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Existence of ideal knots

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Abstract Ideal knots are curves that maximize the scale invariant ratio of thickness to length. Here we present a simple argument to establish the existence of ideal knots for each knot type and each isotopy class and show that they are $C^{1,1}$ curves.

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1 Introduction

Any continuously differentiable, non-self-intersecting curve can be thickened normal to itself to produce a non-self-intersecting tube of constant radius centered on the curve. If the curve is straight there is no upper bound on the tube radius, but for non-straight curves there is a critical value of the radius above which the tube intersects itself. This critical value is a geometrical property of the curve called its *thickness* or *normal injectivity radius* [1],[2]. A natural optimization problem is to find the thickest curve of prescribed length amongst those of a given knot type. The thickness of such a curve is an intrinsic property of the knot, and the curve itself provides a certain *ideal shape* or representation of the knot type [3]. (Notice that some authors prefer the term *tight* over *ideal*.) Approximations of ideal shapes in this sense have been found via a series of computer experiments [4],[5]. These shapes were seen to have intriguing physical features, and even a correspondence to time-averaged shapes of knotted DNA molecules in solution [3]–[6].

Ideal shapes of knots can be defined in various different ways. For example, rather than fix length and maximize thickness over a prescribed class of knotted curves [7], one may instead fix thickness and minimize length [8]. (For other formulations and related problems see Section 4.) These equivalent definitions capture the physical idea that, when a simple knot in a piece of rope is pulled tight, it always achieves a geometrical configuration with a minimum length of rope within the knot. Such a configuration corresponds to an ideal shape; the essential quantity being optimized is a scale invariant ratio between thickness and length. Intuition suggests that there should be at least one such shape depending on the complexity of a given knot.

In this article we prove the existence of ideal shapes for each knot type; indeed, for each knot isotopy class. The basic problem we address is that of maximizing the thickness functional over sets of C^1 curves of prescribed length and topology. For this purpose, we use the observation of [7] that for smooth curves γ, the thickness or normal injectivity radius can be identified with the global radius of curvature functional

$$\Delta[\gamma] \quad = \inf_{\substack{x,y,z\in\gamma \\ x\neq y\neq z\neq x}} R(x,y,z)$$

where $R(x,y,z)$ denotes the radius of the circle through the three distinct points x, y and z. This functional can be defined for parameterized curves in a natural way; for example, as in [8]. Using such a definition we show that $\Delta[\gamma]$ is bounded from above and upper semi-continuous on the set of unit length curves that are parameterized by arclength and satisfy $\Delta[\gamma] \geq \theta > 0$. Because this set and any of its subsets defined by prescribing knot type or isotopy class is closed under convergence in the C^0-norm, we are able to exploit standard direct methods and obtain existence of curves of maximal thickness for each knot type and isotopy class. We find furthermore that these ideal shapes are actually in the class of $C^{1,1}$ curves, which means that their unit tangent fields are Lipschitz continuous.

Similar existence results were recently established in [8] by different techniques. The basic problem studied there was that of minimizing general energy functionals over sets of framed curves subject to a lower bound on thickness. That framework covers not only the ideal knot problem (where the energy being minimized is the arclength functional), but also various other problems in elastic rod theories which are motivated, for example, by the optimal packing of biological filaments [9],[10]. Here we give a more succinct existence proof for ideal shapes using a different variational principle. Our approach is similar to that used in the proof of Tonnelli's theorem on the existence of shortest geodesics in a given homotopy class. Moreover, after our work was completed we were made aware of [11], which contains arguments related to those here.

The presentation is structured as follows. In Section 2 we define and outline various properties of the global radius of curvature functional $\Delta[\gamma]$ as discussed above. In Section 3 we provide a variational characterization of ideal shapes and establish their existence as $C^{1,1}$ curves. In Section 4 we discuss alternative variational formulations for ideal shapes and extend our existence result to cover a class of optimal packing problems as considered in [9].

2 Global curvature

Our definition of ideal shapes is based on the global curvature functions introduced in [7]. Here we define these functions and summarize some of their properties. With the exception of Lemmas 4 and 5, results similar to those below are detailed in [8].

2.1 Preliminaries

Throughout our developments we consider closed curves γ belonging to one or more of the sets $C^0(S,\mathbb{R}^3)$, $C^1(S,\mathbb{R}^3)$ or

$$\mathcal{Q} = \{\gamma \in C^1(S,\mathbb{R}^3) \mid \quad |\gamma'(s)| = 1, \quad s \in S\}$$

where S is the circle with unit perimeter; in particular, $S \cong \mathbb{R}/\mathbb{Z}$. A curve γ will be called *simple* if it has no self-intersections, that is, if the map $\gamma : S \to \mathbb{R}^3$ is injective. Otherwise, the curve γ will be called *non-simple*. In this case there exist pairs $s, t \in S$ $(s \neq t)$ for which $\gamma(s) = \gamma(t)$. Any such pair will be called a *double point* of γ. Since $\mathcal{Q} \subset C^1(S,\mathbb{R}^3) \subset C^0(S,\mathbb{R}^3)$ we use the usual C^0 and C^1 topologies when discussing limits and continuity in $\mathcal{Q}$.

We use $|\cdot|$ to denote the (intrinsic) distance between two points in $\mathbb{R}^3$ or S depending on the context. To denote the angle between two non-zero vectors u and v in $\mathbb{R}^3$ we use $\sphericalangle(u,v) \in [0,\pi]$. The distance between a point $x \in \mathbb{R}^3$ and a subset $\Sigma \subset \mathbb{R}^3$ will be denoted by $\mathrm{dist}(x,\Sigma)$ and the diameter of Σ will be denoted by $\mathrm{diam}(\Sigma)$. For any $r > 0$ we define open neighborhoods of x and Σ by

$$B_r(x) = \{y \in \mathbb{R}^3 \mid |y - x| < r\} \quad \text{and} \quad B_r(\Sigma) = \{y \in \mathbb{R}^3 \mid \mathrm{dist}(y,\Sigma) < r\}.$$

When Σ is the image of a curve $\gamma \in \mathcal{Q}$, we call $B_r(\Sigma) = B_r(\gamma)$ the *tubular neighborhood* of γ with radius $r > 0$. We say that $B_r(\gamma)$ is *non-self-intersecting* or *regular* if the closest-point projection map $\Pi_\gamma : B_r(\gamma) \to \gamma$ is single-valued and continuous. That is to say, for any $x \in B_r(\gamma)$ there is exactly one $s(x) \in S$ such that $\Pi_\gamma(x) := \gamma(s(x))$ satisfies

$$\mathrm{dist}(x,\gamma) = |\gamma(s(x)) - x|,$$

and $\Pi_\gamma(x)$ is a continuous function of $x \in B_r(\gamma)$. The existence of such non-self-intersecting tubular neighborhoods is guaranteed by the tubular neighborhood theorem [12]. For further justification of this notion of non-self-intersecting see the discussion following Lemma 2.

2.2 Global radius of curvature functions

Following [7], [8] we define the global radius of curvature functions ρ_G and Δ for parameterized space curves γ as follows.

Definition 1 *Let $\gamma : S \to \mathbb{R}^3$. Then the global radius of curvature of γ at the point $\gamma(s)$, $s \in S$, is given by*

$$\rho_G[\gamma](s) \;:=\; \inf_{\substack{\sigma,\tau \in S\setminus\{s\} \\ \sigma\neq\tau}} R(\gamma(s), \gamma(\sigma), \gamma(\tau)), \tag{1}$$

and we denote its infimum by

$$\Delta[\gamma] := \inf_{s\in S} \rho_G[\gamma](s). \tag{2}$$

Here $R(x, y, z) \geq 0$ is the radius of the *smallest* circle containing x, y and z. When x, y and z are non-collinear there is a unique circle passing through them and

$$R(x, y, z) = \frac{|x - y|}{|2 \sin[\sphericalangle(x - z, y - z)]|}, \tag{3}$$

which implies that $R(x, y, z)$ is continuous at non-collinear points. When x, y and z are collinear and distinct there is no circle passing through all three points and $R(x, y, z)$ is defined to be infinite. However, if two points coincide, say $x = z$ or $y = z$, then there are many circles through the three points and $R(x, y, z)$ is the smallest possible radius; namely, the distance $|x - y|/2$. A straightforward consequence of Definition 1 is:

Lemma 1 *Consider any $\gamma \in C^0(S, \mathbb{R}^3)$. If γ has a double point at the pair $s, t \in S$ ($s \neq t$), then $\rho_G[\gamma](s) = \rho_G[\gamma](t) = 0$. If $\Delta[\gamma] > 0$, then γ is simple.*

The functional $\Delta[\gamma]$ is invariant under various transformations of the curve γ. From the definition of $R(x, y, z)$ we deduce that $\Delta[\gamma]$ is invariant under translations, rotations and reflections of γ. Moreover, $\Delta[\gamma]$ is invariant under reparameterization in these sense that $\Delta[\gamma \circ \pi] = \Delta[\gamma]$ for any bijection $\pi : S \to S$. The functional $\Delta[\gamma]$ is also covariant under scaling in the sense that $\Delta[\lambda\gamma] = \lambda\Delta[\gamma]$ for any $\lambda > 0$.

2.3 Geometric interpretations

When a closed curve γ is both simple and smooth, the functions $\rho_G[\gamma]$ and $\Delta[\gamma]$ are known to be related to the standard local radius of curvature $\rho[\gamma]$, and to the thickness or normal injectivity radius $\mathrm{Inj}[\gamma]$ as discussed in Section 1. In particular, $0 \leq \rho_G[\gamma](s) \leq \rho[\gamma](s)$ for all $s \in S$ and $\Delta[\gamma] = \mathrm{Inj}[\gamma]$ [7]. Here we generalize these ideas to curves in the set $\mathcal{Q}$. The first result is:

Lemma 2 *Consider a curve $\gamma \in \mathcal{Q}$ and for any $s \in S$ let $D_\theta(\gamma(s), \gamma'(s))$ denote the open planar disk of radius $\theta > 0$ centered at $\gamma(s)$ and contained in the plane perpendicular to $\gamma'(s)$, let $C(s,\theta)$ denote the circular perimeter of $D_\theta(\gamma(s), \gamma'(s))$, and let*

$$M(s,\theta) = \bigcup_{z \in C(s,\theta)} B_\theta(z)$$

(*see Figure 1a*). *Then*

(i) $\gamma \cap M(s,\theta) = \emptyset$ *for all* $s \in S$ *iff* $\Delta[\gamma] \geq \theta$,

(ii) $\mathrm{diam}(\gamma) \geq 2\theta$ *if* $\Delta[\gamma] \geq \theta$,

(iii) $B_\theta(\gamma)$ *is regular iff* $\Delta[\gamma] \geq \theta$,

(iv) Π_γ *has the property* $\Pi_\gamma^{-1}(\gamma(s)) \cap B_\theta(\gamma) = D_\theta(\gamma(s), \gamma'(s))$ *if* $B_\theta(\gamma)$ *is regular.*

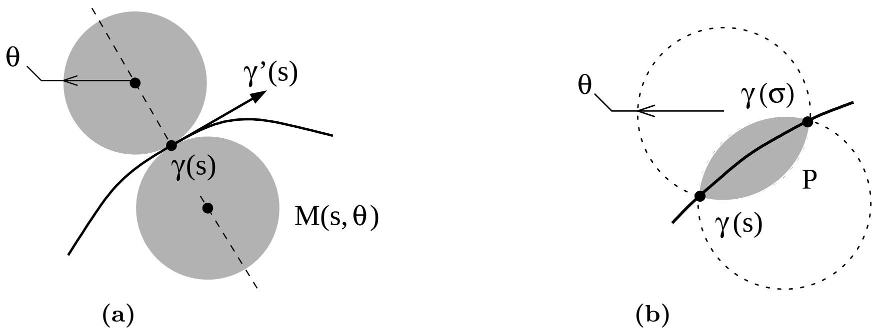

Fig. 1 Two dimensional illustration of (a) the set $M(s,\theta)$ defined in Lemma 2 and (b) the set P defined in the proof of Lemma 3.

The above results follow from the definitions of $\Delta[\gamma]$, $M(s,\theta)$ and $B_\theta(\gamma)$. Item (i) implies that if $\Delta[\gamma] \geq \theta$, then an open ball of radius θ placed tangent at any point $\gamma(s)$ may be rotated around the tangent vector $\gamma'(s)$ without intersecting the curve. On the other hand, if $\Delta[\gamma] < \theta$, then there is a point on the curve about which a similar rotation of such a ball could not be effected. Thus $\Delta[\gamma]$ is the radius of the largest ball that can be rotated tangentially about every point of a curve γ without intersecting it.

According to item (ii) the inequality $\Delta[\gamma] \geq \theta$ imposes a lower bound on the overall size of γ. From this result we conclude that $\Delta[\gamma]$ must be bounded on $\mathcal{Q}$. In particular, because the diameter of curves in $\mathcal{Q}$ cannot exceed one-half their (unit) length, we find that $\Delta[\gamma]$ cannot exceed one-fourth this length.

Items (iii) and (iv) imply that the regularity of the tubular neighborhood $B_\theta(\gamma)$ is equivalent to the condition $\Delta[\gamma] \geq \theta$, and that $B_\theta(\gamma)$ is the union of disjoint disks $D_\theta(\gamma(s), \gamma'(s))$. Since each point $x \in B_\theta(\gamma)$ is in a unique disk $D_\theta(\gamma(s), \gamma'(s))$ normal to the curve, we deduce that $B_\theta(\gamma)$ has the structure of a uniform tube of radius θ centered on γ. Moreover, according to item (iii), any tubular neighborhood of radius larger than $\Delta[\gamma]$ would fail to have this structure. Thus $\Delta[\gamma]$ may be identified with the notion of normal injectivity radius as discussed in [1],[2].

The next result shows that a positive lower bound on $\Delta[\gamma]$ imposes a certain amount of regularity on a curve γ.

Lemma 3 *Consider a curve $\gamma \in \mathcal{Q}$ and suppose $\Delta[\gamma] \geq \theta > 0$. Then γ has a Lipschitz continuous tangent γ' with Lipschitz constant θ^{-1}, that is, $\gamma \in C^{1,1}(S, \mathbb{R}^3)$ and*

$$|\gamma'(s) - \gamma'(\sigma)| \leq \theta^{-1}|s - \sigma| \quad \forall s, \sigma \in S. \tag{4}$$

The condition $\gamma \in C^{1,1}(S, \mathbb{R}^3)$ implies that the standard local curvature of γ exists almost everywhere, and (4) implies that it is bounded by θ^{-1}.

Proof The above result follows from the fact that, when $|s-\sigma|$ is sufficiently small, for example $|s - \sigma| < \theta/2$, the arc of γ between $\gamma(s)$ and $\gamma(\sigma)$ must be contained in (the closure of) the pod-shaped intersection P of all open balls of radius θ containing $\gamma(s)$ and $\gamma(\sigma)$ on their boundaries as illustrated in Figure 1b. This implies that the tangent vector $\gamma'(s)$ is contained in the cone with vertex $\gamma(s)$, axis $\mathcal{L}$ and opening angle α, where $\mathcal{L}$ is parallel to the chord $\gamma(\sigma)-\gamma(s)$ and α is given by $\sin(\alpha/2) = |\gamma(\sigma)-\gamma(s)|/2\theta$. Since $\gamma'(\sigma)$ is in a similar cone with the same opening angle we conclude that (4) holds for the case when $|s - \sigma| < \theta/2$. The result for all $s, \sigma \in S$ is obtained by partitioning an arbitrary interval into a finite number of sufficiently small intervals. $\square$

From the proof of Lemma 3 and the a-priori estimate (4) we deduce that, when $|s - \sigma|$ is sufficiently small, the arc of curve between $\gamma(s)$ and $\gamma(\sigma)$ has a unit tangent field that is nearly parallel to the chord between these points. This leads to the following uniform bound:

Lemma 4 *Let $\theta > 0$ be given. Then there is a constant $C \in (0, 1)$ such that for any $\gamma \in \mathcal{Q}$ with $\Delta[\gamma] \geq \theta$ we have*

$$C|s - \sigma| \leq |\gamma(s) - \gamma(\sigma)| \leq |s - \sigma| \tag{5}$$

for any $s, \sigma \in S$ with $|s - \sigma| \leq \theta/2$.

2.4 Continuity properties of $\Delta[\gamma]$

Here we outline various continuity properties of the functional $\Delta[\gamma]$ for curves $\gamma \in \mathcal{Q}$. While it is natural to consider the C^1 topology on $\mathcal{Q}$, we opt for generality and establish these properties under the C^0 topology by exploiting Lemmas 3 and 4.

Our first result states that the subset of curves satisfying $\Delta[\gamma] \geq \theta > 0$ is closed under C^0 convergence in $\mathcal{Q}$. Moreover, $\Delta[\gamma]$ is upper semi-continuous with respect to C^0 convergence in this set.

Lemma 5 *Let $\{\gamma_n\} \subset \mathcal{Q}$ be a sequence of curves such that $\Delta[\gamma_n] \geq \theta > 0$ for all $n \in \mathbb{N}$ and suppose $\gamma_n \to \gamma$ in $C^0(S, \mathbb{R}^3)$. Then the limit γ is a simple curve in $\mathcal{Q}$ and $\Delta[\gamma] \geq \theta$. Consequently, if $\Delta[\gamma_n] \to \eta$, then $\Delta[\gamma] \geq \eta$.*

Proof The conclusion that $\gamma \in \mathcal{Q}$ follows from the fact that $\{\gamma_n\}$ is an equicontinuous and uniformly bounded family of functions in $C^1(S, \mathbb{R}^3)$. In particular, equicontinuity follows from Lemma 3 since

$$\begin{aligned} |\gamma_n(s) - \gamma_n(\sigma)| &\leq |s - \sigma|, \quad \forall s, \sigma \in S \\ |\gamma_n'(s) - \gamma_n'(\sigma)| &\leq \theta^{-1}|s - \sigma|, \quad \forall s, \sigma \in S, \end{aligned} \tag{6}$$

and uniform boundedness follows from the conditions $\gamma_n \to \gamma$ in $C^0(S, \mathbb{R}^3)$ and $|\gamma_n'(s)| = 1$. Thus we may extract a subsequence $\{\gamma_{n_j}\}$ that converges in $C^1(S, \mathbb{R}^3)$ to a curve μ; moreover, $\mu \in \mathcal{Q}$ since $|\mu'(s)| = 1$. Since $\gamma_n \to \gamma$ in C^0 and $\gamma_{n_j} \to \mu$ in C^1 we must have $\gamma = \mu$ by uniqueness of limits in C^0. Thus γ is in $\mathcal{Q}$.

The fact that γ is simple follows from the observation that it is the C^1-limit of a subsequence $\{\gamma_{n_j}\}$ where, by Lemma 2, each γ_{n_j} has a regular tubular neighborhood of radius $\theta > 0$. More explicitly, we may first pass to the limit in (5) and deduce that, in any small interval $|s - \sigma| < \theta/2$, the arc of curve between $\gamma(s)$ and $\gamma(\sigma)$ must be simple. Next, we suppose for contradiction that there exist parameters $|s_1 - s_3| \geq \theta/2$ such that $\gamma(s_1) = \gamma(s_3) = z$. By (5) again we can find parameters s_2 and s_4 close to s_1 and s_3, respectively, such that $s_1 < s_2 < s_3 < s_4$, $\gamma(s_2) \neq z$ and $\gamma(s_4) \neq z$. Let $2r = \min\{|\gamma(s_2) - z|, |\gamma(s_4) - z|, \theta\}$ and consider the open ball $B_r(z)$. Since $\gamma_n \to \gamma$ in C^0 we find that $\gamma_n(s_1)$ and $\gamma_n(s_3)$ are inside $B_r(z)$ while $\gamma_n(s_2)$ and $\gamma_n(s_4)$ are outside for all n sufficiently large. Since each γ_n is a simple closed curve it must have at least four intersections with the sphere $\partial B_r(z)$. This contradicts the lower bound $\Delta[\gamma_n] \geq \theta$. Thus the limit curve γ must be simple.

The limit curve $\gamma \in \mathcal{Q}$ must also satisfy the bound $\Delta[\gamma] \geq \theta$. Otherwise, we can find three non-collinear points $\gamma(\sigma_i)$ $(i = 1, 2, 3)$ with the property that $R(\gamma(\sigma_1), \gamma(\sigma_2), \gamma(\sigma_3)) < \theta$. Because $\gamma_n \to \gamma$ in C^0 and the function R is continuous at non-collinear points we would then conclude that $\Delta[\gamma_n] < \theta$ for n sufficiently large, which is a contradiction. Thus the limit curve must satisfy $\Delta[\gamma] \geq \theta$. Moreover, if $\Delta[\gamma_n] \to \eta$, then for any $\epsilon > 0$ we have $\Delta[\gamma_n] \geq \eta - \epsilon$ for all n sufficiently large. By the same arguments as before we find that the limit curve must satisfy the bound $\Delta[\gamma] \geq \eta - \epsilon$, which implies $\Delta[\gamma] \geq \eta$ by the arbitrariness of ϵ. This establishes the upper semicontinuity of the functional Δ. $\square$

In our application we will consider curves in $\mathcal{Q}$ that are in a fixed isotopy class in the following sense:

Definition 2 *Two continuous closed curves $K_1, K_2 \subset \mathbb{R}^3$ are isotopic, denoted as $K_1 \simeq K_2$, if there are open neighborhoods N_1 of K_1, N_2 of K_2, and a continuous mapping $\Phi : N_1 \times [0,1] \to \mathbb{R}^3$ such that $\Phi(\cdot, \tau)$ is a homeomorphism for each $\tau \in [0,1]$, $\Phi(x,0) = x$ for all $x \in N_1$, $\Phi(N_1, 1) = N_2$, and $\Phi(K_1, 1) = K_2$.*

Roughly speaking, two curves are in the same isotopy class if one can be continuously deformed onto the other.

Isotopy classes provide a notion of equivalence for knotted curves. In particular, if two curves are isotopic, they have the same knot type. However, the converse is not necessarily true. Here we take knot type to mean the weakest possible notion of equivalence as defined, for example, by homeomorphisms which are not necessarily homotopic to the identity map or orientation-preserving. In this sense a trefoil and its mirror image are of the same knot type, but they are not in the same isotopy class. To indicate that two curves K_1 and K_2 are of the same knot type we use the notation $K_1 \sim K_2$.

The next result states that a C^0-convergent sequence of curves $\{\gamma_n\} \subset \mathcal{Q}$ subject to a uniform, positive lower bound on $\Delta[\gamma_n]$ cannot change isotopy class (a fortiori cannot change knot type) for all sufficiently large n. This will allow us to control the topology of limits.

Lemma 6 *Let $\{\gamma_n\} \subset \mathcal{Q}$ be a sequence of curves such that*

(i) $\Delta[\gamma_n] \geq \theta > 0, \qquad \forall n \in \mathbb{N}$,

(ii) $\gamma_n \to \gamma$ *in* $C^0(S, \mathbb{R}^3)$ *as* $n \to \infty$.

Then $\gamma \simeq \gamma_n$ for all n sufficiently large.

Proof From Lemma 5 we immediately deduce that the limit γ is a simple curve in $\mathcal{Q}$ and $\Delta[\gamma] \geq \theta$. In particular, the proof of Lemma 5 shows that $\{\gamma_n\}$ actually converges to γ in the C^1 sense. The construction of the isotopy map Φ between γ and γ_n for all n sufficiently large then follows because the closest-point projection onto the image of γ_n restricted to γ is bijective. $\square$

3 Variational formulation and main result

Using the global radius of curvature functional $\Delta[\gamma]$ we can formulate variational problems to describe ideal shapes in $\mathcal{Q}$. In particular, let $\mathcal{Q}_k$ be the subset of $\mathcal{Q}$ consisting of all curves of the same isotopy class as a given simple curve $k \in \mathcal{Q}$, and let $\mathcal{Q}_k^0$ be the subset of all curves of the same knot type as k, that is

$$\mathcal{Q}_k = \{\gamma \in C^1(S, \mathbb{R}^3) \mid \quad \gamma(0) = 0, \quad \gamma \simeq k, \quad |\gamma'(s)| = 1, \quad s \in S\},$$
$$\mathcal{Q}_k^0 = \{\gamma \in C^1(S, \mathbb{R}^3) \mid \quad \gamma(0) = 0, \quad \gamma \sim k, \quad |\gamma'(s)| = 1, \quad s \in S\}$$

where, without loss of generality, we fix $\gamma(0) = 0$ to eliminate rigid translations. We consider the problems of finding curves $\gamma_* \in \mathcal{Q}_k$ and $\gamma_*^0 \in \mathcal{Q}_k^0$ such that

$$\Delta[\gamma_*] = \sup_{\gamma \in \mathcal{Q}_k} \Delta[\gamma] \quad \text{and} \quad \Delta[\gamma_*^0] = \sup_{\gamma \in \mathcal{Q}_k^0} \Delta[\gamma]. \tag{7}$$

Any solution γ_* of the first problem is an ideal shape for the isotopy class represented by k, and any solution γ_*^0 of the second is an ideal shape for the knot type. By Lemma 2, these ideal shapes admit the thickest, regular tubular neighborhood within their isotopy class and knot type. Our main existence result is:

Theorem 1 *For any simple curve $k \in \mathcal{Q}$ the maximization problems defined in (7) have solutions $\gamma_* \in \mathcal{Q}_k$ and $\gamma_*^0 \in \mathcal{Q}_k^0$. Every solution to either problem is actually in $C^{1,1}(S, \mathbb{R}^3)$.*

Proof Since every curve $\gamma \in \mathcal{Q}$ has unit length the functional $\Delta : \mathcal{Q} \to \mathbb{R}$ is bounded by Lemma 2(ii). Thus the suprema $\eta_k = \sup_{\mathcal{Q}_k} \Delta[\gamma]$ and $\eta_k^0 = \sup_{\mathcal{Q}_k^0} \Delta[\gamma]$ considered in (7) are finite.

Consider first the problem in $(7)_1$ and let $\{\gamma_n\} \subset \mathcal{Q}_k$ be any maximizing sequence such that $\Delta[\gamma_n] \to \eta_k$. Without loss of generality we may suppose that $\Delta[\gamma_n] \geq \Delta[k] > 0$ where the strict inequality follows from the fact that k is simple. As in the proof of Lemma 5, we claim the sequence $\{\gamma_n\}$ is an equicontinuous family of functions in $C^1(S, \mathbb{R}^3)$. In particular, this sequence satisfies the bounds in (6) with $\theta = \Delta[k] > 0$. Because the sequence is also uniformly bounded in $C^1(S, \mathbb{R}^3)$ we may extract a subsequence that converges in the C^1 sense to a curve γ_*. This convergence implies that $|\gamma_*'(s)| = 1$ and $\gamma_*(0) = 0$.

From Lemma 5 we find that γ_* is a simple curve. Furthermore, from Lemma 6 we deduce that $\gamma_* \in \mathcal{Q}_k$. In particular, γ_* is isotopic to γ_n for all n sufficiently large, and each γ_n is by definition isotopic to k. By the semicontinuity of Δ we have $\Delta[\gamma_*] \geq \eta_k$, which implies $\Delta[\gamma_*] = \eta_k$ since η_k is the supremum. Thus γ_* is an ideal shape for the knot isotopy class represented by k. The $C^{1,1}$ regularity of γ_* follows from Lemma 3.

The same arguments lead to similar results for problem $(7)_2$. In particular, let $\{\gamma_n^0\} \subset \mathcal{Q}_k^0$ be any maximizing sequence such that $\Delta[\gamma_n^0] \to \eta_k^0$. As before, this sequence is equicontinuous and uniformly bounded in $C^1(S, \mathbb{R}^3)$ and we may extract a subsequence that converges in the C^1 sense to a curve γ_*^0. The conclusion that $\gamma_*^0 \in \mathcal{Q}_k^0$ follows from the fact that, by Lemma 6, γ_*^0 is isotopic to γ_n^0 for all n sufficiently large (thus the isotopy class eventually becomes constant along the sequence), and each γ_n^0 is by definition of the same knot type as k. From the semicontinuity of Δ we deduce $\Delta[\gamma_*^0] = \eta_k^0$, which implies that γ_*^0 is an ideal shape for the knot type represented by k, and the $C^{1,1}$ regularity of γ_*^0 follows from Lemma 3. $\square$

Thus for every knot type and isotopy class there exists an ideal shape in $\mathcal{Q}$ whose regularity is at least $C^{1,1}(S, \mathbb{R}^3)$. Similar results are presented in [8],[11].

The above results imply the existence of maximizers for each handedness of any knot that is not isotopic to its mirror image; for example, a trefoil. Furthermore, regardless of its handedness every maximizer for such a knot must have the same thickness since $\Delta[\gamma]$ is invariant under reflections.

Because regularity follows directly from Lemma 3, and does not rely on any extremal properties, one may speculate that ideal shapes are actually smoother than $C^{1,1}$. However, numerical data presented in [7] suggests that the ideal shapes of some composite knots are not C^2. Similarly, examples presented in [11] show that the ideal configurations of some linked (but unknotted) curves are also not C^2. Thus the $C^{1,1}$ regularity established in the above result may be quite sharp.

The variational characterization (7) can be exploited to derive necessary conditions for a knotted curve to be ideal. For example, in [7] it was shown that a smooth curve can be ideal only if its global radius of curvature function ρ_G is constant and minimal on every non-straight segment of the curve. In contrast, the numerical data presented in [7] suggest that the standard local radius of curvature is not constant on ideal shapes.

4 Other topologies, variational principles and results

The key to the existence argument presented here is Lemma 3 which implies equicontinuity in the C^1 topology for maximizing sequences in $\mathcal{Q}$. We point out that there are different variants of the argument that one can follow which, for some purposes, may be preferable to the one presented here. In particular, one may want to work in a space of curves different from $\mathcal{Q}$, and possibly take limits in topologies other than C^1.

One alternative is to consider a space of continuous curves with an upper bound on length together with the C^0 topology. To obtain existence results in this case it suffices that the limit of simple curves which are in a given knot class and satisfy $\Delta \geq \theta > 0$ itself be a simple curve in the same knot class, that Δ be upper semicontinuous under this topology when the limit curve is simple and that bounded sets in $C^{1,1}$ be compact. In this case, one could pass to the limit and use the fact that the length functional is lower semicontinuous in the C^0 topology. Curves that maximize Δ must then achieve the upper bound on length; otherwise, one could rescale the curve until the bound is achieved and therefore increase Δ since it is covariant under scalings.

Other variational principles in which Δ is maximized can also be considered. For example, one can consider maximizing Δ subject to bounds on the diameter of a curve, or on the radius of gyration of a curve and so on. Like Δ and length, these quantities are also covariant under scalings. An example class of problems along these lines would be to find curves $\gamma_* \in \mathcal{Q}_{k,a}$ such that

$$\Delta[\gamma_*] = \sup_{\gamma \in \mathcal{Q}_{k,a}} \Delta[\gamma]$$

where

$$\mathcal{Q}_{k,a} = \{\gamma \in C^1(S, \mathbb{R}^3) \mid \gamma(0) = 0,\ \gamma \simeq k,\ G[\gamma] \leq a,\ |\gamma'(s)| = 1,\ s \in S\}.$$

Here k is a simple curve of prescribed knot type, $G[\gamma]$ is a given functional (for example, radius of gyration) and a is a constant. When $G[\gamma]$ is lower semicontinuous in the C^1 topology on $\mathcal{Q}$, we find that existence of maximizers follows by the same arguments used in the proof of Theorem 1. Thus, for closed curves, we obtain existence for various optimal packing problems as considered in [9].

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