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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 \( \geq 3 \). A spatial graph of Γ is a topological embedding image \( G \) of Γ into \( \mathbb{R}^3 \) such that there is an orientation-preserving homeomorphism \( h : \mathbb{R}^3 \rightarrow \mathbb{R}^3 \) sending \( G \) to a polygonal graph in \( \mathbb{R}^3 \). 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 \( \mathbb{R}^3 \). 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 \( h : \mathbb{R}^3 \rightarrow \mathbb{R}^3 \) such that \( h(G) = G' \). Let \( [G] \) be the class of spatial graphs \( G' \) which are equivalent to \( G \).

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 \( \geq 3 \) of \( G \)) by adding edges or loops \( \alpha_i \) \( (i = 1, 2, \cdots, m) \). Clearly, \( T = \emptyset \) if \( G \) is a link, and \( T \) is...
one vertex if $G$ has just one vertex of degree $\geq 3$. Let $D$ be a diagram of $G$. The subdiagrams of $D$ corresponding to $T$ and $\alpha_i$ 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 $\alpha_i$ \((i = 1, 2, \cdots, m)\). The edge diagram $D\alpha_i$ is monotone if there is an orientation on $\alpha_i$ 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 $\alpha_i$ 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 $D\alpha_i$ \((i = 1, 2, \cdots, m)\). 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 $D\alpha_i$ \((i = 1, 2, \cdots, m)\) needed to obtain a monotone diagram from $D$. For $T = \emptyset$, we denote $d(D; T)$ by $d(D)$.

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 $(c_1(G), \delta_1(G))$ where $c_\gamma(G)$ and $\delta_\gamma(G)$ are called the $\gamma$-crossing number and the $\gamma$-warping degree of $G$, respectively. The minimal crossing number $c(G) = \min_{D \in [D_G]} c(D)$ of $G$ has the inequality $c(G) \leq c_1(G)$.

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 \( \gamma \)-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 \( \gamma \)-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 \( \Gamma \), there are only finitely many unknotted graphs \( G \) of \( \Gamma \) 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 \( \gamma \)-unknotted graph. The \( \gamma \)-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:

\[
\begin{align*}
\mu_\gamma(G) & \leq \delta_\gamma(G) \\
\forall \gamma & \mu(G) \leq \delta(G)
\end{align*}
\]

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 \( \theta \)-curve in Figure 4 has \( \mu(G) = \mu_\gamma(G) = 1 < \delta(G) = \delta_\gamma(G) = 2 \) and \( c_\gamma(G) = 4 < c_\epsilon(G) = 7 \). 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 \( \Gamma \) and any integer \( n \geq 0 \), there are infinitely many spatial graphs \( G \) of \( \Gamma \) such that \( \mu(G) = \mu_\gamma(G) = \delta(G) = \delta_\gamma(G) = n \).

4 A spatial graph with degree one vertices

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

![Figure 3: An edge reduction](image)
homeomorphism $h : \mathbb{R}^3 \rightarrow \mathbb{R}^3$. Let $V$ be the set of degree one vertices of $G$. For the line segment $[a, b]$ between $a, b \in \mathbb{R}^3$ 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 $\gamma$-warping degrees $\delta_\gamma(G, x)$, $\delta_\gamma(G)$ and the $\gamma$-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.

\[
\begin{align*}
\delta(G) &= \mu(G) = 0 \\
\delta(G) &= \mu(G) = 1
\end{align*}
\]

Figure 5: Knotted arcs

References


