ON COMPARING THE WRITHE OF A SMOOTH CURVE TO THE WRITHE OF AN INSCRIBED POLYGON

JASON CANTARELLA

ABSTRACT. We find bounds on the difference between the writhing numbers of a smooth curve and a polygonal curve inscribed within. The proof is based on an extension of Fuller's difference of writhe formula to the case of polygonal curves. The results establish error bounds useful in the numerical computation of writhe.

1. INTRODUCTION

The writhing number measures the wrapping and coiling of space curves. Writhe has proved useful in molecular biology, where it is used to study the geometry of tangled strands of DNA [17]; often with the famous Călugăreanu-White formula for a curve C in space with a normal field V [5, 6, 18, 14]:

$$\operatorname{Lk}(C, C + \epsilon V) = \operatorname{Tw}(C, V) + \operatorname{Wr}(C).$$

In these applications, and in numerical simulations performed by biologists and mathematicians, it is often required to compute writhing numbers using numerical methods.

Several authors have presented algorithms for computing the exact writhing number of an n-edge polygonal curve in a finite number of steps [9, 4, 1, 17]. The fastest of these algorithms runs in time $O(n^{1.6})$, while earlier methods use time $O(n^2)$.

Careful implementations of such algorithms provide acceptable accuracy in computing writhe for polygonal curves. But reliably computing the writhe of smooth curves requires another step: we must be able to bound the error introduced in approximating a smooth curve by an inscribed polygonal curve. The purpose of this paper is to prove:

Theorem 1. *Suppose $C(t)$ is a simple, closed curve of class $\mathcal{C}^4$. We assume $C(t)$ is parametrized so that $|C'(t)| \geq 1$, and that we have upper bounds $B_1, \dots, B_4$ on $|C'(t)|, \dots |C^{(4)}(t)|$. Let $C_n(t)$ be any n-edge polygonal curve inscribed in C with maximum edge length x and $1/x > 5B_2$.*

If the ribbon formed by joining $C_n(t)$ to $C(t)$ for every t is embedded,

$$|\operatorname{Wr}(C) - \operatorname{Wr}(C_n)| < \alpha\, n x^3 + n O(x^4). \tag{1}$$

where α is a numerical constant less than $B_2(5B_2^2 + B_3)$.

That is, if the lengths of the edges of C_n are approximately constant, the error is bounded by a multiple of $1/n^2$.

The proof is based on Fuller's $\Delta\operatorname{Wr}$ formula, which gives the difference in writhing number between two curves as the spherical area of the ribbon bounded by the curves on S^2 swept out by their unit tangent vectors [11]. (Following Bruce Solomon [16], we will refer to such curves as *tantrices*, though they are classically referred to as *tangent indicatrices*.)

We begin by defining the writhing number in Section 2. Sections 3 and 4 then introduce the original form of Fuller's $\Delta\mathrm{Wr}$ formula. In Sections 5 and 6 we extend Fuller's formula to the case where one curve is polygonal and the other is of class $\mathcal{C}^2$ using a natural geometric idea: the tantrix of a polygonal curve should be defined to be the chain of geodesic segments on S^2 joining the (isolated) tangent vectors of the curve (this was pointed out by Chern in [8]). In the process, we discover a surprising fact: the writhe of a polygonal curve is *equal* to the writhe of any smooth curve obtained by carefully rounding off its corners!

Section 7 contains the remainder of our work: estimating the terms in our improved version of the $\Delta\mathrm{Wr}$ formula to obtain Theorem 9. We test our error bounds in Section 8 by computing the writhe of a collection of polygonal curves inscribed in a smooth curve of known writhe.

The last section contains a discussion of some open problems inspired by the present work. We state the most important of them now: Like most of the theory of writhing numbers, the proof of our main theorem depends essentially on the fact that C is closed. Can these methods be extended to open curves?

2. DEFINITIONS

The writhing number of a space curve is defined by:

Definition 2. *The* writhe *of a piecewise differentiable curve $C(s)$ is given by:*

$$\mathrm{Wr}(C) = \frac{1}{4\pi} \int_{C \times C} \frac{C'(s) \times C'(t) \cdot (C(s) - C(t))}{|C(s) - C(t)|^3} \,\mathrm{d}s\,\mathrm{d}t, \tag{2}$$

Definition 2 is inspired by the Gauss formula for the linking number of two space curves, $A(s)$ and $B(s)$ (see Epple [10] for a fascinating discussion of the history of this formula):

$$\mathrm{Lk}(A, B) = \frac{1}{4\pi} \int_{A \times B} \frac{A'(s) \times B'(t) \cdot (A(s) - B(t))}{|A(s) - B(t)|^3} \,\mathrm{d}s\,\mathrm{d}t. \tag{3}$$

When the two curves A and B become a single curve, their linking number becomes the writhing number. This introduces a potential singularity on the diagonal of $C \times C$, but a careful calculation shows that the integral still converges. In fact, the integrand of Equation 2 approaches 0 on the diagonal of $C \times C$, even when the curve C has a corner.

From now on, we'll assume that C is simple. With this assumption, another way to look at the integral of Definition 2 is to observe that the integrand is the pullback of the area form on S^2 under the Gauss map $C \times C \to S^2$ defined by

$$(C(s), C(t)) \mapsto \frac{C(s) - C(t)}{|C(s) - C(t)|}. \tag{4}$$

From this perspective, we can see that the (signed) multiplicity of the Gauss map at any point p on S^2 is just the number of self-crossings of the projection of C in direction p.

3. FULLER'S ΔWr FORMULA

Suppose we have a differentiable curve $C(t)$, with unit tangent vector $T(t)$. As we mentioned in Section 1, the curve $T(t)$ on the unit sphere is known as the tantrix of C. This curve divides the unit sphere into a number of cells. Within each cell, the signed crossing number of the projection of C is constant: changing projection directions within the cell amounts to altering the projection of the knot by a regular isotopy consisting of Reidemeister moves of type II and III (pictured below). Neither of these moves changes the signed crossing number of the knot.

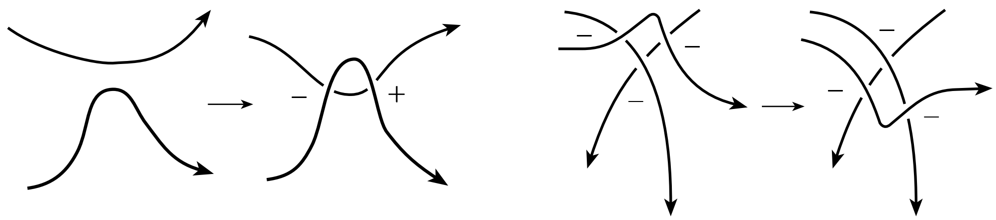

Figure 1. Changing the projection direction within a cell can only alter the diagram by one of these two moves. Neither changes the signed crossing number of the diagram, as we can see by counting the $+$ and $-$ markers at the crossings of C.

This observation motivates the idea that the writhe of a closed space curve is related to the fraction of the sphere's area enclosed by its tantrix. In 1978, Brock Fuller stated the following:

Theorem 3. (Fuller's Spherical Area Formula) *For any closed space curve $C(s)$ of class $\mathcal{C}^3$, let A be the spherical area enclosed by the tantrix of C. Then*

$$1 + \mathrm{Wr}(C) = \frac{A}{2\pi} \mod 2. \tag{5}$$

Fuller used this formula to conclude that the difference in writhe between two curves X_0 and X_1 whose tantrices T_0 and T_1 are sufficiently close is given by a certain formula, which represents the spherical area of the ribbon between T_0 and T_1.

To be more specific, suppose that X_0 and X_1 are simple closed space curves of class $\mathcal{C}^2$, with regular parametrization (that is, parametrized so that X_0' and X_1' never vanish), and unit tangent vectors T_0 and T_1. Let $F : S^1 \times [0,1] \to \mathbf{R}^3$ be a continuous deformation of X_0 into X_1, where $F(t,\lambda) = X_\lambda(t)$ and the X_λ are simple curves of class $\mathcal{C}^1$, with unit tangent vectors $T_\lambda(t)$ continuous in (t,λ).

Theorem 4. (Fuller's ΔWr Formula) *If $T_1(t)$ and $T_\lambda(t)$ are not antipodal for all (t,λ), then*

$$\mathrm{Wr}(X_1) - \mathrm{Wr}(X_0) = \frac{1}{2\pi} \int_C \frac{T_0(t) \times T_1(t)}{1 + T_0(t) \cdot T_1(t)} \cdot [T_0'(t) + T_1'(t)] \, \mathrm{d}t. \tag{6}$$

We observe that this formula does not require an arc-length parametrization of X_0 and X_1.

4. JUSTIFYING FULLER'S INTERPRETION OF THE ΔWr FORMULA

While Fuller stated both these theorems in 1978, he did not provide complete proofs for either. The first rigorous proofs of Theorems 3 and 4 were given by Aldinger, Tabor, and Klapper [2] in 1995. While these authors proved both theorems as stated, they did not show that the formula in Theorem 4 represents the spherical area of the ribbon between T_0 and T_1 (in [2], the right-hand side of Equation 6 describes the difference between the twist of two frames on X_0 and X_1.)

In the spirit of their paper, we now justify Fuller's original intuition about Equation 6.

Proposition 5. *Given two curves $T_0(t), T_1(t) : [0,1] \to S^2$ where $T_0(t)$ and $T_1(t)$ are never antipodal, the area of the spherical region R bounded by T_0, T_1 and the great circle arcs joining their endpoints is given by*

$$\text{Area}(R) = \int \frac{T_0(t) \times T_1(t)}{1 + T_0(t) \cdot T_1(t)} \cdot (T_0' + T_1')\ \mathrm{d}t. \tag{7}$$

Proof. We let

$$u(\theta, t) = \cos\theta\ T_0(t) + \sin\theta\ T_1(t),$$

and parametrize the region R by

$$v(\theta, t) = \frac{u(\theta, t)}{|u(\theta, t)|}$$

where θ ranges from 0 to $\pi/2$. Plugging this parametrization into the area form on S^2, and using the properties of the triple product, we find

$$\mathrm{d}\,\text{Area} = \frac{1}{|u|^3} \left(\frac{\partial u}{\partial \theta} \times \frac{\partial u}{\partial s} \cdot u \right) \mathrm{d}\theta \wedge \mathrm{d}t.$$

Using the definition of $u(\theta, t)$, this simplifies to

$$\mathrm{d}\,\text{Area} = T_0 \times T_1 \cdot \left(\frac{\cos\theta}{(1 + 2\cos\theta\sin\theta\ T_0 \cdot T_1)^{\frac{3}{2}}} T_0' + \frac{\sin\theta}{(1 + 2\cos\theta\sin\theta\ T_0 \cdot T_1)^{\frac{3}{2}}} T_1' \right) \mathrm{d}\theta \wedge \mathrm{d}t.$$

Using the formula $\sin 2\theta = 2\cos\theta\sin\theta$, and the fact that the definite integrals of each of the trigonometric expressions above from 0 to $\pi/2$ are equal, we have

$$\text{Area}(R) = \int_0^1 T_0 \times T_1 \cdot \left[\int_0^{\pi/2} \frac{\cos\theta}{(1 + \sin 2\theta\ T_0 \cdot T_1)^{3/2}} \,\mathrm{d}\theta \right] (T_0' + T_1')\,\mathrm{d}t.$$

This can be solved by the general integration formula

$$\int \frac{\cos\theta}{(1 + a\sin 2\theta)^{3/2}}\,\mathrm{d}\theta = \frac{-a\cos\theta - \sin\theta}{(a^2 - 1)\sqrt{1 + a\sin 2\theta}}, \tag{8}$$

which yields the formula in the statement of the Proposition. □

5. Extending Fuller's formula to polygonal curves: I

To measure the difference in writhe between a smooth curve and a polygonal curve inscribed in the smooth curve, we must extend Theorem 4 to polygonal curves. To do so, we intend to approximate each polygonal curve with a family of smooth curves so that the writhe of the smooth curves converges to the writhe of the polygonal curve.

Examining Definition 2, it might seem that this result follows from general principles. For instance, one might conjecture that Wr was continuous in the C^1 norm on curves, and hope to obtain an approximating family using standard techniques. Unfortunately, the situation is not so simple; as the example in Figure 2 shows, writhe is not continuous in any C^k norm on curves. Thus, our proof depends explicitly on the hypothesis that the limit curve is polygonal; it cannot be easily extended to the case where the limit curve is merely piecewise C^2.

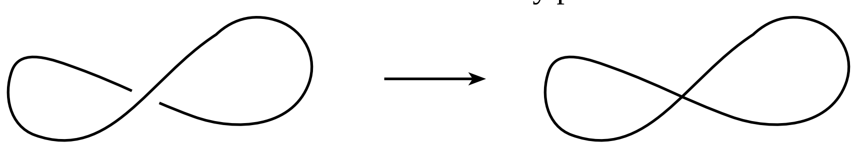

Figure 2. The family of almost-planar curves on the left converge in any C^k norm to the planar figure eight curve on the right. However, the writhe of the curves on the left approaches one, while the writhe of the planar figure eight is zero. This shows that writhe is not continuous in any C^k norm on curves.

To prepare for the proof, we establish some notation for polygonal curves. Let $C(t)$ be a polygonal curve with corners at cyclically ordered parameter values $t_0 < t_1 < \cdots < t_n = t_0$. We let $T(t)$ denote the unit tangent to C, and set up the convention that $T(t_i)$ will be the tangent vector *leaving* $C(t_i)$.

We now construct a family of smooth curves approximating our polygonal curve.

Proposition 6. *Given an embedded polygonal curve C with corners at $t_0, \dots, t_{n-1}, t_n = t_0$, there exists a family of smooth curves C_i converging pointwise to C with*

(1) *$C_i = C$ outside a neighborhood of each corner point $C(t_j)$ of radius $1/i$.*
(2) *Near each corner, the tangent vectors of C_i interpolate between $T(t_{j-1})$ and $T(t_j)$.*
(3) $\mathrm{Wr}(C_i) \to \mathrm{Wr}(C)$.

Proof. It is easy to construct a family of $C_i \to C$ obeying conditions (1) and (2) by rounding off each corner of C. We claim that this can be done in such a way that the writhe integrand has a uniform upper bound on all the C_i. Since condition (1) implies that the $C_i \to C$ pointwise in the $\mathcal{C}^1$ norm, the bounded convergence theorem [15, p.81] will then yield condition (3).

Since any pair of adjacent edges is planar, we can choose the C_i so that the region of each C_i approximating a pair of adjacent edges is also planar. This means that for some universal ϵ, the writhe integrand of each C_i vanishes in an ϵ-neighborhood of the diagonal of $C_i \times C_i$.

Since C has no self-intersections and the angle at each corner of C_i is positive, the distance between any pair of non-adjacent edges of C is bounded below by some constant. Since the C_i converge to C pointwise, we may assume the same for the portions of the C_i approximating any pair of disjoint edges. Throwing away finitely many of the C_i if necessary, this means that for any $\delta > 0$, there exists a universal lower bound (depending on δ) on the distance between any pair of points in $C_i \times C_i$ *outside* an δ-neighborhood of the diagonal.

But for any pair of points on C_i, the writhe integrand is bounded above by the inverse square of the distance between them. Thus, our lower bound on self-distances yields a universal upper bound on the writhe integrand for C and all the C_i outside a δ-neighborhood of the diagonal. Choosing $\delta < \epsilon$, this completes the proof of the proposition. □

6. Extending Fuller's formula to polygonal curves: II

We now state our extension of Fuller's theorem. Our formula will apply to the following situation (c.f. Section 3): Suppose that X_0 and X_1 are simple closed space curves, with X_0 of class $\mathcal{C}^2$ and X_1 polygonal, with regular parametrization (that is, parametrized so that X_0' and X_1' never vanish where they are defined), and unit tangent vectors T_0 and T_1.

Let $F : S^1 \times [0,1] \to \mathbf{R}^3$ be a C^0 deformation of X_0 into X_1, where $F(t,\lambda) = X_\lambda(t)$, so that the X_λ are simple curves of class C^1 for $\lambda \in [0,1)$, with unit tangent vectors $T_\lambda(t)$ continuous in (t,λ). As above, we take the corners of X_1 to be at parameter values $t_0, t_1, \dots, t_n = t_0$. We let T_1 denote the unit tangent vector to X_1, and let $T_1(t_i)$ be the tangent vector *leaving* $X_1(t_i)$.

Theorem 7. *If each corner angle of X_1 is strictly greater than $\pi/2$, and each $T_1(t)$ and $T_\lambda(t)$ are at an angle less than $\pi/2$, then*

$$\mathrm{Wr}(X_1) - \mathrm{Wr}(X_0) = \frac{1}{2\pi}\sum_{i=1}^{n} \mathrm{Area}\, R(T_0(t_i), T_0(t_{i+1}), T_1(t_i)) + \mathrm{Area}\, \triangle T_0(t_i) T_1(t_{i-1}) T_1(t_i),$$

where $R(T_0(t_i), T_0(t_{i+1}), T_1(t_i))$ is the spherical region bounded by geodesics from $T_1(t_i)$ to $T_0(t_i)$ and $T_0(t_{i+1})$ and the portion of T_0 between t_i and t_{i+1}, $\triangle T_0(t_i)T_1(t_{i-1})T_1(t_i)$ is the spherical triangle with these three vertices, and Area *represents oriented area on S^2.*

Proof. Construct a sequence of smooth curves $C_j \to X_1$ using Proposition 6. For large enough j, each of these curves can be homotoped to X_1 through a family of simple $\mathcal{C}^1$ curves with a continuous family of tangent vectors, as in the setup for the statement of this theorem above.

Joining these homotopies to the homotopy from X_1 to X_0 assumed by our hypotheses generates a family of (non-smooth) homotopies from the X_0 to each of the C_j. We wish to smooth each of these to obtain homotopies from X_0 to C_j which obey the conditions of Fuller's $\Delta\mathrm{Wr}$ formula (Theorem 4).

We first prove that the tangent vectors of each of the intermediate curves in each homotopy from X_0 to C_j are never antipodal to the corresponding tangent vectors T_j of C_j. By hypothesis, for each t and λ, $\angle T_\lambda(t), T_1(t) < \pi/2$. On the other hand, since the difference between the tangent vectors to X_1 at any corner is less than $\pi/2$, for large enough j, $\angle T_1(t), T_j(t) < \pi/2$. Putting these equations together, we see that $\angle T_\lambda(t), T_j(t) < \pi$, and so these vectors are never antipodal.

It is easy to smooth the combined homotopy from X_0 to C_j so that each of the intermediate curves is of class $\mathcal{C}^1$ while preserving this condition. Since the smoothed homotopy satisfies the hypotheses of Fuller's $\Delta\mathrm{Wr}$ formula (Theorem 4), Proposition 5 tells us that the difference between $\mathrm{Wr}(X_0)$ and $\mathrm{Wr}(C_j)$ is the spherical area of the ribbon joining T_0 and T_j.

For each i, the contribution to the spherical area from the straight part of C_j between t_i and t_{i+1} comes from the ribbon between $T_1(t_i)$ and the portion of T_0 with $t \in (t_i + 1/j, t_{i+1} - 1/j)$. As $j \to \infty$, this area converges to the area of the ribbon between the portion of T_0 with $t \in (t_i, t_{i+1})$ and $T_1(t_i)$. This is the first term in our sum above.

At each vertex t_i of X_1, the contribution to our spherical area from the curved part of C_j comes from the ribbon between the great circle arc connecting $T_1(t_{i-1})$ and $T_1(t_i)$ and a portion of T_0 of parameter length $2/j$. As $j \to \infty$, the area of this ribbon converges to the area of the spherical triangle with vertices $T_0(t_i)$, $T_1(t_i)$, $T_1(t_{i-1})$. This is the second term in our sum above. Figure 3 shows both these terms on the unit sphere.

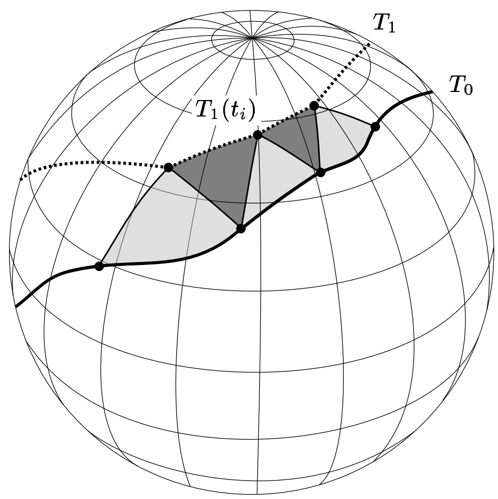

Figure 3. This figure shows the two types of regions in the sum in the statement of Theorem 7. The top (dotted) curve shows the great circle arcs joining the tangent vectors $T(t_i)$ of the polygonal curve X_1. The bottom curve shows the continuous curve of unit tangents T_0 to the smooth curve X_0. The light gray regions show the first terms in the sum, while the dark gray spherical triangles show the second terms.

We have shown that the right-hand side of the statement of the Theorem is equal to the limit $\lim_{j\to\infty}(\mathrm{Wr}(C_j) - \mathrm{Wr}(X_0))$. However, by Proposition 6, $\lim_{j\to\infty} \mathrm{Wr}(C_j) = \mathrm{Wr}(X_1)$. Thus

$$\lim_{j\to\infty} \mathrm{Wr}(C_j) - \mathrm{Wr}(X_0) = \mathrm{Wr}(X_1) - \mathrm{Wr}(X_0), \tag{9}$$

which is the left-hand side in the statement of the Theorem. This completes the proof. □

We now make a surprising observation: Since the tantrices of the C_j differ as curves on S^2 only in parametrization, the area between each of these curves and the tantrix of X_0 is constant. Thus, by Fuller's formula, each C_j has the same writhe! And since (by Proposition 6) these writhing numbers converge to the writhe of X_1, each $\mathrm{Wr}(C_j)$ is equal to $\mathrm{Wr}(X_1)$ as well! So we have the following corollary:

Corollary 8. *If C_n is a polygonal curve, and C is a smooth curve obtained by rounding off the corners of C_n under the conditions of Proposition 6, then*

$$\mathrm{Wr}(C_n) = \mathrm{Wr}(C). \tag{10}$$

7. Bounding the $\Delta\mathrm{Wr}$ Formula

We now prove our main theorem by finding asymptotic bounds for Fuller's $\Delta\mathrm{Wr}$ formula. Our theorem deals with the following situation: Assume that $C(t)$ is a simple closed curve of class $\mathcal{C}^4$, parametrized so that $|C'(t)| \geq 1$. (Given any initial parametrization, this can be accomplished by rescaling.) Further, assume we have upper bounds $B_1, \ldots, B_4$ on the norms of the first four derivatives of C.

Let $C_n(t)$ be any n-edge polygonal curve inscribed in C. We assume that the maximum edge length of C is bounded by x.

Theorem 9. *If the ribbon formed by joining $C_n(t)$ to $C(t)$ for every t is embedded, and $1/x > 5B_2$,*

$$|\,\mathrm{Wr}(C) - \mathrm{Wr}(C_n)| < \alpha\, n x^3 + nO(x^4). \tag{11}$$

where α is a numerical constant less than $B_2(5B_2^2 + B_3)$.

We make a few comments on this theorem before diving into the proof. First, we observe that if the lengths of the edges of C_n are all of the same order of magnitude, the difference between the writhe of C and the writhe of C_n is of order $1/n^2$.

Next, we observe that the form of our theorem was chosen to be of maximal use in applications. In particular, we did not require that C be parametrized by arclength and state our bounds in terms of curvature and torsion because in practice it is very difficult to obtain an arc-length parametrization of a given curve, while it is comparatively easy to obtain values for the derivative bounds given above.

Last, we discuss the role of the additional hypotheses in the statement above; that the ribbon between C and C_n be embedded and that $1/x$ be greater than $5B_2$. Both are intended to exert enough control over the approximation to guarantee the existence of a homotopy from C to C_n obeying the requirements of Theorem 7.

We can guarantee that C_n satisfies the first hypothesis by proving that C_n lies in an embedded tubular neighborhood of C. Since C is of class $\mathcal{C}^4$, and has no self-intersections, such a neighborhood is guaranteed to exist: for a discussion of how to compute the radius of this tube (which is known as the *thickness* of C), see the literature on *ropelength* of knots (*e.g.* [12, 7, 13]).

Proof. We begin by reparametrizing our curve by arclength. This forces us to recompute our bounds for the derivatives of $C(t)$ (a standard computation), arriving at

$$|C'(s)| = 1, \qquad |C''(s)| < K := 2B_2, \qquad |C'''(s)| < T := 2B_3 + 10B_2^2, \tag{12}$$

while $C^{(4)}(s)$ is again bounded above. To remind ourselves of the connection between these bounds and the curvature and torsion of our curve, we will refer to the bound for the second derivative as K, and the bound for the third derivative as T. Further, we note that the curvature $\kappa(s)$ of our curve is bounded above by K, and that our hypotheses imply that $1/x > (5/2)K$.

We also establish the convention that the corners of C_n are at parameter values cyclically ordered as $s_0, \dots, s_{n-1}, s_n = s_0$.

By smoothing the linear interpolation between C and C_n, we can construct a homotopy between C and C_n according to the conditions of Theorem 7 as long as:

(1) the ribbon joining C to C_n is embedded,
(2) the angle at each corner of C_n is at least $\pi/2$,
(3) the angle between $T(s)$ and $T_n(s)$ is at most $\pi/2$ for any s.

Borrowing from Lemma 12 (below), we see that our assumption that $1/x > (5/2)K$ is enough to bound the angle in (3) by $0.20402 < \pi/4$. At any corner s_i, the same Lemma implies that the corner angle is the supplement of at most twice 0.20402, so this is enough to ensure that condition (2) holds as well.

Theorem 7 now tells us that

$$
\begin{aligned}
(13)\quad |\operatorname{Wr}(C) - \operatorname{Wr}(C_n)| \leq \frac{1}{2\pi} \sum_{i=1}^{n} &|\text{Area}\, R\left(T\left(s_i\right), T\left(s_{i+1}\right), T_n\left(s_i\right)\right)| \\
&+ |\text{Area}\, \triangle T\left(s_i\right) T_n\left(s_{i-1}\right) T_n\left(s_i\right)|,
\end{aligned}
$$

where the first term is the area of the spherical region bounded by the geodesics from $T_n(s_i)$ to $T(s_i)$ and $T(s_{i+1})$ and the portion of T between s_i and s_{i+1}, and the second term is the area of the spherical triangle. Our job now is to estimate the areas of these regions. To do so, we first invoke Taylor's Theorem, in the form commonly used in numerical analysis (c.f. [3], Thm.1.4):

Theorem 10. (Taylor's Theorem) *Suppose $C(s)$ is a curve of class $\mathcal{C}^4$, with fourth derivative bounded by B_4'. Then (choosing coordinates so that $C(0)$ is at the origin),*

$$
C(s) = sC'(0) + \frac{s^2}{2}C''(0) + \frac{s^3}{6}C'''(0) + R_4(s), \tag{14}
$$

where $|R_4(s)| < s^4 B_4'$.

We will use this expression for $C(s)$ frequently in our work below.

Lemma 11. *For any s, we have*

$$
|s - |C(s)|| < \frac{K^2}{24}|s^3| + \frac{1}{120}|s^5|, \qquad \textit{and} \qquad |C(s)| \leq |s|. \tag{15}
$$

Further, for any edge of C_n, the difference $|s_{i+1} - s_i|$ is at most $1.01\, x$.

Proof. We assume without loss of generality that s is positive. By Schur's lemma ([8]), since the curvature of C is bounded above by K, $|C(x)|$ is at least the length of a chord across an arc of length s on a circle of radius $1/K$, or $(2/K)\sin(K/2)s$. This means that we have

$$
\frac{2}{K}\sin\frac{K}{2}s = s - \frac{K^2}{24}s^3 + R_5(s),
$$

where $R_5(s)$ is the term of order s^5 which comes from the usual Taylor expansion of $\sin s$. In particular,

$$\begin{aligned} |s - |C(s)|| &< s - \frac{2}{K} \sin \frac{K}{2} s \\ &< \frac{K^2}{24} s^3 - R_5(s), \end{aligned}$$

where $R_5(s) < \frac{1}{120} s^5$. The upper bound on $|C(s)|$ comes from the fact that C is unit-speed.

The second statement is another Schur's lemma calculation; this time invoking our hypothesis that $x > (5/2)K$ and observing that $1.01 \sin y > y$ for y between 0 and $1/5$. □

We will also need an upper bound on the angle between $T(s)$ and $C_n(s)$.

Lemma 12. *The angle between the tangent vector $T(s)$ and the corresponding tangent vector $T_n(s)$ to C_n is bounded above by*

$$\angle T(s) T_n(s) < 0.51005 K x. \tag{16}$$

Proof. Assume that s is between s_i and s_{i+1}. Then

$$\sin \angle T(s) T_n(s) = \frac{|[C(s_{i+1}) - C(s_i)] \times T(s)|}{|C(s_{i+1}) - C(s_i)|}. \tag{17}$$

But we have

$$C(s_{i+1}) - C(s_i) = \int_{s_i}^{s_{i+1}} T(t)\, dt,$$

and for any t, we have

$$T(t) = T(s) + \int_s^t T'(u)\, du.$$

This means that

$$[C(s_{i+1}) - C(s_i)] \times T(s) = \int_{s_i}^{s_{i+1}} T(t) \times T(s)\, dt \tag{18}$$

$$= \int_{s_i}^{s_{i+1}} \int_s^t T'(u) \times T(s)\, du\, dt. \tag{19}$$

Since $|T'(u) \times T(s)| \leq |T'(u)||T(s)| \leq \kappa(u) < K$, and s is between s_i and s_{i+1}, a small computation reveals that this integral is bounded by $\frac{K}{2}(s_{i+1} - s_i)^2$.

Since the length $|C(s_{i+1}) - C(s_i)|$ is bounded below by $(1/1.01)(s_{i+1} - s_i)$ by Lemma 11, we get

$$\sin \angle T(t) T_n(t) < \frac{1.01}{2} K x. \tag{20}$$

Since $1/x > (5/2)K$, this is always bounded above by $1.01/5$, and so

$$\angle T(t) T_n(t) < \frac{1.01^2}{2} K x. \tag{21}$$

□

We are now ready to embark on the main work of the proof: estimating the areas in Equation 13. We begin with the first term: the area bounded by the portion of $T(s)$ between s_i and s_{i+1}, together with the great circle arcs joining $T(s_i)$ and $T(s_{i+1})$ to $T_n(s_i)$. Without loss of generality, we may assume that $i = 0$, that $s_0 = 0$, and that $C(0) = \mathbf{0}$, and apply the Taylor expansion of Equation 14 to C at 0. Our strategy is to prove that this region is contained in a neighborhood of the great circle arc joining $T(0)$ and $T(s_1)$. Suppose s is between 0 and s_1. We want to bound the height of $T(s)$ above the $T(0), T(s_1)$ plane, or

$$h(s) := \frac{C'(s) \cdot C'(0) \times C'(s_1)}{|C'(0) \times C'(s_1)|}. \tag{22}$$

First, we have

$$\begin{aligned} C'(s_1) &= C'(0) + s_1 C''(0) + \frac{s_1^2}{2} C'''(0) + R_3(s_1). \\ C'(s) &= C'(0) + sC''(0) + \frac{s^2}{2} C'''(0) + R_3(s). \end{aligned}$$

Using the triple product identities, we can rewrite $h(s)$ in terms of the inner product of $C'(0)$ and the cross product of these vectors. For the triple product, we get

$$\left[\frac{s_1^2 s}{2} - \frac{s^2 s_1}{2}\right] C'(0) \cdot C''(0) \times C'''(0) + C'(0) \cdot \left[R_3(s_1) \times C'(s) + C'(s_1) \times R_3(s)\right]. \tag{23}$$

Expanding the last term, we see that is the sum of a term of order $s_1 s^3$ and a term of order $s s_1^3$. Thus, to leading order, the norm of the entire triple product is bounded above by

$$|h(s)| < H := \frac{KT}{2|C'(0) \times C'(s_1)|} s_1^3 + O(s_1^4), \tag{24}$$

since $s \in [0, s_1]$. We now consider the height of $T_n(0)$ above the $T(0), T(s_1)$ plane. Since $T_n(0)$ is the normalization of $C(s_1) - C(0) = C(s_1)$, this height is given by

$$\frac{C(s_1)}{|C(s_1)|} \cdot \frac{C'(0) \times C'(s_1)}{|C'(0) \times C'(s_1)|}. \tag{25}$$

As before, we get

$$C'(0) \times C'(s_1) = s_1 C'(0) \times C''(0) + \frac{s_1^2}{2} C'(0) \times C'''(0) + O(s_1^3). \tag{26}$$

Taking the dot product with the Taylor expansion of $C(s_1)$, we get only terms of order $O(s_1^4)$ and higher. Thus, to leading order, this region is contained in a rectangle based on the great circle arc joining $C'(0)$ and $C'(s_1)$ of height H. We now estimate the area of this rectangle.

First, we note that the length of the great circle joining $C'(0)$ and $C'(s_1)$ is given by the angle θ between $C'(0)$ and $C'(s_1)$. Since $s_1 < 1.01\,x$ by Lemma 11, this length is bounded above by $1.01\,Kx$, which is less than 0.404 by our hypotheses on x. Since H is small compared to s, we may assume that the entire rectangle is contained within a spherical disk of radius 0.5.

We project the rectangle to the plane by central projection: this map is increasing on lengths and areas, and increases length by at most a factor of 1.01. The area of the rectangle in the plane is overestimated by the product $1.01\,\theta H$. On the other hand, we have $|C'(0) \times C'(s_1)| = \sin\theta$. And for $\theta < 0.404$, $1.02 \sin\theta > \theta$. Keeping track of the various constants involved, and using the fact that $s_1 < 1.01\,x$ again, the area of this spherical region is overestimated by

$$\text{Area}\, R(T(s_i), T(s_{i+1}), T_n(s_i)) < KT\,x^3 + O(x^4), \tag{27}$$

We now turn to the second term in the Equation 13: the area of the spherical triangle bounded by $T(s_i)$, $T_n(s_{i-1})$ and $T_n(s_i)$. Without loss of generality we assume that $i = 1$, that $s_1 = 0$, and that $C(0) = \mathbf{0}$, and we expand C around 0 using Equation 14. We wish to compute

$$\text{Area}\,\triangle\left(\frac{C(s_0)}{|C(s_0)|}, \frac{C(s_2)}{|C(s_2)|}, C'(0)\right) = \left|\left(\frac{C(s_0)}{|C(s_0)|} - C'(0)\right) \times \left(\frac{C(s_2)}{|C(s_2)|} - C'(0)\right)\right|. \tag{28}$$

If we factor out $1/|C(s_0)||C(s_2)|$, we are left with the norm of the cross product of two terms:

$$\begin{aligned} C(s_0) - |C(s_0)|C'(0) &= (s_0 - |C(s_0)|)\, C'(0) + \frac{s_0^2}{2}C''(0) + \frac{s_0^3}{6}C'''(0) + R_4(s_0) \\ C(s_2) - |C(s_2)|C'(0) &= (s_2 - |C(s_2)|)\, C'(0) + \frac{s_2^2}{2}C''(0) + \frac{s_2^3}{6}C'''(0) + R_4(s_2). \end{aligned}$$

Using Lemma 11, we see that $|s - |C(s)|| < (K^2/24)s^3 + O(s^5)$, and we see that the leading term of this expression contains fifth powers of of s_0 and s_2, and is bounded by:

$$s_0^2 s_2^2 \left(\frac{K^3}{48} + \frac{KT}{12}\right)(s_0 + s_2) \tag{29}$$

However, we must still divide by $|C(s_0)||C(s_2)|$. By Lemma 11, we see that the ratios $s_0/|C(s_0)|$ and $s_2/|C(s_2)|$ are bounded above by 1.01. Thus, using the same Lemma to conclude that s_2 and s_0 are less than $1.01\,x$, and making a central projection argument as before, we are left with

$$\text{Area}\,\triangle(T_n(s_i), T_n(s_{i-1}), T(s_i)) < \frac{K^3 + KT}{3}x^3 + O(x^4). \tag{30}$$

Summing over i, and dividing by 2π, then writing K and T in terms of B_2 and B_3, we obtain the statement of the theorem. Note that we have overestimated the numerical constants to simplify the resulting formula. □

If a curve has a small region of high curvature, and larger regions of low curvature, it may be desirable to approximate the curve more carefully in the regions of high curvature in order to save time in the computation of writhe. Since our error bound is additive along the curve, these methods are well suited to this case. We have

Corollary 13. *Suppose C is a $\mathcal{C}^4$ curve and C_n is a curve inscribed in C so that C and C_n obey the hypotheses of Theorem 9.*

If C and C_n are divided into regions R_i, each containing n_i edges which are bounded above in length by x_i, and so that the derivatives of C are bounded by $B_{1i}, \dots, B_{4i}$ and $1/x_i > 5B_{2i}$, then

$$|\,\text{Wr}(C) - \text{Wr}(C_p)| < \sum_i \alpha_i\, n_i x_i^3 + n_i O(x_i^4).$$

where each α_i is a numerical constant less than $B_{2i}(5B_{2i}^2 + B_{3i})$.

We make one more observation:

Proposition 14. *Let C be a simple, closed space curve of class $\mathcal{C}^2$, and C_p be a polygonal approximating curve as in Theorem 9 or Corollary 13.*

If the arc joining the endpoints of a sequence of n edges of C_p is planar, then the $n-2$ edges interior to this region contribute nothing to the error bound in the Theorem.

In particular, this means that the derivative bounds in both statements can be taken to be bounds on the derivatives of the non-planar *regions of the curve C.*

Proof. On these edges, the tantrix of the smooth curve and the polygonal curve parametrize the same great circle arc on S^2. Thus, the ribbon between these curves has zero area. □

8. Example Computations

We are now prepared to test Theorem 1 by computing the writhing numbers of various polygonal approximations of a smooth curve, and comparing the results to the exact writhe of the smooth curve. To control the numerical error introduced in these calculations, all of these computations were performed using an arbitrary-precision implementation of Banchoff's formula for the writhing number of a polygonal curve. The initial runs were performed with 45 decimal digits of precision. They were checked against runs performed with 54 digits of precision. Since the results agreed, we feel confident that roundoff error does not affect the computations reported on below.

The curve whose writhe we computed is an example of Fuller[11]:

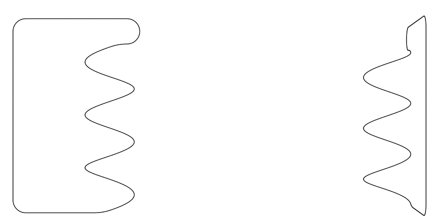

Figure 4. This example of Fuller's "closed helix" is composed of 3 turns of a helix of radius 1 with pitch angle 0.33, with ends joined by a planar curve.

Using Theorem 3, and the Călugăreanu-White formula, it is easy to see that the writhe of this curve is $3(1-\sin 0.33) \simeq 2.0278709$. After all, the area enclosed by the tantrix of this curve C is that of a hemisphere, plus 3 enclosures of a spherical cap of radius $\pi/2 - 0.33$. Thus the writhe of the curve is equal to $1 - \sin 0.33 \mod 2$. To complete the computation, one sets up a frame on the curve, and computes its twist and linking number. (Details for this computation can be found in [11].)

We now take a series of polygonal approximations to C, and compare the difference between their writhing numbers and the writhe of C to the bounds of Theorem 9.

We begin by finding bounds on the derivatives of C and the edge length of our approximations. By Proposition 14, it suffices to find derivative bounds for the helical region of C. Since the helix has unit radius, both B_2 and B_3 can be taken to be one. The curve is parametrized so that $|C'(s)| \geq 1$.

Here are the results of computing writhe with various numbers of edges:

n	$\mathrm{Wr}(C_n)$	$\lvert\mathrm{Wr}(C_n) - \mathrm{Wr}(C)\rvert$	x	$\alpha\, n x^3$
100	2.00541	0.02246	0.506	77.73
250	2.02434	0.00353	0.203	12.55
500	2.02697	0.0009	0.101	3.09
1000	2.02763	0.00024	0.051	0.786

It is worth examing a graph of these results.

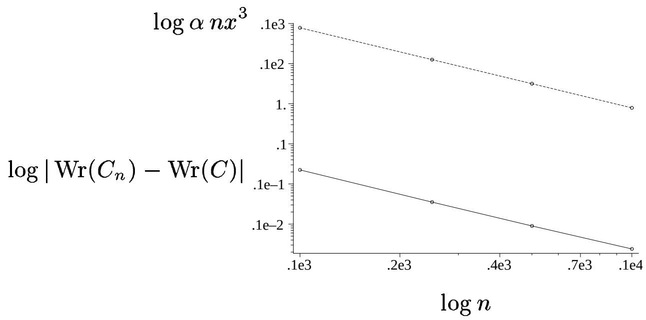

Figure 5. This graph shows a log-log plot of the actual error in computing the writhing number for one of Fuller's "closed helices" with various numbers of edges (lower solid line), together with our error bounds (upper dotted line). The fact that the lines are parallel shows that the convergence is of order n^2, as predicted by Theorem 9.

9. Further Directions

In this paper, we have given a set of asymptotic error bounds which allow us to compute the writhe of a closed space curve with defined accuracy by computing the writhe of a polygonal approximation to this curve. The example we computed in Section 8 shows that our bounds are of the right order of magnitude: roughly speaking, the writhe converges quadratically in the number of edges of the approximation. Our work leaves open several directions for further inquiry.

First, it is puzzling that our approximation theorem for curves with corners (Proposition 6) should depend on the hypothesis that the limit curve is polygonal. To sketch an extension of this result, we recall a definition from Chern ([8]):

Definition 15. *The tantrix of a piecewise C^1 curve $C(s)$ with positive corner angles is the image of $T(s)$ on the unit sphere, together with the great circle arcs joining the pairs of tangent vectors at each corner of the curve.*

We note that our Theorem 7 shows that Fuller's $\Delta\mathrm{Wr}$ formula holds for polygonal curves with the definition of tantrix extended as above. We further suspect that:

Conjecture 16. *Fuller's Spherical Area formula (Theorem 3) and Fuller's* $\Delta\mathrm{Wr}$ *formula (Theorem 4) hold for piecewise* C^2 *curves with the extended definition of tantrix given by Definition 15.*

The proofs of both of these theorems depend on the Călugăreanu-White formula, which only applies to closed curves. Thus all of our results are restricted to closed curves. This leaves open a much more important problem:

Problem 17. *Extend all these theorems (the Călugăreanu-White formula, Fuller's spherical area formula, and Fuller's* $\Delta\mathrm{Wr}$ *formula) to open curves.*

In particular, extending the results of this paper to open curves would be useful for applications in biology, where the curves of interest are not neccesarily closed. We note that while Fuller's $\Delta\mathrm{Wr}$ formula makes sense for open curves, computational examples show that it does not give the correct answer: boundary terms must be added to account for the ends of the curves.

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