The Crossing Probability Knot Energy

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Abstract

The crossing probability energy U_{CP} is defined and properties are explored. The energy is based upon the probability that non-adjacent edge pairings of a polygonal knot P_n do not cross. U_{CP} is found to be asymptotically finite, but not asymptotically smooth. An algorithm is presented to compute U_{CP} as well as minimize the energy using a gradient flow.

1 Introduction

Knot energies were first introduced in 1988 by Fukuhara [3, 4] and deal with measuring the complexity of knot conformations. Within mathematics, energy functions are studied to obtain measures of complexity that turn out to be useful knot invariants [7]. One hopes that energy minimizers will yield ideal knot conformations. Within the scientific world, knot energies are hoped to be applicable to situations found in DNA knotting and polymer science [4, 7]. Further motivation includes the study of electrophoretic mobility of knotted DNA and the knotted flow and field lines in fluids and electromagnetism [4].

Let $\mathcal{S}$ be the set of either simple closed curves or polygonal curves. A function f is *scale invariant* if for any $n \in \mathbb{R}^+$ then $f(nS) = f(s)$ for any $S \in \mathcal{S}$. This implies that any increase or decrease in scale of any knot does not change the value of the function f.

A *knot energy* is a scale invariant function from $\mathcal{S}$ into the positive real numbers:

$$f : \mathcal{S} \to \mathbb{R}^+$$

The knot energy $f(S)$ is the energy of the knot $S \in \mathcal{S}$ [2, 4].

In Section 2 we begin with the background needed to further explore knot energies and develop some intuition for properties that knot energies may possess. Definitions for knot energy properties such as basic, charge, and strong

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are provided and a precise definition of the crossing probability energy U_{CP} is given. In Section 3 some basic results are shown, such as the property that U_{CP} is minimized only for a planar trivial knot. We delve further into U_{CP} properties in Section 4. Here we provide a special construction of a knot, namely a *near diagram knot*, to aid in proving that U_{CP} is asymptotically finite. We also show that U_{CP} is not asymptotically smooth based upon the results in Section 3.

In Section 5 we present an algorithm to compute and locally minimize U_{CP}. The algorithm calculates the value of U_{CP} for the initial knot inputted then attempts to minimize the energy for the given knot representation and type using a gradient flow. Along with discussion of the experimental behavior of U_{CP}, a data table is included for four different knot energies of knots from three to eight crossings. This table provides a side by comparison of U_{CP} with Simon's minimum distance energy U_{MD} [7], as well as two other potential energies discussed in Section 6. Within Section 6, we conclude by discussing two potential knot energies as well as proposing conjectures about U_{CP}. The two potential energies were arrived upon in the investigation of U_{CP}. They are based upon probabilities, but it is not clear what the probabilities are as of yet.

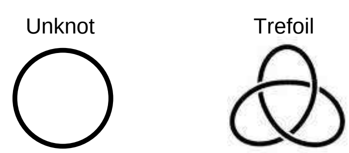
2 Background

Here we provide definitions needed and notational conventions used throughout the paper. A knot's complexity often revolves around how twisted the knot is or how many times the knot crosses over itself, which is denoted as the crossing number of the knot, defined here. Certain desirable knot energy properties are defined.

Definition 2.1. A *knot* is a simple closed curve in 3-dimensional space.

Definition 2.2. The *crossing number* of a knot type $\mathcal{K}$, denoted $c(\mathcal{K})$, is the least number of crossings over all projections of the knot type.

Example 2.3. The crossing number of the unknot is 0. The crossing number of the trefoil knot is 3.



Definition 2.4. The *stick number* of a knot type $\mathcal{K}$, denoted $s(\mathcal{K})$, is the least number of sticks, or edges, needed to construct a knot of type $\mathcal{K}$.

Example 2.5. The unknot has stick number 3 and the trefoil has stick number 6.

2.1 Properties

Define $\mathcal{P}_n$ to be the set of all polygonal knots with n-edges. Define $\mathcal{K}_n$ to be the set of all knots of knot type $\mathcal{K}$ with n-edges. Note that $\mathcal{K}_n \subseteq \mathcal{P}_n$. Throughout the paper, K or P_n is used to denote an arbitrary knot.

Here we define properties that knot energies may possess as in [2, 4].

Definition 2.6. Let $f : \mathcal{P}_n \to \mathbb{R}^+$ be an energy function of polygons. The *n-energy* of a knot type $\mathcal{K}$ is an infimum over all n-gons in $\mathcal{K}_n$:

$$f_n(\mathcal{K}) = \inf \{ f(P_n) \,|\, \text{for all } P_n \in \mathcal{K}_n \}$$

The energy of a knot type $\mathcal{K}$ over all polygons is the infimum:

$$f(\mathcal{K}) = \inf_{n>0} f_n(\mathcal{K})$$

Notation: We denote the infimum of U_{CP} of a knot type $\mathcal{K}$ as $U_{CP_n}(\mathcal{K})$ and call it the $n-$*crossing probability energy*.

Definition 2.7. Let $f : \mathcal{P}_n \to \mathbb{R}^+$ be an energy function of polygons. Then,

(a) f is called a *basic* energy function if $f(P_n)$ is the absolute minimum within $\mathcal{P}_n$ iff P_n is the regular polygon of n-edges (denoted by R_n);

(b) f is called a *strong* energy function if for any given positive number $a > 0$ there are only finitely many knot types $\mathcal{K}$ such that $f(\mathcal{K}) \leq a$. In this case $f(\mathcal{K})$ is defined to be the infimum of f over $\mathcal{P}_n(\mathcal{K})$;

(c) f is called a *charge* energy function if $f(P_n) \to \infty$ as P_n approaches a singular polygon (a polygon with self intersections);

(d) f is called *semi-ideal* energy function if it satisfies conditions (a), (b), and (c).

One expectation of a knot energy is that if we increase the number of edges of a knot, K, of a specified knot type, $\mathcal{K}$, we expect the energy sequence of K not to diverge. In otherwords, we want the infimum of the energy of $\mathcal{K}$ to be bounded. This keeps the knot energy from tending to infinity as we increase the edge number without bound. We call this property *asymptotically finite* and define it below.

Definition 2.8 (Asymptotically Finite). Let f be a knot energy function for $\mathcal{S} = \mathcal{P}_n$. Let $f_n(\mathcal{K})$ be the infimum of the energy of polygons of length n-edges and knot type $\mathcal{K}$. Then f is *asymptoticallly finite* if

$$\limsup_{n\to\infty} f_n(\mathcal{K}) < \infty$$

for any knot type $\mathcal{K}$.

Another desirable property of a knot energy is that of being *asymptotically smooth.*

Definition 2.9 (Asymptotically Smooth). Let f be a knot energy function for $\mathcal{S} = \mathcal{P}_n$ and $f(P_n)$ be the energy of a polygon $P_n \in \mathcal{P}_n$. Let the edges of P_n be labeled $\{e_1, e_2, \ldots, e_n\}$. Let θ_i be the excluded angle between the edges e_i and e_{i+1} and θ_n be the excluded angle between e_n and e_1. The energy function f is *asymptotically smooth* if there exists $M > 0$ such that for all $P_n \in \mathcal{P}_n$ and all $n > 0$,

$$\theta = \max_i(\theta_i) \leq \left[\frac{M}{n}\right] f(P_n)$$

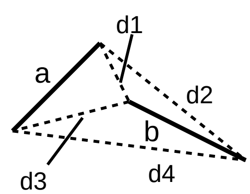
If an energy, f, is asymptotically smooth, then the total curvature of any knot K (defined as the sum of the θ_i's) is bounded by $M \cdot f(K)$. It is important to note that the converse of this statement is not always true [2].

2.2 Crossing Probability Energy

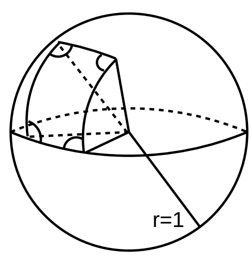
The *crossing probability energy* deals with the probability of whether or not pairs of edges cross. We will first define $n(a, b)$, the probability that the edges a, b don't cross, using two differing definitions to build an intuition for the energy. One definition defines $n(a, b)$ using the dihedral angles of a formed tetrahedron between the edges a, b and the other utilizes a double integral to find the average number of times a crosses b in a given projection. The definition of the total energy immediately follows from the definition of $n(a, b)$.

2.2.1 Dihedral Definition of $n(a, b)$

Let a and b be two non-adjacent edges of $P_n \in \mathcal{P}_n$. Two edges are defined to be non-adjacent if they do not share any vertices. The vertices of a and b create a tetrahedron. We will be concerned with the four dihedral angles along the edges of the tetrahedron other than the knot edges a, b, as shown in the following figure:



If we take each face of the tetrahedron and slice the unit sphere through the origin with each face, then the intersection between the faces of the tetrahedron and the surface of the sphere will create a quadrilateral on the sphere's surface:



The probability that the two edges, a and b, cross is the surface areas of the quadrilateral and its reflection through $\vec{0}$ divided by the total surface area of the sphere, which is 4π. The area of the quadrilateral is just the sum of the four angles minus 2π. Each of the quadrilateral's angles are equal to $\pi - d_i$, where the d_i's are the dihedral angles we defined above. We multiply the quadrilateral's surface area by 2 because of the diametrically opposed quadrilateral on the sphere. Then the probability that the two edges cross $p(a, b)$ is:

$$
\begin{aligned}
p(a,b) &= \frac{1}{4\pi} \cdot 2 \cdot \mathit{Area\ of\ Quadrilateral} \\
&= \frac{1}{2\pi}\Big((\pi - d_1) + (\pi - d_2) + (\pi - d_3) + (\pi - d_4) - 2\pi\Big) \\
&= 1 - \frac{d_1 + d_2 + d_3 + d_4}{2\pi}
\end{aligned}
$$

where each d_i is the dihedral angle between the two faces of the tetrahedron that share the edge i. There are only four of them because we exclude the two edges, a and b, of the knot. The probability, $n(a,b)$, that the two non-adjacent edges a, b do not cross is given by $n(a,b) = 1 - p(a,b)$, or:

$$n(a,b) = \frac{d_1 + d_2 + d_3 + d_4}{2\pi}$$

2.2.2 Integrand Definition of $n(a,b)$

In [7], Simon uses the Gauss map to show that the probability that two edges of a knot cross to be:

$$\frac{1}{2\pi} \int_{I \times I} |J(f)| \, ds \, dt$$

where $f(s,t)$ is the map $f : I \times I \to S^2$, $I = [0,1]$, and S^2 is the unit sphere. $J(f)$ is the Jacobian of f and the integrand term multiplied by $\frac{1}{2\pi}$ is the average number of times two edges are seen to cross over each other in the projection onto S^2. This is the probability that two edges cross, i.e. $p(a,b)$. Then since $n(a,b) = 1 - p(a,b)$:

$$n(a,b) = 1 - \frac{1}{2\pi} \int_{I \times I} |J(f)| \, ds \, dt$$

2.2.3 The Crossing Probability Energy - U_{CP}

Now we define the *crossing probability energy* as:

$$U_{CP}(P_n) = \frac{1}{\displaystyle\prod_{a,b} n(a,b)}$$

where the product is taken for each non-adjacent edge pairing a, b of P_n.

In [8], Trapp showed that U_{CP} is strong by proving that for $K \in \mathcal{P}_n$, $U_{CP}(K) \geq e^c$ where $c = c(K)$, the crossing number of the knot K, and that U_{CP} is not charge.

3 Basic Results

In Section 2.1 we stated that a knot energy is *basic* if and only if the energy is minimized on regular n-gons. Here we present a theorem that not only distinguishes the trivial knot from non-trivial knots but also distinguishes between the planar trivial knot and the non-planar trivial knot. We prove that if K is a planar trivial knot, then $U_{CP}(K) = 1$. This says nothing about K being a regular polygon, therefore U_{CP} is not basic.

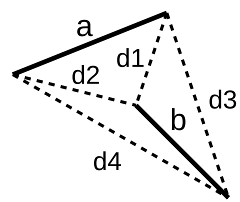
Although U_{CP} is not minimized only on regular polygons, it is nice that the energy is minimized on the trivial knot and that any non-trivial knot has energy $U_{CP} > 1$, a result that directly follows from the following theorem.

Theorem 3.1. *For $K \in \mathcal{P}_n$, $U_{CP}(K) = 1$ iff K is a planar trivial knot.*

Proof. Let $K \in \mathcal{P}_n$.

i.) Let $U_{CP}(K) = 1$. Since $U_{CP}(K) = 1 \geq e^c$, c=0. Then K is a trivial knot. Assume K is non-planar. Then some non-adjacent edge pairing will yield a non-planar tetrahedron. This tetrahedron will yield a volume greater than zero and when each of the four faces of the tetrahedron are embedded into a sphere, the resulting quadrilateral will have a surface area greater than zero. Then $p(a, b) > 0$ and $n(a, b) < 1$. This implies $U_{CP}(K) > 1$, contradicting the fact that $U_{CP} = 1$. Therefore K is a planar trivial knot.

ii.) Let K be a planar trivial knot. Then every edge of K will lie in the same plane. For any two non-adjacent edge pairing a, b, the tetrahedron resulting from connecting the vertices of the edges will also be planar. Then two of the dihedral angles we consider, d_1 and d_2, will be π and the other two, d_3 and d_4, will be 0, as made evident by the following figure:



Then n(a,b) for every non-adjacent edge pairing will be:

$$n(a, b) = \frac{d_1 + d_2 + d_3 + d_4}{2\pi} = \frac{\pi + \pi + 0 + 0}{2\pi} = 1$$

$U_{CP}(K)$ is the reciprocal of the product of $n(a, b)$ for each non-adjacent edge pairing. Therefore $U_{CP}(K) = 1$.

Therefore $U_{CP}(K) = 1$ *iff* K is a planar trivial knot. □

Corollary 3.2. *If $K \in \mathcal{P}_n$ is a non-planar trivial knot, then $U_{CP}(K) > 1$.*

Proof. Let $K \in \mathcal{P}_n$ be a non-planar trivial knot. Since $U_{CP} \geq e^c$ and $c = 0$, then $U_{CP}(K) \geq 1$. Since K is non-planar, by Theorem 3.1, $U_{CP}(K) \neq 1$. Therefore $U_{CP}(K) > 1$. □

Corollary 3.3. *If $K \in \mathcal{P}_n$ is a non-trivial knot, then $U_{CP}(K) > 1$.*

Proof. Proof is similar to Corollary 3.2. □

Theorem 3.4. *U_{CP} is not basic.*

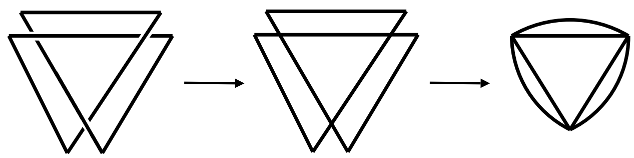
Proof. By Theorem 3.1, a regular polygon, R_n, has energy $U_{CP}(R_n) = 1$ as well as any other planar trivial knot. Therefore U_{CP} is not minimized only for regular n-gons. □

4 U_{CP} Properties

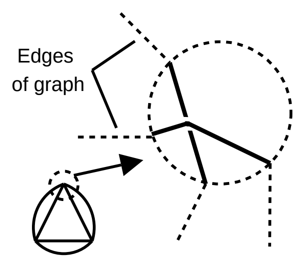
At this point, we know that U_{CP} is strong, though not basic or charge. Here we present a special construction of a knot, given enough sticks, to aid in the presentation that U_{CP} is asymptotically finite. From Theorem 3.1, it follows that U_{CP} is not asymptotically smooth. Through this discussion we arrive at tight bounds for U_{CP_n}, the $\inf U_{CP}$ for a knot type $\mathcal{K}$, bounded below and above by e^c and $\left(\frac{256}{81}\right)^c \approx 3.16^c$. This leads to the fact that U_{CP} is really just the crossing number when we bound the *n-crossing probability energy*, U_{CP_n}, by showing $c \leq \ln(U_{CP_n}) \leq 1.151c$.

4.1 Near Diagram Knot and U_{CP_n}

According to [5], the stick number of a knot is at most twice the crossing number, i.e. $s \leq 2c$. We create a planar graph of the knot P_n by turning all crossings to intersections. Each vertex of the graph corresponds to a crossing of P_n. For example, we obtain something like the following for the trefoil knot (note the resulting diagram has $2c$-edges):

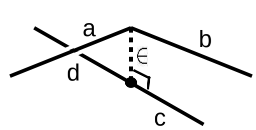


This construction can be done for an arbitrary knot, we just use the trefoil as the example here. If we construct each crossing by laying the undercrossing edge in the plane of the graph (all the non-crossing edges of the graph lie in the same plane) and use two edges for each overcrossing we obtain something similar to:



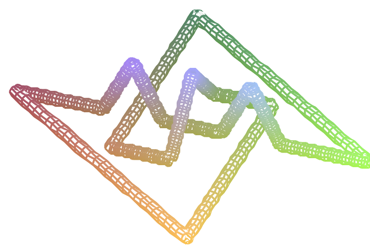
Now insert a vertex on the undercrossing edge so that the new vertex is directly under the crossing vertex. If we continue this way, we will use 4 sticks, or edges, for every crossing of the knot P_n. So the total amount of sticks needed to create this representation of the knot P_n will be $2c + 4c = 6c$. This will be the minimum number of sticks assumed for each knot in the following proofs, i.e. $n \geq 6c$.

Definition 4.1 (Near Diagram Knot). Let $K \in \mathcal{P}_n$. Let each crossing of K be respresented as:



where the crossing vertex, the shared vertex between edges a and b, is exactly above the undercrossing vertex, the shared vertex between the edges c and d. Every vertex except the crossing vertex lies in the same plane as the edges c and d. This plane also contains all undercrossing edges, two vertices from each crossing edge pair, and all non-crossing planar edges. Also, we assume the edge a is orthogonal to the edges c and d, similarly with the edge b. Let $\epsilon > 0$ be the distance between every crossing vertex and undercrossing vertex. We define a knot represented this way as a *near diagram knot.*

Example 4.2. Here is an example of a near diagram knot representation of the trefoil:

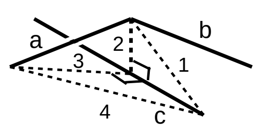


Note that there are $6c$, or 18, sticks used. Recall that the straight undercrossing edges contain vertices directly below the crossing vertices, giving 3 sticks not shown in the picture.

The fact that U_{CP} is not charge [8] is what allows us to exploit a near diagram knot representation by taking the limit of U_{CP} as $\epsilon \to 0$, i.e. as a vertex approaches another vertex. Even though the fact that U_{CP} is not charge is dissapointing, the following theorem will lead us into a proof that U_{CP} asymptotically finite, a property some energies lack. One such example is Simon's minimum distance energy, U_{MD}, which is charge though not asymptotically finite [4]. It is good to note here that the appropriate normalization of U_{MD} does seem to be asymptotically finite [6].

Theorem 4.3. *Let P_n be a near diagram knot, $c(P_n) = c$, and $\epsilon > 0$ be the distance between every crossing vertex and undercrossing vertex, then*
$\lim_{\epsilon \to 0} \big(U_{CP}(P_n)\big) = \left(\frac{4}{3}\right)^{4c} \approx 3.16^c$.

Proof. Let the polygonal knot P_n be a near diagram knot. Near each crossing, the knot looks like:



For each crossing, label the two overcrossing edges a and b and label the two undercrossing edges c and d, as above.

To determine $U_{CP}(P_n)$ there are four different non-adjacent edge pairing types that we have to consider:

- crossing edge - undercrossing planar edge
- crossing edge - planar edge

- crossing edge - crossing edge
- planar edge - planar edge

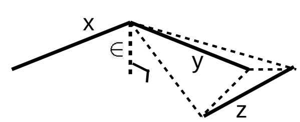
Case i. (crossing edge - undercrossing edge) We will first look at the probability $n(a, c)$. Construct a tetrahedron as in the figure above by connecting the vertices of a to those of c. Remember, we are only concerned with the dihedral angles along the edges that are not a or c. Label every other edge of the tetrahedron 1 through 4 as in the above figure. The triangular faces $\{12c\}$ and $\{23a\}$ are perpendicular to the plane that c lies in. As ϵ decreases, the crossing vertex lowers along the shared edge of the triangles $\{12c\}$ and $\{23a\}$. This causes the dihedral angles along the edges 1, 2, and 3 to approach $\frac{\pi}{2}$ and the dihedral along the edge 4 to approach 0. Thus, the probability that the two non-adjacent edges a and c don't cross approaches the following limit:

$$\lim_{\epsilon \to 0} n(a, c) = \lim_{\epsilon \to 0} \frac{d_1 + d_2 + d_3 + d_4}{2\pi} = \frac{\frac{\pi}{2} + \frac{\pi}{2} + \frac{\pi}{2} + 0}{2\pi} = \frac{\frac{3\pi}{2}}{2\pi} = \frac{3}{4}$$

where each d_i is the dihedral angle along the edge i.

The probabilities $n(a, d)$, $n(b, c)$, $n(b, d) \to \frac{3}{4}$ following the same construction. The crossing contributes a factor of $\left(\frac{4}{3}\right)^4 \approx 3.16$ to the $\lim_{\epsilon \to 0}(U_{CP}(P_n))$. Since each crossing of P_n will contribute a factor of $\left(\frac{4}{3}\right)^4$ to $U_{CP}(P_n)$, there will be a total factor of $\left(\frac{4}{3}\right)^{4c}$ for all crossings.

Case ii. (crossing edge - planar edge) Now we take a look at the same limit between a crossing edge and another planar edge besides the undercrossing edge, as shown:



where $\epsilon > 0$ is again the distance between the crossing vertex, shared between the edges x and y, and the plane in which z lies. As ϵ approaches 0 the edge pairings $\{x, z\}$ and $\{y, z\}$ approach planar edge pairings. The probability that two planar edges cross is 1, as shown in the proof of Theorem 3.1. So as ϵ approaches 0, $n(x, z) \to 1$ and $n(y, z) \to 1$. The contribution to $U_{CP}(P_n)$ is a factor of 1.

Case iii. (crossing edge - crossing edge) Here we have to consider two non-adjacent crossing edge pairings and their energy as $\epsilon \to 0$. As ϵ approaches 0 the crossing edges approach planar edge pairings. The contribution to $U_{CP}(P_n)$ is a factor of 1.

Case iv. (planar edge - planar edge) For every planar edge pairing, the probability $n(a, b) = 1$ and as each crossing height approaches 0, $n(a, b) = 1$. The contribution to $U_{CP}(P_n)$ is a factor of 1.

Now we have looked at every possible non-adjacent edge pairing in P_n and their contribution to the product in the calculation of $U_{CP}(P_n)$ as each of the crossings approach a height of 0. We have:

$$\lim_{\epsilon \to 0} U_{CP}(P_n) = \left(\frac{4}{3}\right)^{4c} \cdot 1 \cdot 1 \cdot 1 = \left(\frac{4}{3}\right)^{4c} \approx 3.16^c \qquad \square$$

This theorem allows us to say that $U_{CP_n}(\mathcal{K})$, the infimum of U_{CP} for a given knot type $\mathcal{K}$, is bounded above by $\left(\frac{4}{3}\right)^{4c}$, leading into the proof that U_{CP} is asymptotically finite.

Theorem 4.4. *If $K \in \mathcal{K}_n$, then $U_{CP}(K)$ is asymptotically finite.*

Proof. Let $K \in \mathcal{K}_n$. For $n \geq 6c$, Theorem 4.3 shows that $U_{CP_n}(\mathcal{K}) \leq \left(\frac{4}{3}\right)^{4c}$. Therefore:

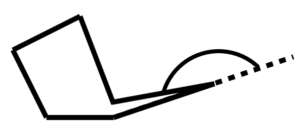
$$\limsup_{n \to \infty} U_{CP_n}(\mathcal{K}) < \infty$$

and $U_{CP}(K)$ is asymptotically finite. $\square$

Theorem 4.5. *If $K \in \mathcal{P}_n$, then $U_{CP}(K)$ is not asymptotically smooth.*

Proof. We will prove this theorem by illustrating a specific example where U_{CP} is not asymptotically smooth.

Let K be a planar trivial knot. Then $K \in \mathcal{P}_n$. By Theorem 3.1, $U_{CP}(K) = 1$. Let $\theta = \max_i(\theta_i)$ where each θ_i is the excluded angle between the edges e_i and e_{i+1} and θ_n is the excluded angle between e_n and e_1. We can construct a representation of K where θ is near π, similar to:



Leave θ fixed near π as $n \to \infty$, where n is the number of edges of K. Then there is no constant $M > 0$ such that $n\theta \leq M$ and since $U_{CP}(K) = 1$ then there is no $M > 0$ such that

$$\theta \leq \frac{M}{n} U_{CP}(K)$$

Therefore $U_{CP}(K)$ is not asymptotically smooth. $\square$

4.2 U_{CP_n} Bounds

We can now discuss bounds for $U_{CP_n}(\mathcal{K})$, the n-crossing probability energy for any $K \in \mathcal{K}_n$. Since $U_{CP}(K) \geq e^c$ [8], where $c = c(K)$, we know that $U_{CP_n}(\mathcal{K}) \geq e^c$. From Theorems 4.2 and 4.3 we have that $U_{CP_n}(\mathcal{K}) \leq \left(\frac{4}{3}\right)^{4c}$. Then the bounds for $U_{CP_n}(\mathcal{K})$ are:

$$e^c \leq U_{CP_n}(\mathcal{K}) \leq \left(\frac{4}{3}\right)^{4c}$$

The following theorem uses this fact to shed some light on what energy U_{CP} actually is.

Theorem 4.6. *Is $\mathcal{K}$ is a knot type, $n \geq 6c$, and $U'_{CP} = \ln(U_{CP})$, then $c \leq U'_{CP_n}(\mathcal{K}) \leq 1.151c$.*

Proof. Assume the given above. From Theorems 4.2 and 4.3 and [8],

$$e^c \leq U_{CP_n}(\mathcal{K}) \leq \left(\frac{256}{81}\right)^c$$

$$\ln e^c \leq \ln\left(U_{CP_n}(\mathcal{K})\right) \leq \ln\left(\frac{256}{81}\right)^c$$

$$c \leq U'_{CP_n}(\mathcal{K}) \leq c\left(\ln\frac{256}{81}\right) \approx c \cdot 1.150728$$

$$\therefore c \leq U'_{CP_n}(\mathcal{K}) \leq 1.151c$$

□

This is interesting because it shows that the infimum of the crossing probability energy is essentially the crossing number of a knot. The upper bound for U'_{CP_n} is tight enough at 1.151c that it is hopeful that the infimum of U'_{CP} is actually lower, closing in on c.

In fact, in the following section, we conjecture that U'_{CP} of the inscribed polygons of a smooth knot approaches the average crossing number of the smooth knot as the inscribed polygons approach the smooth knot.

4.2.1 Conjecture that $\ln(U_{CP}(K)) \rightarrow ACN(K)$

The *average crossing number*, or $ACN(K)$, of a polygonal knot K is defined as:

$$ACN(K) = \sum_{\frac{n(n-3)}{2}} \frac{1}{2\pi}\int_{I\times I} |J(f)|\, ds\, dt$$

(Refer to the Integrand Definition of $n(a,b)$ in Section 2.2.2 and [7].)

If we look at a knot K through all possible projections, we see the knot crossing over itself. For example, if we look at the trefoil knot over all of it's projections, most of the time it appears to cross over itself 3 times. But, through some projections of the knot it may appear to have 4 or 5 crossings. The average of all these crossing numbers over all projections is the *average crossing number* of the knot.

For the following discussion, the notation of $kp - q$ denotes a knot with p-crossings and q is a sequencing number to distinguish between knot types.

For a given parameterization of the trefoil knot, $k3-1$, we inscribe polygonal approximations of $k3-1$ and increase the number of edges of the inscribed polygons, denoted K_i. We look at what happens to $U_{CP}(K_i)$, or rather $\ln(U_{CP}(K_i))$, as the K_is approach the smooth curve of $k3-1$. We already know that the average crossing number, ACN, of the K_is should approach the ACN of the smooth curve $k3-1$. It turns out for this example, that $\ln(U_{CP}(K_i))$ seems to approach $ACN(k3-1)$. The specific parameterization of $k3-1$ we use is:

$$\vec{c}(t) = \left[\cos(2t)\cdot(2+\cos 3t),\ \sin(2t)\cdot(2+\cos 3t),\ \sin 3t\right] \text{ for } 0 \leq t \leq 2\pi$$

For n-edges, we parameterize n-vertices by substituting $t = \frac{2\pi}{n}i$, for $i = \{1, 2, \ldots, n\}$, into $\vec{c}(t)$. The following data table shows the results.

Polygonal $\to$ Smooth Approx. of $k3-1$			
n-edges	U_{CP}	$\ln(U_{CP})$	ACN
10	178.77492	5.18613	4.43745
15	107.85290	4.68077	4.42233
20	95.86474	4.56294	4.42801
25	91.53649	4.51674	4.43300
30	87.82454	4.47534	4.41812
40	89.24765	4.49142	4.45971
50	89.28829	4.49187	4.47172
60	89.07112	4.48944	4.47549
70	88.85005	4.48695	4.47673
75	88.87794	4.48726	4.47837
80	88.91590	4.48769	4.47988
90	88.92345	4.48778	4.48161
100	88.78545	4.48622	4.48123
150	88.80006	4.48639	4.48417
200	88.76220	4.48596	4.48472

The data was computed by a procedure written in Maple, following the algorithm described in the next section.

By looking at the table above, the data shows that as we increase the number of edges of the inscribed polygons, $\ln(U_{CP}(K_i)) \to ACN(K)$ where K is a specific parameterization of $k3-1$.

Let C^2 be the set of smooth curved knots.

Conjecture 4.7. *If $K \in C^2$ and $\{K_1, K_2, K_3, \ldots, K_m\}$ is a sequence of $K-$ inscribed polygonal knots, K_i, that approaches K as edges of the inscribed polygons are increased, then* $\ln(U_{CP}(K_i)) \to ACN(K)$.

5 Algorithm / Experimental Behavior and Data

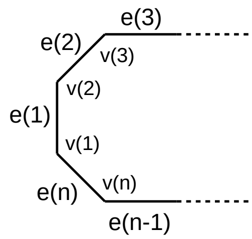
Here we will present a computing algorithm to calculate the value of U_{CP} for a given knot conformation. This algorithm also uses a negative gradient flow to locally minimize the energy.

We also discuss the behavior of U_{CP} for different knots as they flowed to local energy minima. We include a table of data that provides values of U_{CP} for certain knots, as well as comparisons to the minimum distance energy, U_{MD}, and two potential energies discussed in Section 6.

5.1 Algorithm

(a) *Input*: The vertices, $\{v_1, v_2, v_3, \ldots, v_n\}$, of a polygonal knot, K, are input in order.

That the vertices are input in order means you begin with v_1 and travel around the knot labeling the vertices consecutively to v_n. The edges, e_i, are defined as below:



(b) For each $\frac{n(n-3)}{2}$ non-adjacent edge pairing a, b of K compute $n(a, b)$:

(i) Utilize crossproducts to find the normal vectors to each face of the tetrahedron.

(ii) Using dotproducts between the normal vectors, solve the following equation:

$$\cos\theta_i = \frac{n_x \cdot n_y}{||n_x|| \cdot ||n_y||}$$

for θ_i and $i = 1, 2, 3, 4$, where n_x, x_y are the normal vectors to the faces x and y. θ_i is the dihedral angle between the faces x and y. Refer to Section 2.2 for the definition of U_{CP}.

(iii) Sum the θ_is to get:

$$n(a, b) = \frac{\sum \theta_i}{2\pi}$$

(c) The reciprocal of the total product is taken to obtain U_{CP}:

$$U_{CP} = \frac{1}{\prod_{a,b} n(a, b)}$$

There should be $\frac{n(n-3)}{2}$ factors in the product of n(a,b), corresponding to the amount of non-adjacent edge pairings of K.

(d) For the gradient of U_{CP}, we first take the natural logarithm of the energy for ease of derivation:

$$\ln(U_{CP}) = \ln\left(\frac{1}{\prod n(a, b)}\right) = -\sum (\ln n(a, b))$$

Then with respect to each coordinate, x_i, of the ordered vertices of K we take the partial derivative of $\ln(U_{CP})$. The vector of the coordinates of K looks like $K_{coord} = [x_1, x_2, x_3, x_4, \ldots, x_{3n}]$, where (x_1, x_2, x_3) are the coordinates of v_1 and so on. The gradient of U_{CP} is then computed by:

$$\triangledown U_{CP} = \left[\frac{\partial}{\partial x_1} U_{CP},\ \frac{\partial}{\partial x_2} U_{CP},\ \frac{\partial}{\partial x_3} U_{CP},\ \ldots,\ \frac{\partial}{\partial x_{3n}} U_{CP}\right]$$

where

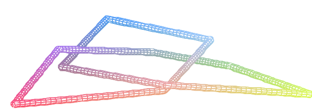
$$\frac{\partial}{\partial x_i} U_{CP} = -\sum_{\frac{n(n-3)}{2}} \left(\frac{1}{n(a, b)} \cdot \frac{\partial}{\partial x_i} n(a, b)\right)$$

for $i = 1, 2, 3, \ldots, 3n$. Then the gradient $\bigtriangledown U_{CP}$ is normalized and multiplied by $(-1 \times \epsilon \times \{\text{minimum of all } MD(a, b)\})$. The term $MD(a, b)$ is the minimum distance between two non-adjacent edges a, b [7]. We take the negative to go in the minimizing gradient direction. The ϵ is chosen small enough so as not to change the knot type when moving the knot. This modified gradient gives a vector, K_{move}, which is added to K_{coor}, the coordinates of the original knot K, to give us a new knot, K'. The algorithm is then started over with K' as the input knot. The minimization is then iterated as desired.

5.2 Experimental Behavior

With the presented algorithm and a procedure in Maple, we experimented with the minimization of 3 and 4 crossing knot representations, namely the trefoil and figure-eight knots. The gradient flow seemed to take vertices to vertices, and in the case where not enough sticks was given, vertices moved toward edges. It is good to note here that the energy will not tend to infinity in either case for these are the cases where U_{CP} fails to be charge. This behavior gave the inspiration for augmenting our definition of a *near diagram knot*, which in turn tightened our bound for U_{CP_n}. We originally had the crossing vertex directly above the undercrossing edge, rather than the crossing vertex directly above the undercrossing vertex.

Since vertices were approaching each other, each knot flattened out, as viewed in the following picture of a 10-stick trefoil knot:



5.3 Experimental Data

Using the procedure in Maple, we looked at some values for the U_{CP} energy function. Starting with the coordinates of well-conformed knots, we calculated the energy of the given knots. The knot conformations are close to being energy minimizers for U_{MD} and the values presented in the following table are all for the same knot conformations over all energy functions for a given knot.

The energy functions U_{LM} and U_{MM} are potential new knot energies and have not been explored at any depth. These functions are presented in Section 6.

Recall that the notation of $kp - q$ denotes a knot with p-crossings and q is a sequencing number to distinguish between knot types.

Table of Knot Energy Functions					
Knot	U_{CP}	lnU_{CP}	U_{MD}	U_{LM}	U_{MM}
k3-1	1.644E+03	7.40473	189.87420	8.12639	0.87163
k4-1	1.125E+05	11.63086	459.60736	12.35743	1.54699
k5-1	3.890E+05	12.87137	401.42316	16.41840	3.43179
k5-2	8.388E+05	13.63968	415.59828	16.71347	3.14407
k6-1	6.141E+07	17.93303	1047.44376	16.51381	3.10040
k6-2	7.390E+07	18.11828	879.22558	17.67741	2.21096
k6-3	1.990E+09	21.41124	1133.78786	18.77077	1.22018
k7-1	2.191E+08	19.20515	836.74345	21.05681	5.61575
k7-2	9.537E+08	20.67581	1115.95756	21.52058	5.02846
k7-3	2.327E+08	19.26533	808.66922	21.37211	5.34382
k7-4	1.283E+09	20.97261	1074.63556	23.27893	3.54120
k7-5	7.627E+08	20.45239	1105.25779	21.91794	4.69760
k7-6	8.517E+09	22.86531	1218.41207	22.48299	4.28959
k7-7	1.410E+10	23.36948	1288.90856	24.78095	1.97130
k8-1	9.464E+10	25.27331	1316.51512	28.01840	6.35780
k8-2	1.478E+10	23.41642	992.70256	27.68798	6.99736
k8-10	3.450E+11	26.56678	1642.11212	30.91567	3.92452
k8-11	4.444E+11	26.81997	1811.83416	28.49527	6.22090
k8-12	2.813E+12	28.66525	1785.68026	29.66231	4.93641
k8-13	8.602E+10	25.17789	1224.17291	29.62817	5.16532
k8-14	4.543E+10	24.53937	1453.29254	29.58777	4.93601
k8-15	1.179E+12	27.79557	1766.10962	30.52967	4.19358
k8-16	2.423E+11	26.21330	2265.81992	25.09231	1.82768
k8-17	6.306E+11	27.16998	2539.80301	25.18404	1.75426
k8-18	3.807E+12	28.96798	2923.48082	25.14591	1.65347
k8-19	9.621E+10	25.28978	1230.54271	19.11277	0.88665
k8-20	9.276E+11	27.55582	2200.24966	19.27186	0.71792
k8-21	3.672E+09	22.02409	1062.18104	24.15931	2.65249

6 Conclusion

Here we list some questions and potential problems, as well as definitions for potential knot energies.

6.1 Potential Problems and Knot Energies

While investigating the properties and the behavior of U_{CP} we came across some interesting questions about U_{CP}. Some were simply questions and others were propositions that we were unable to prove.

The first question is that of the following:

- Can we find an upper bound of U_{CP} involving U_{MD}, Simon's minimum distance energy [7]?

We started with the following relationship for some knot $K \in \mathcal{P}_n$:

$$\begin{aligned} \sum n(a,b) &= \sum (1 - p(a,b)) \\ &= \frac{n(n-3)}{2} - ACN(K) \end{aligned}$$

Note that we are summing $\frac{n(n-3)}{2}$ terms, $ACN(K)$ is the average crossing number of K, and a, b are non-adjacent edges of K. In [7], Simon found the relationship that $2\pi ACN(K) \leq U_{MD}(K)$. We apply this to the above equality to find:

$$\sum n(a,b) \geq \frac{n(n-3)}{2} - \frac{1}{2\pi} U_{MD}(K)$$

where

$$U_{MD}(K) = \sum_{a,b} \frac{l(a) \cdot l(b)}{MD(a,b)^2}$$

The edges a, b are non-adjacent, $l(a)$ is the length of edge a, and we again have $\frac{n(n-3)}{2}$ terms in the sum.

From this we sought out to minimize $n(a,b)$ and came across the following conjecture:

Conjecture 6.1. *If a, b are two non-adjacent edges of some knot $K \in \mathcal{P}_n$, then $n(a,b)$ is minimized when $a \perp b$ and $MD(a,b)$ is the distance along the shared perpendicular between endpoints of a and b.*

Experimentally we found this to be the case but were unable to prove that this truly is the minimizing conformation for $n(a,b)$. We found a generalized formula for $n(a,b)$ and an inequality involving $U_{MD}(a,b)$ for this situation. $U_{MD}(a,b)$ is the energy for the edges a and b. The formula involves the length of the two edges a, b, $l(a)$ and $l(b)$, and the minimum distance along the shared perpendicular between endpoints of a and b, $MD(a,b)$:

$$n(a,b) = \frac{\frac{3\pi}{2} + \theta}{2\pi}$$

where

$$\cos(\theta) = \frac{l(a) \cdot l(b)}{\sqrt{l(a)^2 + MD(a,b)^2} \cdot \sqrt{l(b)^2 + MD(a,b)^2}} < U_{MD}(a,b)$$

We know that $0 \leq \cos(\theta) \leq 1$, so the term involving $l(a)$, $l(b)$, and $MD(a,b)$ seems like it might be a probability. If we let that probability be $p'(a,b)$ we can define an energy, U_{LM}, as follows:

$$U_{LM}(K) = \prod_{a,b} \left(\frac{1}{1 - p'(a,b)} \right)$$

where the product is taken for each non-adjacent edge pairing of K.

U_{LM} is quickly shown to be scale invariant and is charge. It would be interesting to determine if U_{LM} satisfies other knot energy properties as well as to know what the probability:

$$p'(a,b) = \frac{l(a) \cdot l(b)}{\sqrt{l(a)^2 + MD(a,b)^2} \cdot \sqrt{l(b)^2 + MD(a,b)^2}}$$

actually is.

Theorem 6.2. *U_{LM} is charge.*

Proof. Let $K \in \mathcal{P}_n$. As K approaches a singular polygon, for some edges a, b of K, $MD(a,b) \to 0$. Then $p'(a,b) \to 1$ and thus $U_{LM}(K) \to \infty$. Therefore U_{LM} is charge. $\square$

Alternatively we can define $p''(a,b)$ to be:

$$p''(a,b) = \frac{MD(a,b)^2}{\sqrt{l(a)^2 + MD(a,b)^2} \cdot \sqrt{l(b)^2 + MD(a,b)^2}}$$

which is also scale invariant and define the energy U_{MM} as:

$$U_{MM}(K) = \prod_{a,b} \left(\frac{1}{1 - p''(a,b)} \right)$$

Further investigation into these energies would be interesting and could possibly provide meaningful knot energies.

6.2 Acknowledgements

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