SELF-CONTACT SETS FOR 50 TIGHTLY KNOTTED AND LINKED TUBES

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ABSTRACT. We report on new numerical computations of the set of self-contacts in tightly knotted tubes of uniform circular cross-section. Such contact sets have been obtained before for the trefoil and figure eight knots by simulated annealing — we use constrained gradient-descent to provide new self-contact sets for those and 48 other knot and link types. The minimum length of all unit diameter tubes in a given knot or link type is called the ropelength of that class of curves. Our computations yield improved upper bounds for the ropelength of all knots and links with 9 or fewer crossings except the trefoil.

1. INTRODUCTION

The study of knots as abstract topological objects has inspired a great deal of fascinating mathematics. But knots are no less interesting as physical structures tied in flexible ropes and pulled tight. While it is intuitively clear that tight knots organize tension and contact forces to bind tightly and resist unravelling, the details of their structure remain mysterious. Even today, there is no explicit mathematical description of any tight knot.

We define the thickness of a space curve to be the supremal (largest) radius of any embedded tubular neighborhood of the curve, and the ropelength of a curve to be the quotient of its length and thickness. Ropelength provides a scale-invariant way to measure the total flexibility of a given length of rope. It has been established that there is a curve of minimum ropelength in each knot and link type $L((6, 5, 3))$ and the ropelength of that curve is called the ropelength $Rop(L)$ of the knot or link type. These minimum ropelength curves are called tight or ideal knots. In this paper, we give some results from our numerical computations of the shapes of tight knots and links.

Over the past ten years, many authors have found approximate shapes for tight knots and links using numerical methods [9, 7, 4, 1]. We follow previous authors in defining a version of ropelength, $Rop_p$, for space polygons and optimizing this polygonal ropelength functional over the space of polygons in different knot and link types. But while most other others rely on simulated annealing, we introduce the use of constrained gradient descent for ropelength optimization.

This new method has allowed us to significantly expand the scope and accuracy of existing computations of tight knots. In particular, it seems that our method has succeeded at the challenging task of resolving the set of self-contacts in all knot and link types with nine and fewer crossings (212 types in all). In the process, we have produced a new table of upper bounds for the ropelengths of these knot and link types which improves upon previous results. These improvements range from 0.05% for the figure eight knot (compared to the bound of [4]) to more than 8.11% for the $9_{20}$ knot (compared to the bound of [13]). For links, these seem to be the first upper bounds reported for almost all of the link types we consider.

This dataset is likely to be useful in the study of tight knots, so we provide here an early view of our results. This research announcement will be followed by an expanded paper, “Tightening Knots with Constrained Gradient Descent”, which describes our methods and results in detail. The filesize limitations of the arXiv forced us to truncate the data section of this posting, and to use comparatively low-quality image files for the three-dimensional views of tight knots and links in Appendix B. A higher-quality view of these images is provided at http://www.cs.washington.edu/homes/piatek/contact_table/.

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2. BACKGROUND MATERIAL

We start by defining ropelength more precisely. Suppose $\gamma$ is a $C^1$ space curve, parameterized by arclength. The maximum diameter of an embedded tube around $\gamma$ is controlled by two phenomena: “self-contacts” of the tube formed when sections of the curve far away in arclength approach each other in space, and “kinks” formed by points of high curvature on $\gamma$. These effects are shown below in Figure 1.

\[ d(s, t) = \|\gamma(s) - \gamma(t)\|. \]

We then have

**Definition 1.** The set $\text{dcsd}(\gamma)$ of doubly-critical self-distances of $\gamma$ is the set of critical points for $d(s, t)$ with $s \neq t$.

Taking the partial derivatives of $d$, we see that $(s, t) \in \text{dcsd}(\gamma)$ if and only if

\[ \langle \gamma(s) - \gamma(t), \gamma'(s) \rangle = 0 \text{ and } \langle \gamma(s) - \gamma(t), \gamma'(t) \rangle = 0. \]

Denoting the curvature of $\gamma$ at $s$ by $\kappa(s)$, Litherland et al. proved

**Theorem 2.1.** [8] The thickness of $\gamma$ is the minimum of

\[ \min_s \frac{1}{\kappa(s)} \text{ and } \min_{(s, t) \in \text{dcsd}(\gamma)} \frac{d(s, t)}{2}. \]

We can now define the primary object of interest in our computations:

**Definition 2.** The self-contact set or strut set of a space curve $\gamma$ is the set of $(s, t) \in \text{dcsd}(\gamma)$ with $\|\gamma(s) - \gamma(t)\| = 2 \text{Thi}(\gamma)$.

The term “strut”, borrowed from tensegrity theory, comes from the fact that minimum-length chords in $\text{dcsd}(\gamma)$ “hold the curve apart from itself” as the knot tightens.

In our polygonal knot-tightening problem, we will replace the curve $\gamma$ with a space polygon $\mathcal{V}$ with vertices $v_1, \ldots, v_V$ and edges $e_1, \ldots, e_V$. To define the polygonal thickness $\text{Thi}_p(\mathcal{V})$ of $\mathcal{V}$, we will need an idea of curvature.

**Definition 3.** The minimum radius of curvature (or MinRad) of $\mathcal{V}$ at $v_i$ is given by the radius of the unique circle tangent to both of the edges which meet at $v_i$ and passing through the midpoint of the shorter one.

If $\theta_i$ is the turning angle of $\mathcal{V}$ at $v_i$, then $\text{MinRad}(v_i)$ is given by

\[ \text{MinRad}(v_i) = \frac{\min\{|e_{i-1}|, |e_i|\}}{2 \tan(\theta_i/2)}. \]
We will also need a definition of doubly-critical self-distances:

**Definition 4.** Let \( \text{dcsd}(V) \) be the set of \((p, q)\) on \( V \) with \( p \neq q \) which are local minima of the self-distance function.

We now define a thickness measure for polygons:

**Definition 5.** The thickness \( \text{Thi}_p(V) \) of a space polygon \( V \) without self-intersections is given by the minimum of

\[
\min_i \text{MinRad}(v_i) \quad \text{and} \quad \min_{(p, q) \in \text{dcsd}(V)} \frac{d(p, q)}{2}.
\]

The polygonal ropelength \( \text{Rop}_p \) of \( V \) is then the quotient of the length of \( V \) and \( \text{Thi}_p(V) \). As expected, when polygons \( V_n \) with increasing numbers of edges are inscribed in a space curve \( \gamma \), it is known that \( \text{Rop}_p(V_n) \to \text{Rop}(\gamma) \) under some mild geometric hypotheses [10, 12, 13]. We define self-contact sets for polygons like we do for smooth curves.

### 3. Quantities Computed and How the Computation Was Validated

Our algorithm minimizes the length of \( V \) subject to a family of constraints derived from the distance and \( \text{MinRad} \) functions in Definition 5. We report the polygonal ropelengths of the minimized configurations in summary form in Appendix A. We also report preliminary computations of the ropelengths of piecewise-smooth curves obtained from our polygons by replacing the corners of the polygon with small circular arcs. These provide tentative upper bounds on the ropelengths of the knot and link types listed. We also provide self-contact sets for 50 of these knots and links.

Though our ropelength bounds for knots improve on those of previous authors, this is an uncertain measure of their quality. After all, there is no way to check the accuracy of an upper bound for the ropelength of any knot, since no exact value for the minimum ropelength of any knot type is known. On the other hand, the minimum ropelength is known or explicitly conjectured for some link types [3, 2]. A comparison of our results to some of these known examples appears below.

| Link name           | Hopf link \((2_1)\) | 3-link chain \((2_1 \# 2_1)\) | Borromean rings \((6_2^3)\) |
|---------------------|---------------------|-------------------------------|-----------------------------|
| Edges               | 216                 | 384                           | 630                         |
| Polygon length      | 25.1439             | 41.7131                       | 58.0300                     |
| Upper bound         | 25.1388             | 41.7086588                    | 58.0145                     |
| Smooth length       | \(8\pi\)           | \(12\pi + 4\)                 | 58.006                      |
| Relative error      | 0.02%               | 0.02%                         | 0.01%                       |

The results above lead us to suspect that most of our smooth ropelength bounds are within 1 to 2 hundredths of a percent of the corresponding minimum ropelength values, but we must be cautious. The ropelength “landscape” for knots is quite complicated, and we have already discovered a number of local ropelength minima for 8 and 9-crossing knots which are very different from the (apparent) global ropelength minima for these knot types. If our gradient descent algorithm has been trapped by one of these local minima, the figures we report might be an accurate computation of the ropelength of the local minimizer, but far off from the true minimum ropelength value for the knot type.

We checked our computation of the self-contact sets by comparing our computed self contact set for the Borromean rings to the contact set for the ropelength-critical configuration provided by [2]. The results appear in the Figure below.
The polygonal configuration of the Borromean rings discovered by our software has total length about $29.01$. The top plot shows the lower triangle of the square $[0, 29.01] \times [0, 29.01]$ representing pairs of arclength values $(s, t)$ on these polygonal rings. To describe the position of a point on this 3-component link with a single arclength value, we use the convention that arclength values in $[0, 9.67)$ refer to points on the first component, values in $[9.67, 19.34)$ refer to points on the second component, and values in $[19.34, 29.01)$ refer to points on the third component of the link. These breaks are reinforced by the colored bands running up the diagonal of the plot, which correspond to the colors of the different components of our tight links in the 3d renderings of Appendix B.

The $s$ and $t$ position of points on the plot is indicated by the labels running up the diagonal, where the three special values representing breaks between components are lifted away from the other labels. The breaks between components are also shown on the plot by the alternating checkerboard pattern of the background colors.

We then locate every pair $(s, t) \in \text{dcsd}(\mathcal{V})$ with $\|\mathcal{V}(s) - \mathcal{V}(t)\| \leq \text{Th}_{ip}(\mathcal{V}) + 10^{-5}$. In the context of our gradient descent algorithm, these points represent active distance constraints. Our code computes Lagrange multipliers for all these active constraints, which represent self-contact forces borne by these tube contacts in the tight knot. We center
a dark green box at every such \((s, t)\) value with a nonzero Lagrange multiplier. The size of the box represents the average\(^1\) edgelength of the polygon \(\mathcal{V}\). We chose this size to represent the expected error in computed self-contact positions introduced by approximating a \(C^1\) ropelength-minimizer by the polygon \(\mathcal{V}\).

As we see from the plot, no tube around a component of the link is in contact with itself (so the three cream-colored triangles near the diagonal are empty). But each of the components makes contact with the other two, as shown by the boxes plotted in the purple and cream-colored rectangles forming the remainder of the plot. We can see that the contacts break up naturally into “lantern-shaped” structures.

This link has been studied by Cantarella, Fu, Kusner, Sullivan, and Wrinkle, who provide a ropelength-critical configuration in [2]. In the bottom plot, we compare one “lantern” formed by 608 of these boxes to the self-contact set predicted by these authors, which is represented by a red line. In this plot, the arclength distances labelled on the \(s\) and \(t\) axes do not correspond to a region of the plot above, but merely indicate the scale of the plot. We can see that the agreement between theory and computation is generally within one edgelength.

Appendix B contains similar plots of our computed self-contact sets for 50 knots and links from our collection of minimized examples. To the left of each self-contact plot, we provide a 3d rendering of the corresponding tight shape. For links, the diagonal and right-hand side of the triangular self-contact plot are colored gray, orange and green in correspondence with the colors of the components in the rendering. The start of each component in the rendering is denoted by the tube coming to a point. The black bands on the tubes correspond to the arclength tick marks on the plot at right. The table also contains the polygonal ropelength of the knot (top number, slightly higher) and the corresponding smooth ropelength upper bound (bottom number, slightly lower), as well as the number of edges in the configuration plotted.

4. CONCLUSIONS

The major contribution of Appendix A is the provision of ropelength figures for links. This allows us to check the accuracy of numerical ropelength minimizations against theoretical results for the first time. We are happy to report that our method passes this test for the cases we examined.

The pictures in Appendix B are considerably more evocative. It is evident from first inspection that the contact sets of tight knots and links seem to contain a fairly small number of commonly repeated patterns. Some of these, such as the “steps” pattern first seen in the trefoil knot, change shape from knot to knot. But others (such as the “winged” pattern in the figure eight knot or the “lantern” shape seen in the Borromean rings) seem to remain remarkably consistent throughout our computations. The reader may notice many other examples as well. Isolating and understanding some of these structures could provide us with a “construction kit” for tight knots, much like the analysis of the simple chain in [3] led to the construction of an infinite family of tight links.

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\(^1\)Our final polygons are almost-equilateral, so this is a good approximation of the lengths of the edges incident to the pair \((s, t)\).
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The table shows new polygonal ropelengths and ropelength upper bounds for 212 knots and links with 9 or fewer crossings. From left to right, there are four columns: the name of the knot or link, the polygonal ropelength $R_{op}$, the corresponding ropelength upper bound $Rop$, and the previous best ropelength upper bound we could find in the literature together with the percentage improvement in ropelength. For these last figures, we used the papers [1, 4, 11].

| Link | $R_{op}$ | $Rop$ | Previous |
|------|----------|-------|----------|
| $2^2_1$ | 25.1439 | 25.1388 | 
| $3_1$ | 32.7490 | 32.7448 | 32.7433864 (−%) |
| $4_1$ | 42.0997 | 42.0928 | 42.1158845 (0.05%) |
| $4^2_1$ | 40.0247 | 40.0169 | 
| $5_1$ | 47.2156 | 47.2016 | 47.51 (0.64%) |
| $5_2$ | 49.4840 | 49.4704 | 49.73 (0.52%) |
| $5^2_1$ | 49.7874 | 49.7723 | 
| $6_1$ | 56.7316 | 56.7150 | 57.11 (0.69%) |
| $6_2$ | 57.0451 | 57.0271 | 57.44 (0.71%) |
| $6_3$ | 57.8602 | 57.8435 | 58.48 (1.08%) |
| $6^2_1$ | 54.4068 | 54.3893 | 
| $6^2_2$ | 56.7132 | 56.7028 | 
| $6^2_3$ | 58.1161 | 58.1044 | 
| $6^3_1$ | 57.8334 | 57.8170 | 
| $6^3_2$ | 58.0300 | 58.0145 | 
| $6^3_3$ | 50.5865 | 50.5745 | 
| $7_1$ | 61.4319 | 61.4109 | 61.89 (0.77%) |
| $7_2$ | 63.9165 | 63.8956 | 65.36 (2.24%) |
| $7_3$ | 63.9539 | 63.9327 | 64.35 (0.64%) |
| $7_4$ | 64.2960 | 64.2724 | 65.63 (2.06%) |
| $7_5$ | 65.2802 | 65.2609 | 65.70 (0.66%) |
| $7_6$ | 65.7183 | 65.7012 | 66.17 (0.7%) |
| $7_7$ | 65.6316 | 65.6108 | 66.09 (0.72%) |
| $7^2_1$ | 64.2585 | 64.2353 | 
| $7^2_2$ | 65.0467 | 65.0274 | 
| $7^2_3$ | 65.3743 | 65.3561 | 
| $7^2_4$ | 65.0971 | 65.0759 | 
| $7^2_5$ | 66.2400 | 66.2186 | 
| $7^2_6$ | 66.3494 | 66.3372 | 
| $7^2_7$ | 55.5451 | 55.5311 | 
| $7^2_8$ | 57.8043 | 57.7948 | 
| $7^3_1$ | 65.8275 | 65.8090 | 
| $8_1$ | 71.0484 | 71.0241 | 71.44 (0.58%) |
| $8_2$ | 71.4327 | 71.4107 | 71.91 (0.69%) |

**APPENDIX A. TABLE OF POLYGONAL ROPELENGTHS AND ROPELENGTH UPPER BOUNDS**

The table shows new polygonal ropelengths and ropelength upper bounds for 212 knots and links with 9 or fewer crossings. From left to right, there are four columns: the name of the knot or link, the polygonal ropelength $R_{op}$, the corresponding ropelength upper bound $Rop$, and the previous best ropelength upper bound we could find in the literature together with the percentage improvement in ropelength. For these last figures, we used the papers [1, 4, 11].
| Link  | $\text{Rop}_p$ | Rop   | Previous     |
|-------|----------------|-------|--------------|
| $s^{8}_{8}$ | 65.0637       | 65.0444 |             |
| $s^{8}_{9}$ | 70.1904       | 70.1810 |             |
| $s^{8}_{10}$ | 68.9823       | 68.9694 |             |
| $s^{8}_{1}$ | 75.2901       | 75.2677 |             |
| $s^{8}_{2}$ | 67.4772       | 67.4571 |             |
| $s^{8}_{3}$ | 66.4140       | 66.4046 |             |
| $s^{9}_{1}$ | 75.7507       | 75.7252 | 76.43 (0.92%) |
| $s^{9}_{2}$ | 79.3035       | 79.2794 | 79.92 (0.8%)  |
| $s^{9}_{3}$ | 78.5867       | 78.5591 | 79.05 (0.62%) |
| $s^{9}_{4}$ | 78.1117       | 78.3861 | 78.84 (0.57%) |
| $s^{9}_{5}$ | 79.7877       | 79.7586 | 80.32 (0.69%) |
| $s^{9}_{6}$ | 80.1326       | 80.0822 | 80.65 (0.7%)  |
| $s^{9}_{7}$ | 80.6597       | 80.6357 | 82.65 (2.43%) |
| $s^{9}_{8}$ | 80.5651       | 80.5384 | 81.14 (0.74%) |
| $s^{9}_{9}$ | 79.9574       | 79.9323 | 80.85 (1.13%) |
| $s^{9}_{10}$ | 79.8161      | 79.7946 | 80.33 (0.66%) |
| $s^{9}_{11}$ | 80.3650       | 80.3418 | 81.98 (1.90%) |
| $s^{9}_{12}$ | 80.1275       | 80.1047 | 80.71 (0.74%) |
| $s^{9}_{13}$ | 80.6525       | 80.6246 | 81.33 (0.86%) |
| $s^{9}_{14}$ | 80.1512       | 80.1259 | 80.73 (0.74%) |
| $s^{9}_{15}$ | 82.1665       | 82.1396 | 82.70 (0.67%) |
| $s^{9}_{16}$ | 80.1446       | 80.1211 | 80.67 (0.68%) |
| $s^{9}_{17}$ | 80.5792       | 80.5537 | 81.90 (1.64%) |
| $s^{9}_{18}$ | 81.6230       | 81.5960 | 82.68 (1.31%) |
| $s^{9}_{19}$ | 82.1828       | 82.1593 | 82.72 (0.67%) |
| $s^{9}_{20}$ | 80.2543       | 80.2288 | 87.31 (8.11%) |
| $s^{9}_{21}$ | 81.1336       | 81.1098 | 81.64 (0.64%) |
| $s^{9}_{22}$ | 81.0714       | 81.0464 | 81.60 (0.67%) |
| $s^{9}_{23}$ | 81.3164       | 81.2898 | 81.84 (0.67%) |
| $s^{9}_{24}$ | 80.9933       | 80.9701 | 81.54 (0.69%) |
| $s^{9}_{25}$ | 81.1873       | 81.1612 | 81.85 (0.84%) |
| $s^{9}_{26}$ | 80.9352       | 80.9137 | 81.94 (1.25%) |
| $s^{9}_{27}$ | 81.9473       | 81.9092 | 83.21 (1.56%) |
| $s^{9}_{28}$ | 81.5694       | 81.5467 | 82.25 (0.85%) |
| $s^{9}_{29}$ | 81.8708       | 81.8470 | 83.45 (1.92%) |
| $s^{9}_{30}$ | 81.8567       | 81.8344 | 82.46 (0.75%) |
| $s^{9}_{31}$ | 81.7436       | 81.6915 | 82.22 (0.64%) |
| $s^{9}_{32}$ | 81.5775       | 81.5555 | 82.34 (0.95%) |
| $s^{9}_{33}$ | 82.8451       | 82.7989 | 83.37 (0.68%) |
| $s^{9}_{34}$ | 82.3213       | 82.2744 | 82.99 (0.86%) |
| $s^{9}_{35}$ | 79.2495       | 79.2216 | 80.85 (2.01%) |
| $s^{9}_{36}$ | 81.0579       | 81.0297 | 81.57 (0.66%) |
| $s^{9}_{37}$ | 81.5845       | 81.5562 | 82.10 (0.66%) |
| $s^{9}_{38}$ | 81.8119       | 81.7909 | 82.43 (0.77%) |
| $s^{9}_{39}$ | 81.9490       | 81.9266 | 85.55 (4.23%) |
| $s^{9}_{40}$ | 81.7008       | 81.6806 | 82.67 (1.19%) |
| $s^{9}_{41}$ | 81.4929       | 81.4399 | 82.11 (0.81%) |
| $s^{9}_{42}$ | 69.6133       | 69.5939 | 70.02 (0.6%)  |
| $s^{9}_{43}$ | 71.7062       | 71.6863 | 72.20 (0.71%) |

| Link  | $\text{Rop}_p$ | Rop   | Previous     |
|-------|----------------|-------|--------------|
| $s^{9}_{44}$ | 71.6516       | 71.6305 | 72.23 (0.82%) |
| $s^{9}_{45}$ | 74.9154       | 74.8959 | 75.51 (0.81%) |
| $s^{9}_{46}$ | 68.6579       | 68.6369 | 69.35 (1.02%) |
| $s^{9}_{47}$ | 75.1289       | 75.0875 | 75.61 (0.69%) |
| $s^{9}_{48}$ | 74.2918       | 74.2477 | 74.94 (0.92%) |
| $s^{9}_{49}$ | 74.0530       | 74.0127 | 74.50 (0.65%) |
| Link | $Rop_p$ | Rop | Previous |
|------|---------|-----|----------|
| $9^2_6$ | 71.3593 | 71.3490 |
| $9^2_6$ | 73.9646 | 73.9377 |
| $9^2_7$ | 69.9602 | 69.9432 |
| $9^2_8$ | 73.6781 | 73.6545 |
| $9^2_9$ | 66.0806 | 66.0658 |
| $9^2_{10}$ | 69.3690 | 69.3483 |
| $9^2_{11}$ | 70.5942 | 70.5699 |
| $9^2_{12}$ | 72.9916 | 72.9685 |
| $9^2_{13}$ | 68.0369 | 68.0305 |
| $9^2_{14}$ | 71.0385 | 71.0185 |
| $9^2_{15}$ | 73.8423 | 73.8217 |
| $9^2_{16}$ | 75.2439 | 75.2245 |
| $9^2_{17}$ | 73.8408 | 73.8194 |
| $9^2_{18}$ | 74.1911 | 74.1697 |
| $9^2_{19}$ | 73.0481 | 73.0305 |
| $9^2_{20}$ | 73.5734 | 73.5553 |
| $9^2_{21}$ | 69.3978 | 69.3840 |
| $9^3_1$ | 81.2897 | 81.2323 |
| $9^3_2$ | 82.4507 | 82.4004 |
| $9^3_3$ | 82.3127 | 82.2861 |
| $9^3_4$ | 82.5449 | 82.5208 |
| $9^3_5$ | 80.7974 | 80.7714 |
| $9^3_6$ | 81.0235 | 81.0054 |
| $9^3_7$ | 82.1986 | 82.1535 |
| $9^3_8$ | 81.1631 | 81.1408 |
| $9^3_9$ | 81.6200 | 81.5735 |
| $9^3_{10}$ | 82.3446 | 82.3259 |
| $9^3_{11}$ | 82.0323 | 82.0137 |
| $9^3_{12}$ | 82.6345 | 82.5740 |
| $9^3_{13}$ | 72.2098 | 72.2008 |
| $9^3_{14}$ | 74.5697 | 74.5492 |
| $9^3_{15}$ | 74.3877 | 74.3655 |
| $9^3_{16}$ | 75.0664 | 75.0430 |
| $9^3_{17}$ | 74.2972 | 74.2779 |
| $9^3_{18}$ | 72.5059 | 72.4741 |
| $9^3_{19}$ | 72.7143 | 72.6859 |
| $9^3_{20}$ | 76.3557 | 76.1829 |
| $9^3_{21}$ | 74.9369 | 74.9212 |
| $9^4_1$ | 85.5620 | 85.5115 |
Appendix B. Table of Self-Contact Sets

3_1

Poly(K): 32.75
Bound: 32.75
Vertices: 400

4_1

Poly(K): 42.10
Bound: 42.10
Vertices: 400

5_1

Poly(K): 47.22
Bound: 47.21
Vertices: 400
