UNDERGRADUATE STUDENT RESEARCH IN KNOT THEORY USING MULTIPLE COMPUTATIONAL PLATFORMS

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Introduction. Problems in knot theory are frequently approachable by undergraduates who have just completed multivariable calculus. The computational power of computer algebra systems and knot theoretic software further enables undergraduate students to observe knot theoretic phenomena, make conjectures, and design and perform sophisticated calculations to solve research questions. This paper describes the work I have done with three undergraduates over the summers of 2003-2005 on determining stick numbers of knots using Derive, Maple, and the knot theoretic program, *KnotPlot*, designed by R. Scharein [5].

Let K be a topological knot or link. The *stick number* of K, $S(K)$, is the minimal number of sticks (line segments) needed to form K in three-dimensional space. Our work is concerned with investigating a variation of the concept of the stick number. Analogous to the definition of a regular polygon as a polygon with equal-length sides and equal interior angles, we use the term *regular* to describe polygonal knots that have equal-length sticks and equal angles between adjacent sticks. Let $\alpha \in (0, \pi)$. An α*−regular conformation* of K is a polygonal embedding of the K in space such that each stick (polygonal edge) has the same length and that the angle at each vertex joining two adjacent sticks is α. The α*−regular stick number* of K, denoted $S_{r,\alpha}(K)$, is the minimal number of sticks needed to construct an α−regular conformation of K. Moreover, part of the interest in polygonal knot conformations outside mathematics is that these conformations may serve as mathematical models for particular molecules: the vertices represent the atoms in the molecule, and the sticks represent the bonds (the bond axes). For most of this paper, we will use the value $\alpha = \cos^{-1}(-1/3)$, which does appear as a bond angle in molecular conformations. This particular value of α is the bond angle at an sp^3 carbon and is the bond angle between two carbon-hydrogen bonds in methane [4]. The results we discuss here are summarized in the following theorem.

Theorem 1 (**[1]**) *The* $\cos^{-1}(-1/3)$*−regular stick number of the trefoil knot is 11, and the* $\cos^{-1}(-1/3)$*−regular stick number of the granny knot is 16.*

A key ingredient to proving this theorem is a lower bound formula [1] for the regular stick number of K in terms of the angle α and the bridge index of K. The result above is proved by constructing such $\cos^{-1}(-1/3)-$regular conformations and then by noting that 11 and 16 are the lower bounds for bridge index two and bridge index three knots, respectively. We describe the construction of the knot conformations below.

Constructing the Knots. We now provide a brief overview of the process we followed to construct regular conformations of the trefoil and granny knots. Before using any computational technology, we began by physically constructing the knots using molecular modeling kits [3]. This physical approach guided us to choose reasonable parameter values once we began to use Derive and Maple. The process we used to obtain the regular conformations of the trefoil and granny knots followed the same general strategy and began the same way, which we now describe explicitly in the case of the trefoil.

Let $\alpha = \cos^{-1}(-1/3)$. To show the existence of an eleven-stick $\alpha-$regular conformation K_r of a right-handed trefoil knot, we first denote the eleven vertices of K_r by $v_0, v_1, \ldots, v_{10}$. We denote the stick joining vertex v_{i-1} to $v_{i(\text{mod } 11)}$ by e_i where $i = 1, \ldots, 11$. For each e_i, we denote the vector from v_{i-1} to $v_{i(\text{mod } 11)}$ by $\mathbf{e}_i$. We will construct seven of vertices (and the connecting sticks), and obtain the remaining vertices by a rotation of π about the $y-$axis. Let $R : \mathbf{R}^3 \to \mathbf{R}^3$ denote this rotation, which in coordinates, is represented by $R(x, y, z) = (-x, y, -z)$. To begin, let $v_0 = (0,0,0)$, $v_1 = (0, \cos(\alpha/2), \sin(\alpha/2)) = (0, \sqrt{3}/3, \sqrt{6}/3)$, and $v_{10} = R(v_1) = (0, \sqrt{3}/3, -\sqrt{6}/3)$. Notice that $||\mathbf{e}_1|| = ||\mathbf{e}_{10}|| = 1$ and $\angle v_1 v_0 v_{10} = \alpha$.

We then successively determine the vertices v_2, v_3, v_4, and v_5 as follows. Assume that v_j is determined for $0 \le j \le i$ and that $||\mathbf{e}_j|| = 1$ for $1 \le j \le i$. To ensure that the angle $\angle v_{i-1} v_i v_{i+1}$ between e_i and e_{i+1} is α, we observe that v_{i+1} must lie on the circle of radius $\sin(\alpha)$ centered at the point $c_{i+1} = v_i - \cos(\alpha)\mathbf{e}_i$ lying in the plane P_i, which is orthogonal to $\mathbf{e}_i$ and passes through c_{i+i}. Let $\mathbf{e}_i = \langle a_i, b_i, c_i \rangle$. We set

$$\mathbf{q}_{1,i+1}(t) = \begin{cases} \langle 1, 0, 0 \rangle & \text{if } a_i^2 + b_i^2 = 0, \\ \left\langle \frac{-b_i}{\sqrt{a_i^2+b_i^2}}, \frac{a_i}{\sqrt{a_i^2+b_i^2}}, 0 \right\rangle & \text{if } a_i^2 + b_i^2 \neq 0 \end{cases}$$

and

$$\mathbf{q}_{2,i+1}(t) = \begin{cases} \langle 0, 1, 0 \rangle & \text{if } a_i^2 + b_i^2 = 0, \\ \left\langle \frac{-a_i c_i}{\sqrt{a_i^2+b_i^2}}, \frac{-b_i c_i}{\sqrt{a_i^2+b_i^2}}, \sqrt{a_i^2 + b_i^2} \right\rangle & \text{if } a_i^2 + b_i^2 \neq 0, \end{cases}$$

where $-\pi \le t < \pi$. Now $< \mathbf{q}_{1,i+1}, \mathbf{q}_{2,i+1}, \mathbf{e}_i >$ is an orthonormal basis for $\mathbf{R}^3$ such that $\mathbf{q}_{1,i+1} \times \mathbf{q}_{2,i+1} = \mathbf{e}_i$ and that $\mathbf{q}_{1,i+1}$ and $\mathbf{q}_{2,i+1}$ span the plane parallel to P_i passing through the origin. We now parametrize the circle of unit vectors orthogonal to $\mathbf{e}_i$ by

$$\mathbf{NV}_{i+1}(t) = \cos(t)\mathbf{q}_{1,i+1} + \sin(t)\mathbf{q}_{2,i+1}, \quad \text{where } -\pi \le t < \pi.$$

Now the possible candidates for the vertex v_{i+1} can be parametrized by

$$\begin{aligned} v_{i+1} &= \mathbf{NV}_{i+1}(t) + c_{i+1} \\ &= \sin(\alpha)\mathbf{NV}_{i+1}(t) - \cos(\alpha)\mathbf{e}_i + v_i \\ &= \frac{2\sqrt{2}}{3}\mathbf{NV}_{i+1}(t) + \frac{1}{3}\mathbf{e}_i + v_i. \end{aligned}$$

It follows from this recursive process that $||v_{i+1} - v_i|| = ||\mathbf{e}_{i+1}|| = 1$, for $i = 2, \ldots, 5$ and that $\angle v_{i-1}v_iv_{i+1} = \alpha$, for $i = 1, 2, 3, 4$. Now for $i = 2, \ldots, 5$, let t_i be the parameter that determines v_i on $\mathbf{NV}_i$. As these four vertices are determined recursively, v_2 is a function of t_2, and v_i is a function of $t_2, \ldots, t_i$, $i = 3, 4, 5$. Similarly, $\mathbf{NV}_2$ is a function of t_2, and $\mathbf{NV}_i$ is a function of $t_2, \ldots, t_i$, $i = 3, 4, 5$.

This is where Derive and subsequently Maple became important tools in this investigation. Calculating the coordinate of each vertex v_i by hand would be unwieldy and inefficient. Instead, we programmed the formulas above to calculate (approximations of) the coordinates of the vertex v_i in terms of the parameters $t_2, t_3, \ldots t_i$. At this stage of the project, Derive was able to compute the vertices, but Derive was noticeably slow when computing v_i for $i \geq 5$. Maple was able to do the same computation with the same code almost instantly.

The remaining vertices $v_6, \ldots, v_9$ are be determined by the rotation R: $v_6 = R(v_5)$, $v_7 = R(v_4)$, $v_8 = R(v_3)$, and $v_7 = R(v_2)$. As $v_6, \ldots, v_9$ are determined via an isometry of $\mathbf{R}^3$, it follows that $||\mathbf{e}_i|| = 1$, for $i = 7, 8, 9, 10$, that $\angle v_{i-1}v_iv_{i+1} = \alpha$, for $i = 7, 8, 9, 10$, and that $\angle v_{10}v_0v_1 = \alpha$. To show that this conformation is indeed regular, we still need to find an ordered 4–tuple of values of (t_2, t_3, t_4, t_5) so that $||\mathbf{e}_6|| = 1$ and $\angle v_4v_5v_6 = \alpha$. (The rotation R ensures that $\angle v_4v_5v_6 = \angle v_5v_6v_7$.) The proof will be complete after finding such a 4–tuple, verifying that the eleven resulting sticks have no intersections at any interior points of the sticks, and finally confirming that the resulting knot is indeed a trefoil knot. We will now proceed to demonstrate the existence of the 4–tuple (t_2, t_3, t_4, t_5).

At this stage of the process, we went back to our physical models to help us choose values for the first two parameters t_2 and t_3. We made reasonable "eyeball" estimates for these parameters and input them into our vertex formulas in Maple to see if indeed these parameters would lead to the intended regular knot conformation. To check whether or not our estimates were viable, we created a system of two nonlinear equations in the variables t_4 and t_5, which we describe below. The reason that we relied on equations in two variables for both the trefoil and the granny knot (for which need additional parameters) is that we can easily plot functions of two variables in Maple and observe whether or not we have a solution. When it appeared that a solution did indeed exist, we then solved our system numerically. It turned out that our expressions below were too complicated for Derive to compute and plot. Maple still could take over ten minutes to complete these calculations and subsequent plots.

Let $k_2 = -1.30899693899575$ and $k_3 = -1.83259571459404$. We use these two numbers for t_2 and t_3, respectively. (Note that these values are approximations of $-5\pi/12$ and $-7\pi/12$.) The conditions $v_6 = R(v_5)$ and $||\mathbf{e}_6|| = 1$ imply that v_5 must lie on a circle of radius $1/2$ that is centered on the $y-$axis and lies in a plane perpendicular to the $xz-$plane. That is, the distance from v_5 to the $y-$axis must be $1/2$. We define a function

$$L(t_4, t_5) = (v_5(k_2, k_3, t_4, t_5)_x)^2 + (v_5(k_2, k_3, t_4, t_5)_z)^2 - \frac{1}{4}.$$

The two conditions above are satisfied when $L(t_4, t_5) = 0$. Assuming $L(t_4, t_5) = 0$, we now have $||\mathbf{e}_5|| = ||\mathbf{e}_6|| = 1$. Hence, the law of cosines implies that the condition $\angle v_4 v_5 v_6 = \alpha$ is equivalent to the condition $||v_6 - v_4|| = 2\sqrt{6}/3$. We now define a function

$$\begin{aligned} A(t_4, t_5) &= ||v_6 - v_4||^2 - \frac{8}{3} \\ &= (v_4(k_2, k_3, t_4, t_5)_x + v_5(k_2, k_3, t_4, t_5)_x)^2 \\ &\quad +(v_4(k_2, k_3, t_4, t_5)_z + v_5(k_2, k_3, t_4, t_5)_z)^2 \\ &\quad +(v_4(k_2, k_3, t_4, t_5)_y - v_5(k_2, k_3, t_4, t_5)_y)^2 - \frac{8}{3}. \end{aligned}$$

The angle condition is satisfied when $A(t_4, t_5) = 0$ and $L(t_4, t_5) = 0$. On the rectangle $[-2.1628, -2.1627] \times [1.0274, 1.0276]$, a solution to the system of equations is $t_4 = t_4^\star \approx t_4' - 2.16271575011929$ and $t_5 = t_5^\star \approx t_5' = 1.02754761268067$. This now proves that the conformation K_r is indeed regular. At this stage, we have not yet shown that nonadjacent sticks are disjoint, nor have we shown that K_r is indeed a conformation of a trefoil knot.

We next must show that the eleven sticks in the conformation K_r do not intersect each other at any interior points of the sticks and that K_r is indeed a conformation of a trefoil knot. We do this by considering an *approximate* $\alpha-$regular conformation, denoted by K_a and showing that K_a has the two desired properties and that K_a can be deformed to K_r without introducing any self-intersections throughout the deformation. The conformation K_a is determined by vertices $v_0', v_1', \ldots, v_{10}'$ as follows. First $v_0' = v_0 = (0,0,0)$. For $i = 1, 2, 3, 8, 9, 10$, v_i' is obtained from v_i by rounding each coordinate of v_i to thirteen decimal places. Note that for each of these six values of i, corresponding coordinates v_i and v_i' differ by no more than 10^{-12}. Now v_4' and v_5' are obtained by rounding $v_4(k_2, k_3, t_4')$ and $v_5(k_2, k_3, t_4', t_5')$ to thirteen decimal places, respectively.

We then input the coordinates of K_a into *KnotPlot* to view a projection of K_a, which was readily seen to be the right-handed trefoil knot. (*KnotPlot* can also confirm that

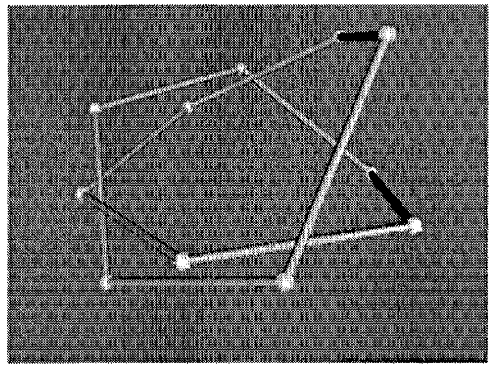

Figure 1: The 11-stick trefoil K_a created with *KnotPlot* [5].

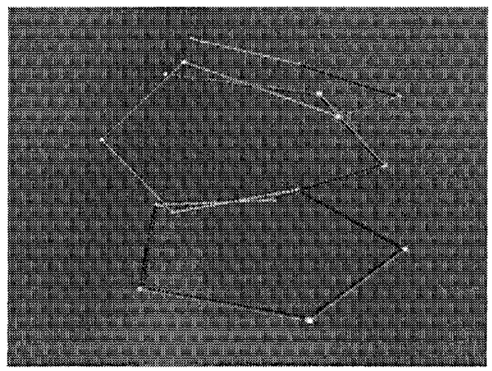

Figure 2: The 16-stick granny knot K_a plotted with *KnotPlot* [5].

this is the right-handed trefoil knot by computing the HOMFLY [2] polynomial, which is a good (but not complete) knot invariant. Several technical lemmas were then needed to confirm that since K_a is indeed a trefoil knot, then so is K_r. Below are figures of the trefoil knot and granny knot created with *KnotPlot.*

References

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