamma(G)$ the complexity of G :

- (1) $c_\gamma(G) = 0$ if and only if $c(G) = 0$, i.e., G is equivalent to a graph in a plane. If $c_\gamma(G) > 0$, then there is a spatial graph G' with $c_\gamma(G') < c_\gamma(G)$ by a splice on G , so that $\gamma(G') < \gamma(G)$.
- (2) $\delta_\gamma(G) = 0$ if and only if G is equivalent to G' with a monotone diagram $(D'; T')$ with $c(D'; T') = c_\gamma(G)$. If $\delta_\gamma(G) > 0$, then by a crossing change on G there is a spatial graph G' with $\gamma(G') < \gamma(G)$.

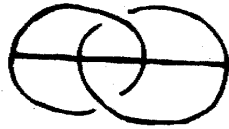


Figure 2: An unknotted plane graph with a Hopf constituent link

3 Warping degree and unknotting number

The *warping degree* $\delta(G)$ of G is the minimum of the warping degrees $d(D; T)$ for all based diagrams $(D; T) \in [D_G]$. Then $\delta(G)$ is a topological invariant and we have $\delta(G) \leq \delta_\gamma(G)$. A spatial graph G is *unknotted* if $\delta(G) = 0$, and γ -*unknotted* if $\delta_\gamma(G) = 0$. A link L is unknotted in this sense 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 . We note that there is an unknotted plane graph with a non-trivial constituent link. For example, the spatial plane graph G in Figure 2 has $\delta(G) = 0$, but has a Hopf constituent link and $\delta_\gamma(G) = 1$. We also note the Conway-Gordon Theorem in [1]: 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. Nevertheless, we have the following properties on an unknotted graph: *For every graph Γ , there are only finitely many unknotted graphs G of Γ up to equivalences. Further, we have the following properties (1) and (2) on an unknotted graph G : (1) By a sequence of edge reductions illustrated in Figure 3, G is deformed into a maximal tree. In particular, every edge of G is contained in a trivial constituent knot. (2) G is equivalent to a trivial bouquet of circles after some edge contractions.* Let $u(D)$ be the minimal number of crossing changes of a diagram D needed to obtain a diagram of an unknotted graph. The *unknotting number* $\mu(G)$ of G is the minimum of the numbers $u(D)$ for all diagrams $D \in [D_G]$. Let $u_\gamma(D)$ be the minimal number of crossing changes of a diagram D needed to obtain a diagram of a γ -unknotted graph. The γ -*unknotting number* $\mu_\gamma(G)$ of G is the minimum of the numbers $u_\gamma(D)$ for all diagrams $D \in [D_G]$. The topological invariants $\mu(G)$, $\mu_\gamma(G)$, $\delta(G)$ and $\delta_\gamma(G)$ are mutually distinct topological invariants satisfying the following square:

$$\begin{array}{ccc} \mu_\gamma(G) & \leq & \delta_\gamma(G) \\ \vee \parallel & & \vee \parallel \\ \mu(G) & \leq & \delta(G) \end{array}$$

For example, the spatial graph G in Figure 2 has $\mu(G) = \delta(G) = 0$ and $\mu_\gamma(G) = \delta_\gamma(G) = 1$. On the other hand, we see that *Kinoshita's θ -curve* in Figure 4 has $\mu(G) = \mu_\gamma(G) = 1 < \delta(G) = \delta_\gamma(G) = 2$ and $c(G) = 4 < c_\gamma(G) = 7$. The proof of this assertion is omitted here, but our proof uses H. Moriuchi's classification of algebraic tangles in [6]. Also, we can show the following result by using a technique in [2]: *For every graph Γ and any integer $n \geq 0$, there are infinitely many spatial graphs G of Γ such that $\mu(G) = \mu_\gamma(G) = \delta(G) = \delta_\gamma(G) = n$.*

4 A spatial graph with degree one vertices

Let Γ be a finite polygonal graph with degree 1 vertices, for simplicity, which has just one connected component with vertices of degrees ≥ 3 . A *spatial graph* of Γ is a topological embedding image G of Γ into $\mathbf{R}^3$ such that $h(G)$ is a polygonal graph in $\mathbf{R}^3$ for an orientation-preserving

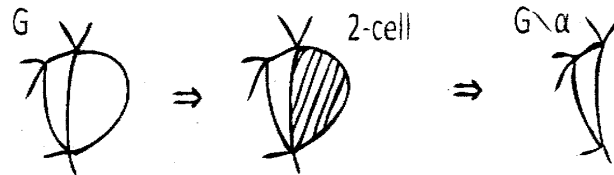


Figure 3: An edge reduction

Figure 4: Kinoshita's θ -curve

homeomorphism $h : \mathbf{R}^3 \rightarrow \mathbf{R}^3$. 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* $\delta(G, x)$ and the *unknotting number* $\mu(G, x)$ of (G, x) are defined by $\delta(G, x) = \max_{v \in V} \delta(G_v(x))$ and $\mu(G, x) = \max_{v \in V} \mu(G_v(x))$, which are called the *warping degree* and the *unknotting number* of G and denoted by $\delta(G)$ and $\mu(G)$, respectively, when $x \in V$. An example is illustrated in Figure 5. In a similar way, the γ -*warping degrees* $\delta_\gamma(G, x)$, $\delta_\gamma(G)$ and the γ -*unknotting numbers* $\mu_\gamma(G, x)$, $\mu_\gamma(G)$ are defined. Different invariants taking the minimum or the average in place of the maximum are also defined.

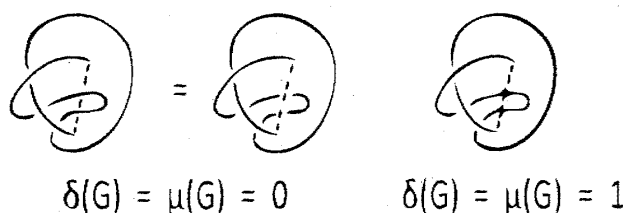


Figure 5: Knotted arcs

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