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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 \( \gamma \)-warping and warping degrees as well as the \( \gamma \)-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 \( \Gamma \) 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 \( \Gamma \) is a topological embedding image \( G \) of \( \Gamma \) into \( \mathbb{R}^3 \) such that there is an orientation-preserving homeomorphism \( h: \mathbb{R}^3 \to \mathbb{R}^3 \) 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 \( \Gamma \) 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 \( \Gamma \) 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 \( h: \mathbb{R}^3 \to \mathbb{R}^3 \) 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 \( [G] \).

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

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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 \textit{maximal tree diagram} \( DT \) and the \textit{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 \textit{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 \textit{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 \textit{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 \textit{monotone} if \( \alpha_i \) 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 \( \alpha_i \). 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 \textit{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 \( d(D) \). When the edges or loops \( \alpha_i \) are previously oriented, we can also define the \textit{oriented warping degree} \( d^+(D; T) \) \((d^+(D) \text{ for } T = \emptyset)\) of \( D \) by considering only the crossing changes on the oriented edge or loop diagrams \( D\alpha_i \) \((i = 1, 2, \cdots, m)\). 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 \textit{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 \((D; T) \in [DG] \). 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 \textit{\( \gamma \)-crossing number} and the \textit{\( \gamma \)-warping degree} of \( G \), respectively. The minimal crossing number \( c(G) = \min_{D \in [DG]} c(D) \) 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 $\delta(G) \leq \delta_r(G)$. A spatial graph $G$ is unknotted if $\delta(G) = 0$, and $\gamma$-unknotted if $\delta_r(G) = 0$. 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 $\delta_r(G) = 1$. 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 $u_r(D)$ 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 $\mu_r(G)$ of $G$ is the minimum of the numbers $u_r(D)$ for all diagrams $D \in [D_G]$. The topological invariants $\mu(G)$, $\mu_r(G)$, $\delta(G)$ and $\delta_r(G)$ are mutually distinct topological invariants satisfying the following square:

\[
\begin{align*}
\mu_r(G) & \leq \delta_r(G) \\
\mu(G) & \leq \delta(G)
\end{align*}
\]

For example, the spatial graph $G$ in Figure 2 has $\mu(G) = \delta(G) = 0$ and $\mu_r(G) = \delta_r(G) = 1$. On the other hand, we see that Kinoshita’s $\theta$-curve in Figure 4 has $\mu(G) = \mu_r(G) = 1 < \delta(G) = \delta_r(G) = 2$ and $c(G) = 4 < c_r(G) = 7$. 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 $\mu(G) = \mu_r(G) = \delta(G) = \delta_r(G) = n$.

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
homeomorphism \( h : \mathbb{R}^3 \to \mathbb{R}^3 \). 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 \textit{warping degree} \( \delta(G, x) \) and the \textit{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 \textit{warping degree} and the \textit{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 \textit{\gamma-warping degrees} \( \delta_\gamma(G, x), \delta_\gamma(G) \) and the \textit{\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


