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COMPUTING THE WRITHE OF A KNOT

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ABSTRACT

We study the variation of the Tait number of a closed space curve according to its different projections. The results are used to compute the writhe of a knot, leading to a closed formula in case of polygonal curves.

Keywords: PL knot, Tait number, writhe, lattice knot.

1. Introduction

Since Crick and Watson's celebrated article in 1953, the local structure of DNA is well understood; its visualization as a double helix suggests the mathematical model of a ribbon in $\mathbb{R}^3$. But what about the global structure of DNA, that is, what kind of closed curve does the core of the ribbon form? It appears that these curves can show a great complexity (supercoiling) and are of central importance in understanding DNA (see [1] and [2]).

In 1961, Călugăreanu [3] made the following discovery: take a ribbon in $\mathbb{R}^3$, let Lk be the linking number of its border components, and Tw its total twist; then the difference $Lk - Tw$ depends only on the core of the ribbon. This real number, later called *writhe* by Fuller [4], is of great interest for biologists, as it gives a measure of supercoiling in DNA.

Several techniques have been developed to estimate the writhe of a given space curve, particularly by Aldinger, Klapper and Tabor [5]. The aim of the present paper is to give a new way of computing the writhe (see proposition 3). Moreover, this method will lead to a closed formula for the writhe of any polygonal space curve.

2. Definitions

Definition 1. *A polygonal knot (or PL knot) is the union of a finite number of* *segments in* $\mathbb{R}^3$*, homeomorphic to* S^1*. A point* $x \in K$ *is either a vertex or an interior point of* K*.*

Let us fix a PL knot K. Take a point ξ in S^2; let d_ξ be the oriented vector line containing ξ and $p_\xi\colon K \to \mathbb{R}^2$ the orthogonal projection with kernel d_ξ.

Definition 2. *The map* p_ξ *is a good projection (or generic projection) if, for all* v *in* $\mathbb{R}^2$*,* $p_\xi^{-1}(v)$ *is empty, one point, or two interior points of* K*.*

Clearly, the good projections form an open dense subset $\mathcal{O}_K$ of S^2; given $\xi \in \mathcal{O}_K$, we get a diagram of the PL knot K by pointing out which segment lies on the top of the other at double points, according to the orientation of d_ξ.

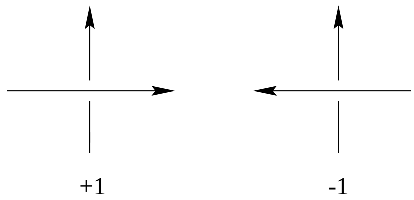

Fig. 1.

To each double point v of a diagram, it is possible to give a sign $s(v) = \pm 1$ by the following rule: we (temporarily) orientate K, and set $s(v) = +1$ if the oriented upper strand has to be turned counterclockwise to coincide with the lower one, $s(v) = -1$ in the other case (see figure 1). The sign obviously does not depend on the orientation of the knot.

Definition 3. *Let* K *be a PL knot and* $\xi \in \mathcal{O}_K$*; the Tait number of* K *relatively to* ξ *is the integer* $T_K(\xi) = \sum_v s(v)$*, where the sum runs through all double points of the diagram associated with* ξ*.*

Given K, let us define a function $T_K\colon S^2 \to \mathbb{R}$ by

$$T_K(\xi) = \begin{cases} T_K(\xi), & \text{if } \xi \in \mathcal{O}_K; \\ 0, & \text{otherwise.} \end{cases}$$

This function is not continuous, but it is integrable (see proposition 1).

Definition 4. *The writhing number (or writhe) of a PL knot* K *is the real number* $Wr(K) = \frac{1}{4\pi} \iint_{S^2} T_K(\xi)\, d\xi$*.*

Since $S^2 \backslash \mathcal{O}_K$ is of measure zero, we can extend the Tait number in any way without changing the value of the writhe; the first proposition will give a very natural way to do so.

The study of $T_K(\xi)$ requires one more object: the indicatrix of a knot, that we define now. Let K be a PL knot; an orientation of K allows us to number its segments $S_1, \ldots, S_n$. For all i, S_i determines a direction, that is, a point s_i in S^2. For $1 \leq i \leq n-1$, let Γ_i be the oriented arc of great circle on S^2 joining s_i to s_{i+1}, and Γ_n the one joining s_n to s_1. The union $\Gamma = \cup_{i=1}^{n} \Gamma_i$ is a closed oriented curve on S^2. Of course, the opposite orientation of K produces the antipodal curve $-\Gamma$.

Definition 5. *The (spherical) indicatrix I of a PL knot is the oriented curve of S^2 given by $I = \Gamma \cup -\Gamma$.*

It is important to notice that the indicatrix may run several times on a fixed arc of great circle.

We can easily check that p_ξ is locally injective if and only if $\xi \in S^2 \backslash I$.

3. The Results

Proposition 1. *If ξ and $\xi\prime$ in $\mathcal{O}_K$ belong to the same connected component of $S^2 \backslash I$, then $T_K(\xi) = T_K(\xi\prime)$.*

Remarks.

- It is possible to extend the definition of the Tait number to all locally injective projections in a very natural way by setting $T_K(\xi) = T_K(A)$, where $T_K(A)$ is the value of the Tait number on the connected component A of $S^2 \backslash I$ containing ξ.
- This proposition directly implies that T_K is integrable on S^2.

Proof. Let Ω be a connected component of $S^2 \backslash I$, and $\xi, \xi\prime \in \Omega \cap \mathcal{O}_K$. If $\Omega \cap \mathcal{O}_K$ were connected, a simple continuity argument would do, but this is not the case in general. Indeed, $\Omega \backslash (\Omega \cap \mathcal{O}_K)$ is the union of a finite number of curves on S^2 that can separate ξ and $\xi\prime$. We need to describe all these curves, and check that crossing them does not change the value of T_K.

Let us first consider the non-generic projections that do not send coplanar segments onto the same line; we call $C_{(m,n)}$ the set of points $\xi \in S^2$ such that there exists $v \in \mathbb{R}^2$ with $p_\xi^{-1}(v)$ consisting of m interior points and n vertices of K. It is easy to check that if $m \geq 4$ or $n \geq 2$, $C_{(m,n)}$ is a finite number of points, as well as $C_{(2,1)}$ and $C_{(3,1)}$. Since $C_{(0,0)}$, $C_{(1,0)}$ and $C_{(2,0)}$ are the constituents of $\mathcal{O}_K$, the only potential trouble makers are $C_{(1,1)}$ and $C_{(3,0)}$ (see figure 2).

We also have to study projections sending $k \geq 2$ coplanar (pairwise non-adjacent) segments of K onto a line d of the plane. Let $D_{(m,n)}$ be the set of $\xi \in S^2$ such that there exists $v \in d$ with $p_\xi^{-1}(v)$ consisting of m interior points and n vertices of K. This time, only $D_{(0,0)}$, $D_{(0,1)}$ and $D_{(1,0)}$ need to be considered.

Thus, there are five types of non-generic projections that can separate ξ and $\xi\prime$; they are illustrated in figure 2.

We now study $\Delta T = T_K(\eta) - T_K(\eta\prime)$, where η and $\eta\prime$ are good projections on each side of a curve in S^2 formed by one type of non-generic projection. Crossing $C_{(1,1)}$ (resp. $C_{(3,0)}$) corresponds to the second (resp. third) Reidemeister move; the Tait number being unchanged by these transformations, the first two cases are

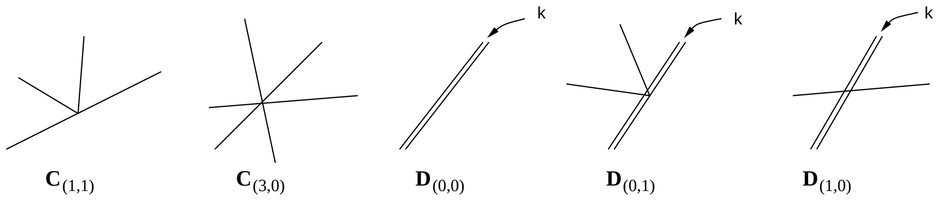

Fig. 2.

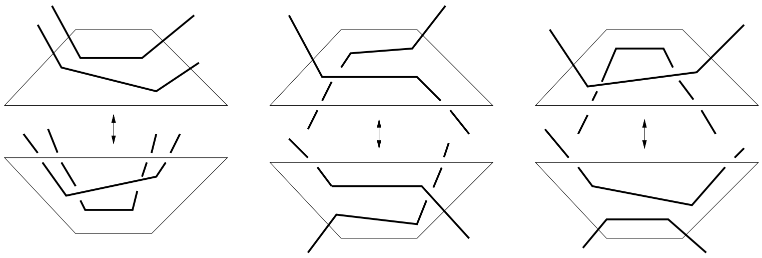

Fig. 3.

settled. It is trivial that $\Delta T = 0$ for $D_{(1,0)}$, while $D_{(0,1)}$ can be seen as k second Reidemeister moves.

It remains to show that $\Delta T = 0$ for $D_{(0,0)}$. If $k = 2$, all the possible cases are described in figure 3; each time, $\Delta T = 0$. For $k \geq 3$, the segments being pairwise non-adjacent, we can apply the same argument (k-1) times. This concludes the proof. □

What about the behavior of $T_K(\xi)$ when ξ crosses the indicatrix? Let α be an open segment of the indicatrix I on S^2, p_1 and p_2 two distinct points on α. Let n be the algebraic number of times that the indicatrix runs from p_1 to p_2. We will say that $\xi \in S^2 \backslash \alpha$ is to the north of α if $(p_1 \times p_2) \cdot \xi$ is strictly positive, to the south if it is strictly negative.

Proposition 2. *Let Ω_0 be the component of $S^2 \backslash I$ to the south of α, Ω_1 to the north; then: $T_K(\Omega_1) = T_K(\Omega_0) + n$.*

Proof. To simplify the exposition, we will give the demonstration only when α is covered once by the indicatrix.

Since K is polygonal, I is the union of a finite number of arcs of great circles; α is an open arc of great circle produced by two adjacent segments A and B of K (we will say: the site AB). Let U be an open path-connected subset of S^2 such that $U \backslash (U \cap \alpha) \subset \mathcal{O}_K$, and let us take $\xi_0 \in \Omega_0 \cap U, \xi_1 \in \Omega_1 \cap U$, c a path in U joining ξ_0 to ξ_1, crossing α at ξ (see figure 4). Since the indicatrix runs only once through

α and since $Im(c)\backslash\xi \subset \mathcal{O}_K$, the site AB alone influences the variation ΔT of the Tait number along c.

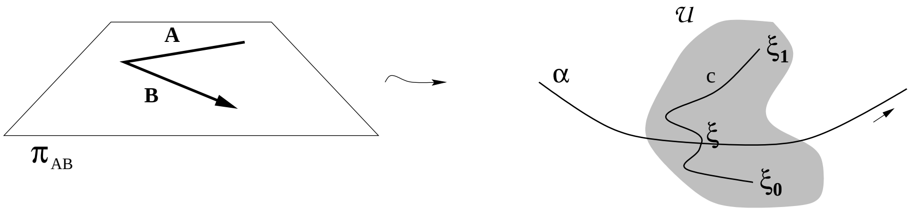

Fig. 4.

Thus, we have to look at the site projected by p_{ξ_0} and by p_{ξ_1}, and check that $T(\xi_1) = T(\xi_0) + 1$.

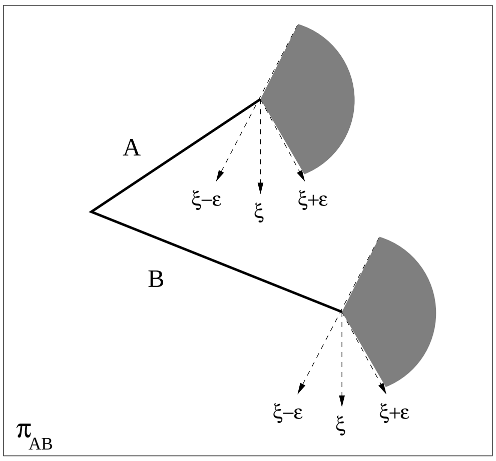

Fig. 5.

Let $N =]\xi - \epsilon; \xi + \epsilon[$ be a neighborhood of ξ in α such that the indicatrix travels only once along N. One or several segments adjacent to A or B can remain in the plane π_{AB} generated by A and B, but these segments lie in the shaded area in figure 5. Indeed, any segment outside the shaded area would make the indicatrix cover N one more time.

Clearly, the transformation illustrated in figure 6 does not change $T(\xi_0)$ and $T(\xi_1)$; therefore, we only need to consider the case where the segments adjacent to A and B leave the plane π_{AB}.

Let us check all the different possibilities. By proposition 1, the four cases illustrated in figure 7 are sufficient. They correspond to the first Reidemeister

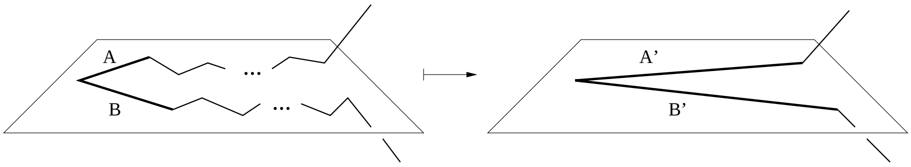

Fig. 6.

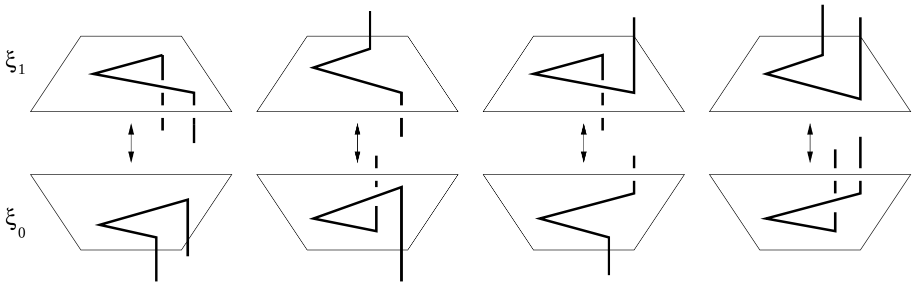

Fig. 7.

move, and we see that $T(\xi_1) = T(\xi_0) + 1$. □

Corollary. *Let $\xi, \xi\prime \in S^2 \backslash I$; then $T_K(\xi) = T_K(\xi\prime) + n$, where n stands for the intersection number of the indicatrix with a path joining ξ to $\xi\prime$.* □

The previous results were stated for PL knots; nevertheless, they remain true for a wider class of knots.

Definition 6. *A piecewise C^2 knot is the image of a closed space curve $\gamma \colon [0;1] \to \mathbb{R}^3$ twice continuously differentiable everywhere except on a finite number of points, satisfying for all $t_0 \in [0;1]$:*

(a) $\lim_{t \to t_0^+} \dot{\gamma}(t)$ *and* $\lim_{t \to t_0^-} \dot{\gamma}(t)$ *exist and are non-zero;*
(b) $\lim_{t \to t_0^+} \frac{\dot{\gamma}(t)}{||\dot{\gamma}(t)||} \neq - \lim_{t \to t_0^-} \frac{\dot{\gamma}(t)}{||\dot{\gamma}(t)||}$.

The indicatrix of a piecewise C^2 knot K is defined in the obvious way, and it is always possible to approach K with a sequence $\{K_n\}$ of PL knots such that $I_{K_n} \to I_K$. Hence, proposition 1 and 2 are true for piecewise C^2 knots, as well as the corollary.

Illustration. The picture shown on figure 8 was obtained by Akos Dobay at the University of Lausanne. It represents S^2 via cylindrical coordinates with 360×900 evaluations of the function T_K associated with a given smooth trefoil knot. For this

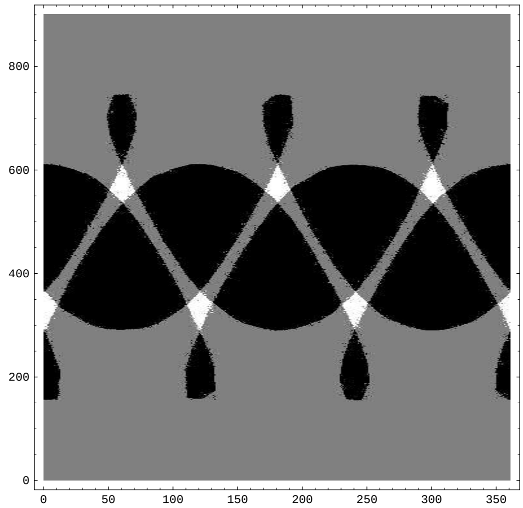

Fig. 8.

particular space curve, these calculations provide a kind of "experimental check" of our results.

4. The Writhe of a Knot

Let K be a piecewise C^2 knot in $\mathbb{R}^3$; since $T_K(\xi) = T_K(-\xi)$ for all ξ in $S^2 \backslash I$,

$$Wr(K) = \frac{1}{4\pi} \iint_{S^2} T_K(\xi)\, d\xi = \frac{1}{2\pi} \iint_{\frac{1}{2}S^2} T_K(\xi)\, d\xi.$$

By the corollary, we get the following formula, related to proposition 4 from Aldinger *et al.*:

Proposition 3. *Let K be a piecewise C^2 knot, I its indicatrix, $A_0, A_1, \ldots, A_r$ the connected components of a hemisphere minus I, and $T_K(\xi_0)$ the Tait number of K relatively to some $\xi_0 \in A_0$. Then, the writhe of K is given by*

$$Wr(K) = T_K(\xi_0) + \frac{1}{2\pi} \sum_{i=1}^{r} n_i \cdot area(A_i),$$

where n_i stands for the intersection number of the indicatrix with a path joining A_0 to A_i. □

Let us now suppose that K is a PL knot. In this case, the A_i are domains of S^2 delimited by arcs of great circles, that is, geodesics. By Gauss-Bonnet: $area(A_i) = 2\pi - \sum_j \theta_{ij}$, where the θ_{ij} are the exterior angles of A_i (see figure 9). Given K,

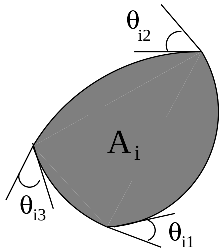

Fig. 9.

the computation of these angles is very easy. With the notations of the previous proposition, we get:

Proposition 4. *The writhe of a PL knot K is given by*

$$Wr(K) = T_K(\xi_0) + \frac{1}{2\pi} \sum_{i=1}^{r} n_i \cdot (2\pi - \sum_j \theta_{ij}). \qquad \square$$

For lattice knots, the calculation is immediate.

Definition 6. *A lattice knot is a PL knot on a cubic lattice in* $\mathbb{R}^3$.

Let K be a lattice knot; its indicatrix divides a hemisphere into four connected components $A_1, \ldots, A_4$, each of area $\frac{\pi}{2}$. Hence:

$$Wr(K) = \frac{1}{2\pi} \sum_{i=1}^{4} T_K(A_i) \cdot \frac{\pi}{2} = \frac{T_K(A_1) + T_K(A_2) + T_K(A_3) + T_K(A_4)}{4}.$$

Using only the first proposition, we have proved:

Proposition 5. *If K is a lattice knot, then* $4 \cdot Wr(K)$ *is an integer.* $\square$

Furthermore, using the second proposition, it is an easy exercise to implement a program computing the writhe, given a diagram of the lattice knot.

Final Remark

The average crossing number of a PL knot K is defined by

$$A(K) = \frac{1}{4\pi} \iint_{S^2} |T_K(\xi)| \, d\xi.$$

Our method also applies to the computing of this number, leading to a closed formula. Here, all the curves on S^2 corresponding to the second Reidemeister move have to be taken into account, as well as the indicatrix I.

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