Computing the Writhing Number of a Polygonal Knot *

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Abstract

The writhing number measures the global geometry of a closed space curve or knot. We show that this measure is related to the average winding number of its Gauss map. Using this relationship, we give an algorithm for computing the writhing number for a polygonal knot with n edges in time roughly proportional to $n^{1.6}$. We also implement a different, simple algorithm and provide experimental evidence for its practical efficiency.

Keywords. Computational topology, differential geometry, knots, Gauss maps, winding number, algorithms, implementation, proteins.

1 Introduction

The writhing number is an attempt to capture the physical phenomenon that a cord tends to form loops and coils when it is twisted. We model the cord by a knot, which in this paper is, by definition, an oriented closed curve in three-dimensional space. We consider its two-dimensional family of parallel projections. In each projection, we count $+1$ or -1 for each crossing depending on whether the overpass requires a counterclockwise or a clockwise rotation to align with the underpass. The writhing number is then the signed number of crossings averaged over all parallel projections. It is a conformal invariant of the knot and useful as a measure of its global geometry.

The writhing number attracted much attention after its relationship with the linking number, expressed by the White formula, was discovered independently by Călugăreanu [6], Fuller [15], Pohl [21], and White [26]:

$$Lk = Tw + Wr. \tag{1}$$

Here Lk is the linking number between the two boundary curves of a closed ribbon in space, Tw is its twisting number, and Wr is the writhe of the axis of the ribbon. A small subset of the mathematical literature on the subject can be found in [2, 14]. Besides the mathematical interest, the White Formula and the writhing number have received attention both in physics and in biochemistry [12, 17, 20, 23]. For example, they are relevant in understanding the various geometric conformations we find for circular DNA in solutions, as illustrated in Figure 1 taken from [5]. By representing

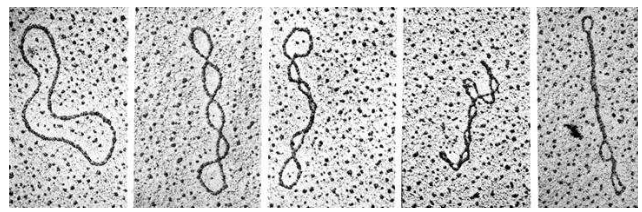

Figure 1: Circular DNAs take on different supercoiling conformations in solutions.

DNA as a ribbon, the writhing number of its axis measures the amount of supercoiling, which characterizes some of the DNA's chemical and biological properties [3].

This paper studies algorithms for computing the writhing number of a polygonal knot. Section 2 introduces background work and states our results. Section 3 relates the writhing number of a knot with the winding number of its Gauss map. Section 4 shows how to compute the writhing number in time less than quadratic in the number of edges of the knot. Section 5 discusses a simpler sweep-line algorithm and presents initial experimental results. Section 6 concludes the paper.

2 Prior and New Work

In this section, we formally define the writhing number of a knot and review prior algorithms used to compute or approximate that number. We conclude by presenting our results.

Definitions. A *knot* is a continuous injection $K : \mathbb{S}^1 \to \mathbb{R}^3$ or, equivalently, an oriented closed curve embedded in three-dimensional real space. We use the two-dimensional sphere of directions, $\mathbb{S}^2$, to represent the family of parallel projections in $\mathbb{R}^3$. Given a knot K and a direction $z \in \mathbb{S}^2$, the projection of K is a possibly self-intersecting, oriented closed curve in a plane normal to z. We assume z to be generic, that is, each crossing of K in the direction z is simple and identifies two oriented intervals along K, of which the one closer to the viewer is the *overpass* and the

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other is the *underpass*. We count the crossing as $+1$ if we can align the two orientations by rotating the overpass in a counterclockwise order by an angle between 0 and π. Similarly, we count the crossing as -1 if the necessary rotation is in a clockwise order. Both cases are illustrated in Figure 2. The *Tait* or *directional writhing number* of K

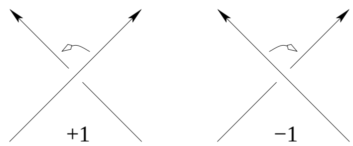

Figure 2: The two types of crossings when two oriented intervals intersect.

in the direction z, denoted as $Dw(z)$, is the sum of crossings counted as $+1$ or -1 as explained. The *writhing number* is the directional writhing number, averaged over all directions $z \in \mathbb{S}^2$,

$$(2) \qquad Wr = \frac{1}{4\pi} \int_{\mathbb{S}^2} Dw(z)\ \mathrm{d}z.$$

We note that a crossing in the projection along z also exists in the opposite direction, along $-z$, and that it has the same sign. Hence $Dw(z) = Dw(-z)$, which implies that the writhing number can also be obtained by averaging the directional writhing number over all points of the projective plane or, equivalently, over all antipodal points pairs $\{z, -z\}$ of the sphere.

Computing the writhing number. Several approaches to computing or estimating the writhing number of a smooth knot have been developed. Consider a path-length parameterization $K : \mathbb{S}^1 \to \mathbb{R}^3$, and use K_t and T_t to denote the position and the unit tangent vectors for $t \in \mathbb{S}^1$. The following double integral formula for the writhing number can be found in [21, 24]:

$$(3) \quad Wr = \frac{1}{4\pi} \int_{\mathbb{S}^1} \int_{\mathbb{S}^1} \frac{\langle T_t \times T_s, K_t - K_s \rangle}{\|K_t - K_s\|^3}\ \mathrm{d}t\ \mathrm{d}s.$$

If the smooth knot is approximated by a polygonal knot, we can turn the right hand side of (3) into a double sum and thus approximate the writhing number of the smooth knot [4, 20]. This can also be done in a way such that the double sum gives the exact writhing number of the polygonal knot [18, 25].

Alternatively, we may base the computation of the writhing number on the directional version of the White formula, $Lk = Dw(z) + Tw(z)$ for $z \in \mathbb{S}^2$. We get (1) by integrating over $\mathbb{S}^2$ and noting that the linking number does not depend on the direction. This implies

$$\begin{aligned} Wr &= Lk - Tw \\ (4) \qquad &= Dw(z) + Tw(z) - \frac{1}{4\pi} \int_{\mathbb{S}^2} Tw(x)\ \mathrm{d}x. \end{aligned}$$

Expressions for the directional and the (average directional) twisting numbers that depend on the second knot nearby K can be found in [18]. Le Bret [19] suggests to fix a direction z and define the second knot such that in the projection it runs always to the left of K. In this case we have $Tw(z) = 0$ and the writhing number is the directional writhing number for z minus the twisting number.

A third approach to computing the writhing number is based on a result by Cimasoni [10], which states that the writhing number is the directional writhing number for a fixed direction z, plus the average deviation of the other directional writhing numbers from $Dw(z)$. By observing that $Dw(x)$ is the same for all directions x in a cell C of the decomposition of $\mathbb{S}^2$ formed by the Gauss maps T and $-T$, we get

$$(5) \quad Wr = Dw(z) + \frac{1}{4\pi} \sum_C [Dw_C - Dw(z)] A_C,$$

where Dw_C is $Dw(x)$ for any one point x in the interior of C, and A_C is the area of C.

If applied to a polygonal knot, all three algorithms take time at least proportional to the square of the number of edges in the worst case.

Our results. We present two new results. The first can be viewed as a variation of (4) and a strengthening of (5). First we need some notation. For a non-critical direction $x \in \mathbb{S}^2$, let $w(x)$ be its winding number with respect to T and $-T$. As explained in Section 3, this means that T and $-T$ wind $w(x)$ times around x.

THEOREM A. For a knot K and a direction z, we have

$$Wr = Dw(z) - w(z) + \frac{1}{4\pi} \int_{\mathbb{S}^2} w(x)\ \mathrm{d}x.$$

Observe the similarity of this formula with Equation (4), which suggests that the winding number can be interpreted as the directional twisting number for a special second knot constructed nearby K. We will prove Theorem A in Section 3. We will also extend the relation in Theorem A to open knots and give an algorithm that computes the average winding number in time proportional to the number of edges. Our second result is an algorithm that computes the directional writhing number in time less than quadratic in the number of edges.

THEOREM B. Given a polygonal knot K with n edges and a direction $z \in \mathbb{S}^2$, $Dw(z)$ can be computed in time $\mathrm{O}(n^{1.6+\varepsilon})$, where ε is an arbitrarily small positive constant.

Theorems A and B imply that the writhing number for a polygonal knot can be computed in time $\mathrm{O}(n^{1.6+\varepsilon})$. As

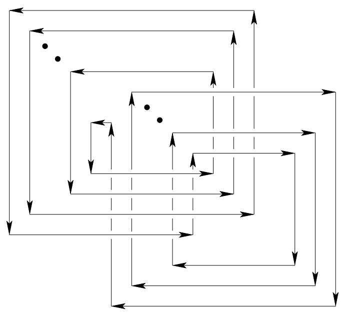

Figure 3: A knot whose directional writhing number is quadratic in the number of edges.

shown in Figure 3, the number of crossings in a projection can be as large as quadratic in n. The sub-quadratic running time is achieved because the algorithm avoids looking at each crossing individually. We also present a simpler sweep-line algorithm that looks at each crossing individually and therefore does not achieve the worst-case running time of the algorithm in Theorem B. It is, however, fast when there are few crossings.

3 Writhing and Winding

In this section, we develop our geometric understanding of the relationship between the writhing number of a knot and the winding number of its Gauss map. We describe the Gauss map as the curve of critical directions, prove Theorem A, and give a fast algorithm for computing the average winding number.

Critical directions. We specify a polygonal knot K by the cyclic sequence of its vertices, $p_0, p_1, \ldots, p_{n-1}$. We use indices modulo n and write $t_i = (p_{i+1} - p_i)/\|p_{i+1} - p_i\|$ for the unit vector along the edge $p_i p_{i+1}$. Note that t_i is also a direction in $\mathbb{R}^3$ and a point in $\mathbb{S}^2$. Any two consecutive points t_i and t_{i+1} determine a unique arc, which, by definition, is the shorter great circle piece that connects them. The cyclic sequence $t_0, t_1, \ldots, t_{n-1}$ thus defines an oriented closed curve T in $\mathbb{S}^2$. We also need the antipodal curve, $-T$, which is the central reflection of T through the origin.

The directions y on T and $-T$ are critical, in the sense that the directional writhing number changes when we pass through y along a generic path in $\mathbb{S}^2$, and these are the only critical directions [10]. It is clear that y is critical only if it is parallel to a line that passes through a vertex p_i and a point on an edge $p_j p_{j+1}$ of the knot. There are $n(n-2)$ vertex-edge pairs defining the same number of great circles in $\mathbb{S}^2$. First we note that only n of these great circles actually carry critical points, namely the great circles that correspond to $j = i+1$. The reason for this is shown in Figure 4, where we see that the writhing number does not change

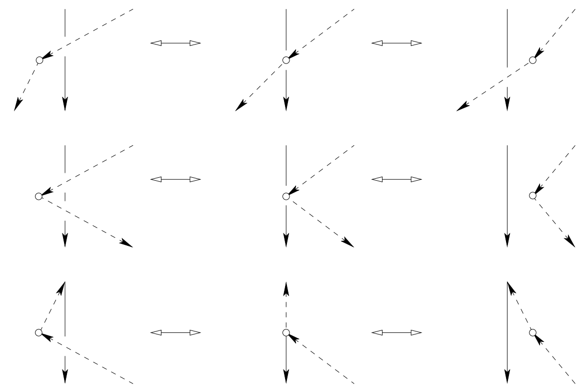

Figure 4: Three cases in sliding the viewpoint sideways over the great circle of directions defined by the hollow vertex and the solid edge. The directional writhing number changes only in the third case.

unless p_i is separated from $p_j p_{j+1}$ by only one edge along the knot. Second, we observe that the subset of directions along which p_i projects onto $p_{i+1}p_{i+2}$ is the arc $t_i u_i$ from t_i to the direction $u_i = (p_{i+2} - p_i)/\|p_{i+2} - p_i\|$ in $\mathbb{S}^2$, and symmetrically the arc $-t_i u_i$ from $-t_i$ to $-u_i$. The subset of directions along which p_{i+2} projects onto $p_i p_{i+1}$ are the arcs $u_i t_{i+1}$ and $-u_i t_{i+1}$. The points t_i, u_i, and t_{i+1} lie on a common great circle and u_i lies on the arc $t_i t_{i+1}$. This implies that the concatenation of $t_i u_i$ and $u_i t_{i+1}$ is the arc $t_i t_{i+1}$, and that of $-t_i u_i$ and $-u_i t_{i+1}$ is the arc $-t_i t_{i+1}$. It follows that T and $-T$ indeed comprise all critical directions.

Decomposition. The curves T and $-T$ are both oriented, which is essential. We say a direction $x \in \mathbb{S}^2$ lies to the *left* of an oriented arc uv if it lies in the open hemisphere locally to the left of the oriented great circle that contains uv. Equivalently, x sees that great circle oriented in a counterclockwise order. If x passes from the left of an arc uv of T to its right, then we either lose a positive crossing (as in the third row of Figure 4), or we pick up a negative crossing. Either way the directional writhing number decreases by one. This motion corresponds to $-x$ passing from the right of the arc $-uv$ of $-T$ to its left. Since the directional writhing numbers at x and $-x$ are the same, this implies that also in the opposite view we decrease the directional writhing number by one. In other words, if x moves from the left of an arc of $-T$ to its right then the effect on the directional writhing number is the opposite from what it is for an arc of T. These simple rules allow us to keep track of the directional writhing number while moving around in $\mathbb{S}^2$. The curves T and $-T$ decompose $\mathbb{S}^2$ into cells within which the directional writhing number is invariant. We can thus rewrite

Equation (2) as

$$Wr = \frac{1}{4\pi} \sum_C Dw_C A_C,$$

where the sum ranges over all cells C of the decomposition, and Dw_C is the directional writhing number of any one point in the interior of C. Equation (5) of Cimasoni can now be obtained by subtracting $Dw(z)$ from Dw_C inside the sum and adding it outside the sum. This reformulation provides an algorithm for computing the writhing number.

`Step 1.` Compute $Dw(z)$ for an arbitrary but fixed direction z.

`Step 2.` Construct the decomposition of $\mathbb{S}^2$ into cells, label each cell C with $Dw_C - Dw(z)$, and form the sum as in Equation (5).

The running time for Step 2 is at least proportional to n^2 in the worst case as there can be quadratically many cells. We improve the running time to $O(n)$ and, at the same time simplify the algorithm. First we prove Theorem A.

Winding numbers. We now introduce a function w over $\mathbb{S}^2$ that may be different from Dw but changes in the same way. In other words, $w(x) - w(z) = Dw(x) - Dw(z)$ for all $x, z \in \mathbb{S}^2$. This function is the winding number of a point $x \in \mathbb{S}^2$ with respect to the two curves T and $-T$. We fix non-critical, antipodal directions z and $-z$ and define $w(x)$ equal to the number of times T winds around the annulus between x and $-z$ plus the number of times $-T$ winds around the annulus between x and z. This is illustrated in Figure 5, where $w(z) = w(-z) = 1$ and $w(x) = 0$. Here we count the winding of T in a counterclockwise order

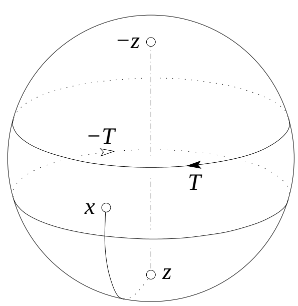

Figure 5: The winding number counts the number of times T separates x from $-z$ and $-T$ separates x from z.

as seen from x positive, and winding in a clockwise order negative. Symmetrically, we count the winding of $-T$ in a clockwise order as seen from x positive, and winding in a counterclockwise order negative. Imagine moving a point y along T and connecting x to y with the arc of the circle passing through x, y, and $-z$ that does not contain $-z$. Symmetrically, we move $-y$ along $-T$ and connect x to $-y$ with the arc of the circle passing through x, $-y$, and z that does not contain z. Locally at x we observe continuous movements of the two arcs. Clockwise and counterclockwise movements cancel, and $w(x)$ is the number of times the first arc rotates in a counterclockwise order plus the number of times the second arc rotates in a clockwise order. The winding number of x is necessarily an integer but can be negative.

Observe that w indeed changes in the same way as Dw does. Specifically, w drops by 1 if x crosses T from left to right, and it increases by 1 if x crosses $-T$ from left to right. Starting from the definition (2) of the writhing number, we thus get

$$\begin{aligned}
Wr &= \frac{1}{4\pi} \int_{\mathbb{S}^2} Dw(x)\, \mathrm{d}x \\
&= Dw(z) + \frac{1}{4\pi} \int_{\mathbb{S}^2} [Dw(x) - Dw(z)]\, \mathrm{d}x \\
&= Dw(z) + \frac{1}{4\pi} \int_{\mathbb{S}^2} [w(x) - w(z)]\, \mathrm{d}x \\
&= Dw(z) - w(z) + \frac{1}{4\pi} \int_{\mathbb{S}^2} w(x)\, \mathrm{d}x,
\end{aligned}$$

which completes the proof of Theorem A.

Signed area modulo 2. Observe that the writhing number changes continuously under deformations of the knot, as long as K does not pass through itself. When K passes through itself there is a ± 2 jump in $Dw(z)$, while $w(z)$ and the average winding number change continuously. We use these observations to give a new proof of Fuller's relation [16],

$$(6) \qquad 1 + Wr = A_T / 2\pi \pmod 2,$$

where $A_T = \frac{1}{2}\int w(x)\, \mathrm{d}x$ is the *signed area* of the curve T in $\mathbb{S}^2$. Note first that $1 + Wr = A_T/2\pi \pmod 1$ because both $Dw(z)$ and $w(z)$ are integer. We start with K being a circle in $\mathbb{R}^3$, in which case (6) holds because $Wr = 0$ and $A_T = \pm 2\pi$. Other than continuous changes, we observe jumps of ± 2 in Wr when K passes through itself. Theorem A together with the fact that the fractional parts of $1 + Wr$ and $A_T/2\pi$ are the same implies that (6) is maintained during the deformation. Fuller's relation follows because every knot can be obtained from the circle by continuous deformation.

Computing the average winding number. Three generic points $a, b, c \in \mathbb{S}^2$ define three arcs, which bound the spherical triangle abc. Recall that the area of abc is the sum of angles minus π. We define the *signed area* of abc as $A = \alpha + \beta + \gamma - \pi$ if a lies to the left of the oriented arc

bc, and as $A = -\alpha - \beta - \gamma + \pi$ if it lies to the right. Let $z \in \mathbb{S}^2$ be a direction not on T and not on $-T$. As shown in Figure 6, every arc $t_i t_{i+1}$ forms a unique spherical triangle $z t_i t_{i+1}$. Let A_i be its signed area. The corresponding arc $-t_i t_{i+1}$ of $-T$ forms the antipodal spherical triangle $-z t_i t_{i+1}$ with signed area $-A_i$. The winding number of

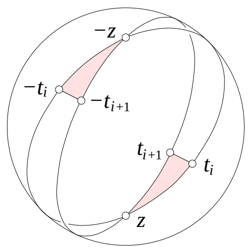

Figure 6: The two spherical triangles defined by an arc of T and its antipodal arc of $-T$.

a direction $x \neq z$ can be obtained by counting the number of spherical triangles that contain it. To be more specific, we call a spherical triangle *positive* if its signed area is positive and *negative* if its signed area is negative. Let $P_T(x)$ and $N_T(x)$ be the numbers of positive and negative spherical triangles $z t_i t_{i+1}$ that contain x, and similarly let $P_{-T}(x)$ and $N_{-T}(x)$ be the numbers of positive and negative spherical triangles $-z t_i t_{i+1}$ that contain x. Then

$$w(x) \quad = \quad [P_T(x) - N_T(x)] - [P_{-T}(x) - N_{-T}(x)].$$

To see this note that the equation is correct for $x = z$ and remains correct as x moves around and crosses arcs of T and of $-T$. The average winding number is thus

$$\begin{aligned} \frac{1}{4\pi} \int_{\mathbb{S}^2} w(x) \; \mathrm{d}x \quad &= \quad \frac{1}{4\pi} \sum_{i=0}^{n-1} A_i - \frac{1}{4\pi} \sum_{i=0}^{n-1} (-A_i) \\ &= \quad \frac{1}{2\pi} \sum_{i=0}^{n-1} A_i. \end{aligned}$$

Computing the sum in this equation is straightforward and takes only time $O(n)$.

Open knots. We define an *open knot* as a continuous injection $J : [0,1] \to \mathbb{R}^3$. Equivalently, it is an oriented curve with endpoints embedded in three-dimensional real space. The directional writhing number of J is well-defined, and the writhing number is the directional writhing number averaged over all parallel projections, as before. Assume J is a polygon specified by the sequence of its vertices, $p_0, p_1, \ldots, p_{n-1}$, and let K be the knot obtained by adding the edge connecting the last vertex to the first. The directions defined by p_1 and an interior point of the additional edge $p_0 p_{n-1}$ are critical for K but not for J, and the directions defined by p_0 and an interior point of the polygon from p_1 to p_{n-1} are critical for J but not for K. By symmetry, the same is true for the directions defined by p_{n-2} and $p_{n-1} p_0$ and by p_{n-1} and the polygon from p_{n-2} back to p_0. As

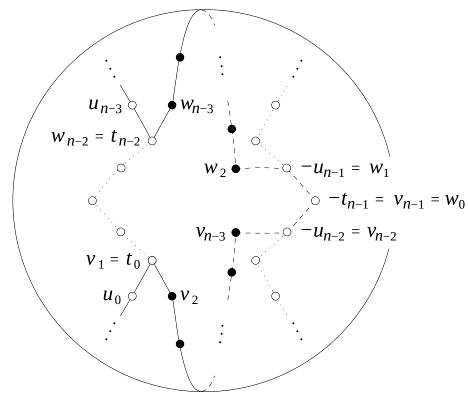

Figure 7: The critical curves of the knot K are marked by hollow vertices, and the additions required for the critical curves of the open knot J are marked by solid black vertices.

illustrated in Figure 7, changing the critical curve T of K to the critical curve S of J can be achieved by removing some arcs and adding others. To describe the process, we define $v_i = (p_i - p_0)/\|p_i - p_0\|$, for $1 \leq i \leq n-1$, and $w_j = (p_{n-1} - p_j)/\|p_{n-1} - p_j\|$, for $0 \leq j \leq n-2$. Observe that $v_1 = t_0$, $v_{n-2} = -u_{n-2}$, $v_{n-1} = w_0 = -t_{n-1}$, $w_1 = -u_{n-1}$, and $w_{n-2} = t_{n-2}$. We get the critical curve S from T by

1. removing the arcs $t_{n-2} t_{n-1}$ and $t_{n-1} t_0$,
2. adding the new path $t_0 = v_1, v_2, \ldots, v_{n-2} = -u_{n-2}$,
3. adding the two partial arcs $-u_{n-2} t_{n-1}$ and $-t_{n-1} u_{n-1}$ of $-T$, and
4. adding the new path $-u_{n-1} = w_1, w_2, \ldots, w_{n-2} = t_{n-2}$.

Symmetrically, we get $-S$ from $-T$. Everything we said earlier about the winding number of the critical curve T of K applies equally well to the critical curve S of J. Similarly, all algorithms described in the subsequent sections apply to knots as well as to open knots.

4 Computing Directional Writhing

In this section, we present an algorithm that computes the directional writhing number of a polygonal knot with n edges in time roughly proportional to $n^{1.6}$. The algorithm uses complicated subroutines that may not lend themselves to easy implementation.

Reduction to five dimensions. Assume without loss of generality that we view the knot K from above, that is, in the direction of $z = (0, 0, -1)$. Each edge $e_i = p_i p_{i+1}$ of K is oriented. Another edge $e_j = p_j p_{j+1}$ that crosses e_i in the projection either passes above or below and it either passes from left to right or from right to left. The four cases are illustrated in Figure 8 and classified as positive and negative crossings according to Figure 2. Letting P_i and N_i be the

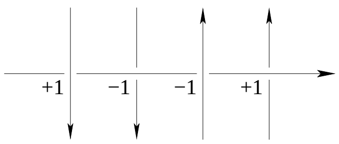

Figure 8: The four ways an oriented edge can cross another.

numbers of edges that form positive and negative crossings with e_i, the directional writhing number is

$$Dw(z) \quad = \quad \frac{1}{2} \left(\sum_{i=0}^{n-1} P_i - \sum_{i=0}^{n-1} N_i \right).$$

To compute the sums of the P_i and N_i efficiently, we map edges in three to points and half-spaces in five dimensions. Specifically, let ℓ_i be the oriented line that contains the oriented edge e_i and use Plücker coordinates as explained in [9] to map ℓ_i to a point $q_i \in \mathbb{R}^5$ or alternatively to a half-space h_i in $\mathbb{R}^5$. The mapping has the property that ℓ_i and ℓ_j form a positive crossing iff q_i lies in the interior of h_j. We use this correspondence to compute $\sum_i P_i$ in two stages: first we collect the pairs of oriented lines that form positive crossings, and second we count among them the pairs of edges that cross.

Recursive algorithm. It is convenient to explain the algorithm in a slightly more general setting, where X and Y are sets of x and y oriented edges in $\mathbb{R}^3$. Let $P(X, Y)$ denote the number of pairs $(e, f) \in X \times Y$ that form positive crossings, and note that $\sum_i P_i = P(X, Y)$ if X is the set of edges of the knot K and $Y = X$. We map X to a set Q of points and Y to a set H of half-spaces in $\mathbb{R}^5$. Let $r > 0$ be a sufficiently large constant. A $\frac{1}{r}$-*cutting* of H and Q is a collection of pairwise disjoint five-dimensional simplices that cover Q such that each simplex intersects at most $\frac{y}{r}$ of the hyperplanes bounding half-spaces in H. We use the algorithm in [1] to compute a $\frac{1}{r}$-cutting consisting of s simplices in time $\mathrm{O}(x + y)$, where s is at most some constant times $r^4 \log r$. For each simplex Δ_k in the cutting define

$$\begin{aligned} X_k &= \{e_i \in X \mid q_i \in \Delta_k\}, \\ Y_k &= \{f_j \in Y \mid \mathrm{bd}\, h_j \cap \Delta_k \neq \emptyset\}, \\ Z_k &= \{f_j \in Y \mid \Delta_k \subseteq h_j\}. \end{aligned}$$

Letting x_k and y_k be the cardinalities of the first two sets, we have $\sum_k x_k = x$ and $y_k \leq \frac{y}{r}$. By construction, every $(e, f) \in X_k \times Z_k$ defines a pair of lines that form a positive crossing. For each simplex Δ_k, we count the edge pairs $(e, f) \in X_k \times Z_k$ that form positive crossings and let P_k be the number of such pairs. Then

$$P(X, Y) \quad = \quad \sum_{k=1}^{s} [P(X_k, Y_k) + P_k].$$

We use the algorithm in [8] to compute all numbers P_k in time $\mathsf{S}(x, y) = \mathrm{O}(x^{2/3} y^{2/3} \log x + x \log x + y \log y)$, and we recurse to compute the $P(X_k, Y_k)$, stopping the recursion when $y \leq r$. The running time of this algorithm is at most

$$\begin{aligned} \mathsf{T}(x, y) &= \mathsf{S}(x, y) + \sum_{k=1}^{s} \mathsf{T}(x_k, y/r) \\ &= \mathrm{O}(y^{4+\epsilon} + x \log^2 x), \end{aligned}$$

for any $\epsilon > 0$, provided $r = r(\epsilon)$ is sufficiently large.

Improving the running time. We improve the running time of the algorithm by taking advantage of the symmetry of the mapping to $\mathbb{R}^5$. Specifically, a point q_i lies in the interior of a half-space h_j iff the point q_j lies in the interior of the half-space h_i. We proceed as above, but when the fourth power of the number of edges in X dips below the number of edges in Y then we switch roles. In other words, if $x^4 < y$ then we map the edges in X to half-spaces and the edges in Y to points. By our above analysis, the running time is then less than $\mathsf{T}(y, x) = \mathrm{O}(x^{4+\epsilon} + y \log^2 y) = \mathrm{O}(y^{1+\epsilon})$. The overall running time is thus less than

$$\begin{aligned} \mathsf{T}(x, y) &= \begin{cases} \mathsf{S}(x, y) + \sum_{k=1}^{s} \mathsf{T}(x_k, \frac{y}{r}) & \text{if } x^4 \geq y, \\ c y^{1+\epsilon} & \text{if } x^4 < y \end{cases} \\ &= \mathrm{O}((xy)^{0.8+\delta} + (x + y)^{1+\delta}), \end{aligned}$$

where c is a positive constant and δ is any real larger than ϵ. It follows that $\sum_i P_i$ can be computed in time $\mathrm{O}(n^{1.6+\varepsilon})$, for any constant $\varepsilon > 0$. Similarly, $\sum_i N_i$ and therefore the directional writhing number, $Dw(z)$, can be computed within the same time bound.

We remark that the technique described in this section can also be used to compute the linking number between two polygonal knots with n and $m \leq n$ edges in time $\mathrm{O}(n^{1.6+\varepsilon})$.

5 Experiments

In this section, we sketch a sweep-line algorithm that computes the writhing number of a polygonal knot using Theorem A. We implement the algorithm in C++ using the LEDA software library and compare it with two versions of the algorithm based on the double integral in Equation (3). We did not implement any version of Le Bret's algorithm mentioned in Section 2 since it is based on a formula similar to Theorem A and can be expected to perform about the same as our sweep-line algorithm.

Sweep-line algorithm. Theorem A expresses the writhing number of a knot K as the sum of three terms. Accordingly, we compute the writhing number in three steps.

`Step 1.` Compute the directional writhing number for an arbitrary but fixed, non-critical direction z, $Dw(z)$.

`Step 2.` Compute the winding number of z relative to the Gauss maps T and $-T$, $w(z)$.

`Step 3.` Compute the average winding number by summing the signed areas of the spherical triangles zt_it_{i+1}, $\frac{1}{2\pi}\sum_i A_i$.

`Return` the alternating sum of the three results, $Dw(z) - w(z) + \frac{1}{2\pi}\sum_i A_i$.

Instead of using the algorithm described in Section 4, we implement Step 1 using a sweep-line algorithm [13], which reports the m crossing pairs formed by the n edges in time $\mathrm{O}((n+m)\log n)$. Steps 2 and 3 are both computed in a single traversal of the spherical polygons T and $-T$, keeping track of the accumulated angle and the signed area as we go. The running time of the traversal is only $\mathrm{O}(n)$.

Double-sum algorithm. We compare the implementation of the sweep-line algorithm with two implementations of Equation (3). Write $e_i = p_{i+1} - p_i$ for the unnormalized tangent vector. Following [4, 20], we discretize Equation (3) to

$$(7) \qquad Wx = \frac{1}{4\pi}\sum_{i=0}^{n-1}\sum_{j\neq i}\frac{\langle e_j \times e_i, p_j - p_i\rangle}{\|p_j - p_i\|^3}.$$

We note that Wx is not the writhing number of the polygonal knot, but it converges to the writhing number of a smooth knot if the polygonal approximation is progressively refined to approach that knot.

Alternatively, we may discretize the double integral in such a way that the result is the writhing number of the approximating polygonal knot. Given two edges e_i and e_j, we measure the area of the two antipodal quadrangles in $\mathbb{S}^2$ along whose directions we see the edges cross. The area of one of the quadrangles is the sum of angles minus one full angle, $\alpha + \beta + \gamma + \delta - 2\pi$. The absolute value of the signed area A_{ij} is the same, and its sign depends on whether we see a positive or a negative crossing. We thus have

$$(8) \qquad Wr = \frac{1}{4\pi}\sum_{i=0}^{n-1}\sum_{j\neq i}A_{ij}.$$

Straightforward vector geometry and trigonometry can be used to derive analytical formulas for the A_{ij} [18].

Comparison. We compare the three implementations using a sequence of polygonal approximations of an artificially created smooth knot. It has the form of the infinity symbol, ∞, and is fairly flat in $\mathbb{R}^3$, with only a small gap in the middle. Because the knots are fairly flat, most of their parallel projections have one crossing and the writhing number is just a little smaller than 1.0. Figure 9 shows that the algorithms

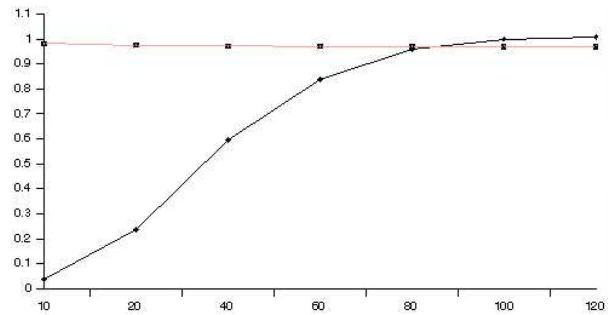

Figure 9: Comparing convergence rates between Wr (upper curve) and Wx (lower curve).

that compute the exact writhing numbers for polygonal approximations converge faster to the writhing number of the smooth knot than the algorithm implementing (7). Figure 10 shows how much faster the sweep-line algorithm is than both implementations of the double-sum algorithm. Let n be the number of edges. The graphs suggest the obvious, namely that the running time of the sweep-line algorithm is $\mathrm{O}(n\log n)$ and those of the two implementations of the double-sum algorithm are $\Theta(n^2)$. We observe the $n\log n$ bound whenever we approximate a smooth knot by a polygon, since for generic projections the number of crossings is independent of the number of edges.

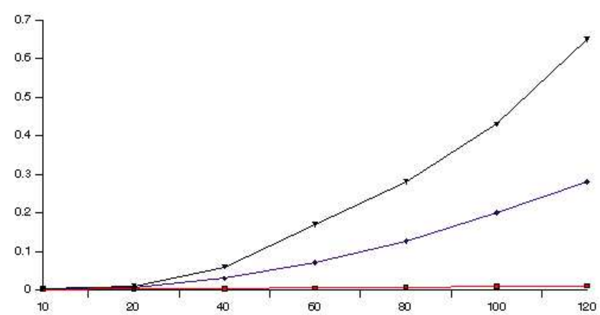

Figure 10: Comparing the running times of the sweep-line algorithm (lower curve) and the two implementations of the double-sum algorithm: approximate (middle curve) and exact (upper curve).

Protein backbones. We present some preliminary experimental results obtained with the three implementations. All

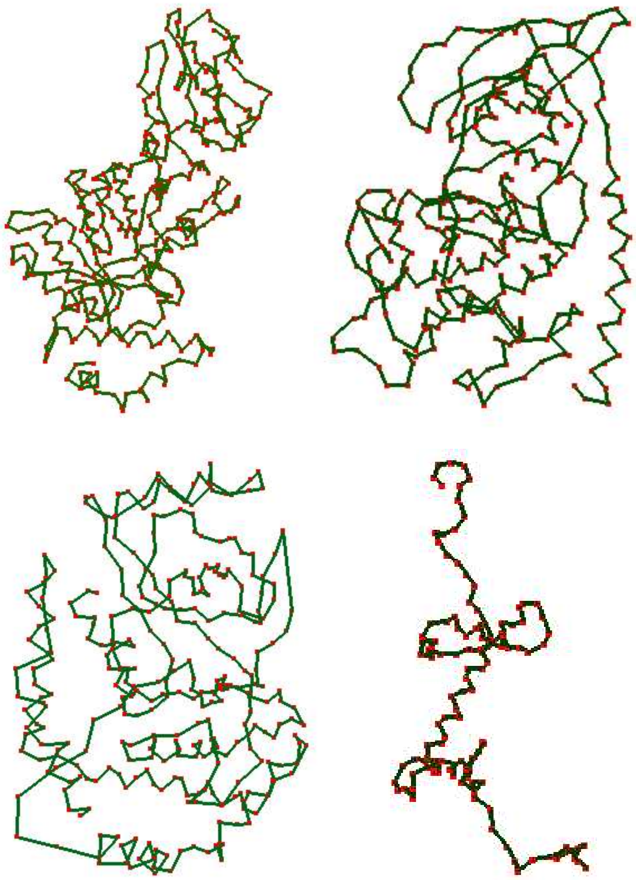

Figure 11: The open knots modeling the backbone of the protein conformations stored in the PDB files 1AUS.pdb (upper left), 1CDK.pdb (upper right), 1CJA.pdb (lower left), and 1EQZ.pdb (lower right).

Data	Size		Time			Writhing #	
	n	m	SwL	$\mathrm{DS_a}$	$\mathrm{DS_e}$	Wr	Wx
1AUS	439	122	0.09	3.93	9.28	22.70	17.87
1CDK	343	111	0.06	2.39	5.62	7.96	6.01
1CJA	327	150	0.06	2.19	5.10	12.14	10.43
1EQZ	125	18	0.02	0.31	0.73	4.78	3.37

Table 1: Four protein backbones modeled by open polygonal knots. The size of the problem is measure by the number of edges, n, and the number of crossings in the chosen projection, m. The time the sweep-line (SwL), the approximate double-sum ($\mathrm{DS_a}$), and the exact double-sum ($\mathrm{DS_e}$) algorithms take is measured in seconds. Wx is an approximation of the writhing number for polygonal data.

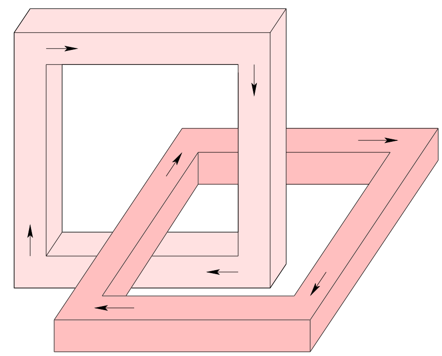

Figure 12: Two linked window-frames outlining a knot whose length is L, whose cross-section radius is R, and whose writhing number is some constant times the ratio of the two to the power $\frac{4}{3}$.

experiments are carried out on a SUN workstation, with a 333 MHz UltraSPARC-IIi CPU, and 256 MB memory. Short of conformation data of long DNA strands, we decided to run our algorithms on a modest collection of open knots representing protein backbones down-loaded from the protein data bank [22]. We modified the algorithms to account for the missing edge in the data, as explained in Section 3. Figure 11 displays the four backbones chosen for our experimental study. Table 1 presents some of our findings.

Thick knots. Even though the writhing number of a polygonal knot can be as large as quadratic in the number of edges, all four protein backbones in Figure 11 have writhing numbers that are significantly smaller than the numbers of edges. If a knot is made out of rope with non-zero thickness, then the quadratic bound can be achieved only if the ratio of length over cross-section radius is sufficiently high. Specifically, a knot of length L that has an embedded tubular neighborhood of radius R has writhing number less than $\frac{1}{4}(L/R)^{4/3}$ [7]. Such 'thick' knots can be used to capture the fact that the edges of a protein backbone are about as long as they are thick. A backbone with n edges thus has writhing number at most some constant times $n^{4/3}$. The example indicated in Figure 12 shows that this upper bound is asymptotically tight. Replace each window-frame by a spiral that intersects a cross-section of the frame in a k-by-k grid of points, and connect the two spirals to form a single knot. The length once around a frame is some constant times k, which implies that L/R is at most some constant times k^3. The directional writhing number for the direction shown in Figure 12 is $2(k^2)^2$. We have the same directional writhing number in almost every direction, which implies that the writhing number is some constant times $(L/R)^{4/3}$, as claimed.

6 Discussion

In this paper, we have described the relationship between the writhing number of a knot in $\mathbb{R}^3$ and the winding number of its Gauss map. Based on this relationship, we have given an algorithm that computes the writhing number of a polygonal knot in time less than quadratic in the number of edges. We implemented a different algorithm whose running time depends on the number of crossings in a projection and tested the software on open knots describing protein backbones. It would be interesting to expand these experiments to see whether there is a correlation between the writhing numbers and the common categorization of folding patterns into protein families. To approach this question, it might be necessary to consider knots on a range of scale levels and look at the writhing number as a function of scale.

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