Lower Bounds for the Ropelength of Reduced Conformations

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Abstract

This paper generalizes the results of Sadjadi [4] and Alley [1] by providing an algorithm to find a lower bound on the ropelength of any knot which admits a reduced diagram. This lower bound is found by changing this problem of geometry into one of linear programming, which is then solved by the simplex algorithm.

1 Introduction

The task of finding a lower bound for the ropelength of a conformation that admits a reduced diagram by means of a taut diagram has been undertaken by several authors. Sadjadi [4] has found a lower bound for the ropelength for reduced alternating diagrams ($4 \cdot$ crossing number), while Alley [1] has found a lower bound for the ropelength for paired diagrams ($4 \cdot$ bridge number). Here, we extend these results by providing an algorithm to find a lower bound for any reduced diagram.

The ultimate goal of this study is to simply relate ropelength to invariants of knot type, as well as to prove that the ropelength of alternating knots is at least linear in the crossing number. Since it is forseeable that there exist non-paired diagrams of alternating knots which could stem from conformations with minimal ropelength, expanding past studies to include non-paired diagrams is necessary. Please see [1], [4] for details.

2 Definitions and Terminology

A **conformation** is an embedding of the unit circle in $\mathbb{R}^3$. A **knot diagram** is a projection of a conformation onto the xy-plane; a **crossing** occurs when two points on the knot have the same x- and y-coordinates. A diagram is said to be **reduced** if it has no crossings that are removable as in Figure 1.

At a crossing, the arc corresponding to the point with the larger z-value is drawn with a solid line through the crossing; the arc corresponding to the point with the smaller z-value is drawn as a line with a break at the crossing. These

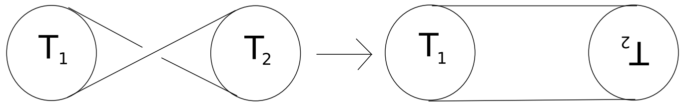

Figure 1: The form of a non-reduced diagram, with (knotted) arcs T_1 and T_2 and removable crossing in the middle.

two arcs are called an **overpass** and an **underpass**, respectively. An overpass (underpass) is called a **maximal overpass (underpass)** if it cannot be extended to cross over more underpasses (overpasses). The number of crossings occuring in a knot diagram is called the **crossing number** c of the diagram; the number of maximal overpasses is called the **bridge number** n. We will let p_i denote the point with the maximum z-value on the arc corresponding to the ith maximal overpass encountered as one traverses the knot from some starting point. Similarly, let q_i denote the point with the minimum z-value on the arc corresponding to the ith maximal underpass encountered as one traverses the knot from the same starting point. For our convenience, we will assume that q_i is encountered before p_i $\forall i$. Let o_i and u_i denote the height (on the z-axis) of p_i and q_i, respectively. If the ith maximal overpass crosses over the jth maximal underpass, then the ordered pair (p_i, q_j) will be called a **pairing**.

At times it will be convenient to relabel the p_i and q_i as $\{v_1, \ldots, v_{2n}\}$, where the subscripts indicate the order in which the maximal overpasses and underpasses are encountered as one travels along the knot beginning at a maximal *underpass* v_1. It follows that v_i corresponds to an underpass when i is odd, and to an overpass when i is even. See Figure 2 for an example.
To each knot diagram, we define a **crossing information graph (CIG)** constructed as such: there is a vertex for each p_i and q_j, and two such vertices are connected by an edge if (p_i, q_j) is a pairing. An example is given in Figure 3. Such a graph is necessarily bipartite, meaning that the set of vertices can be partitioned into two nonempty subsets such that no two vertices from the same subset are joined by an edge. The two subsets correspond to the set of maximal overpasses and the set of maximal underpasses, which we will denote by X and Y respectively. A **matching** is a set of edges from a bipartite graph with no common endpoints. An **X-matching** is a matching involving all vertices in the graph. A knot diagram is called a **paired diagram** if its CIG admits an X-matching.

For any conformation K, define the **ropelength** of K as $Rop(K) = \frac{\ell(K)}{r(K)}$, where $\ell(K)$ is the arc length of K and $r(K)$ is the injectivity radius of K ($r(K)$ is the maximum radius a tube surrounding the knot could have without the tube intersecting itself). It has been proven that $Rop(K)$ is scale invariant, so we will assume that $r(K) = 1$. With this assumption, it is known that in a reduced diagram, $o_i - u_j \geq 2$ for each pairing (o_i, u_j). Define the height function $h : K \to \{0\} \times \{0\} \times \mathbf{R}$ by $h(x, y, z) = (0, 0, z)$. Denote the length of $h(K)$ by

$\ell(h(K))$; clearly $\ell(h(K)) \leq Rop(K)$. Define the **taut image** of K by replacing the arc of h(K) between each $h(p_i)$ and $h(q_i)$ (as well as between each $h(q_i)$ and $h(p_{i+1})$, where the subscripts are modulo n) with a straight line segment. It will be convenient to graph the taut image of K as the **taut diagram** $t(K)$ of K, where the v_i are placed at their respective heights on the z-axis as in Figure 4 (strictly speaking, it is the $h(v_i)$ that are at these points on the z-axis, but it drawing the taut diagram we will write v_i for brevity). The p_i and q_i will be referred to as the vertices of $t(K)$; the edges joining consecutive arcs will be called the edges of $t(K)$. The **length** $\ell(t(K))$ of $t(K)$ is defined to be $\sum_{i=1}^{2n} |h(v_{i+1}) - h(v_i)|$, where the subscripts of the vertices are modulo $2n$ (that is, $v_{2n+1} = v_1$). It follows that $\ell(t(K)) \leq \ell(h(K))$.

3 A Lower Bound for Ropelength of Conformations that Admit a Reduced Diagram

Definition 3.1: Given any taut diagram $t(K)$, we define the **reduced taut diagram** $rt(K)$ by redefining $h(v_i)$ for $i = 1, \ldots, 2n$ (in that order) as follows: for each underpass q_i in $t(K)$, let $h(q_i) = u_i$, and let the heights of the overpasses immediately following and preceding q_i have heights o_j, o_k respectively. Then in

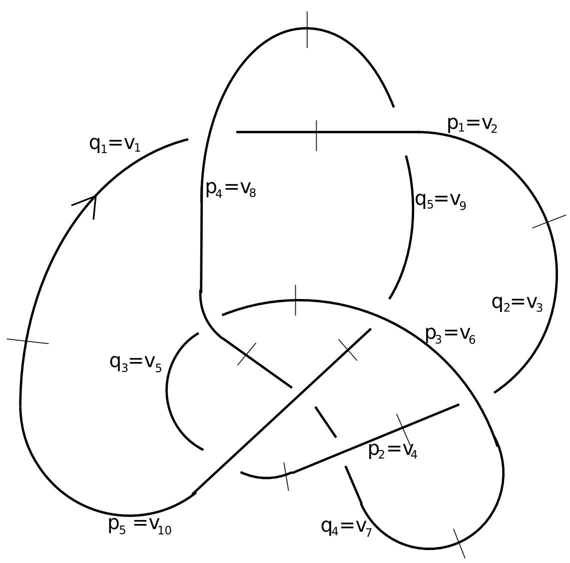

Figure 2: A knot diagram with labelled overpasses and underpasses of a conformation of the knot 8_{19}

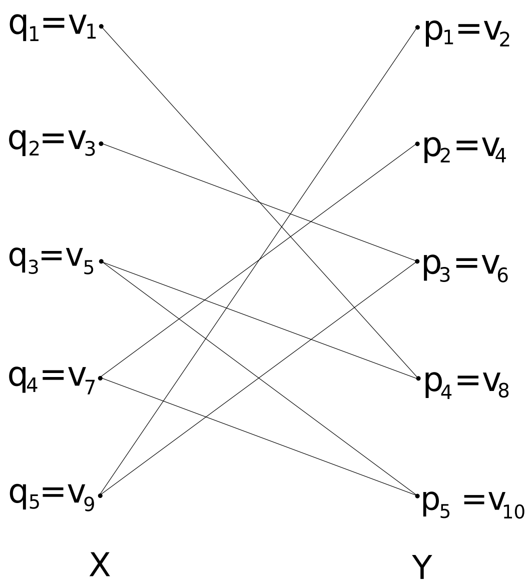

Figure 3: The CIG for the diagram in Figure 2, which is paired via the X-matching $(v_1, v_8), (v_3, v_6), (v_5, v_{10}), (v_7, v_4), (v_9, v_2)$

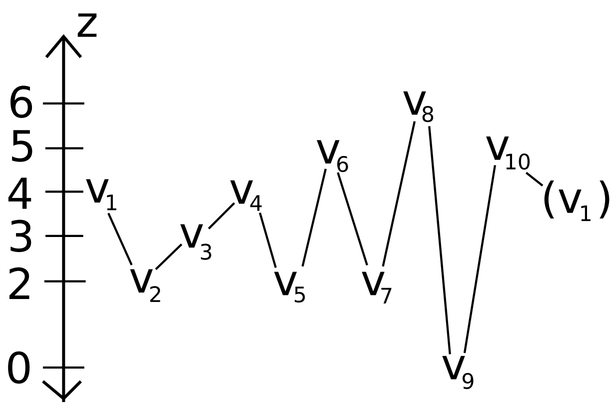

Figure 4: One feasible taut diagram for the example of Figures 2 and 3; note that any two connected vertices of the CIG are at least 2 units apart. Here, $\ell(t(K)) = 28$.

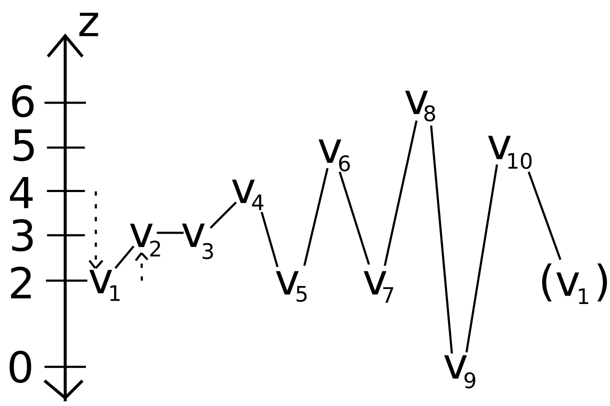

Figure 5: The reduced taut diagram obtained from the taut diagram of Figure 4. Note that each overpass is at or above the heights of its adjacent underpasses, and each underpass is at or below the heights of its adjacent overpasses. $\ell(rt(K)) = 28$.

$rt(K)$ redefine $h(q_i) = min(u_i, o_j, o_k)$. Thus, we move q_i down by the smallest possible distance such that the overpasses immediately following and preceding q_i do not lie below q_i. Similarly, for each overpass p_i in $t(K)$, let $h(p_i) = o_i$, and let the heights of the underpasses immediately following and preceding p_i have heights u_j, u_k respectively. Then, in $rt(K)$ redefine $h(p_i) = max(o_i, u_j, u_k)$. We also define the length of $rt(K)$ $\ell(rt(K))$ with the same formula as for $\ell(t(K))$, but with new values for some of the $h(v_i)$.

See Figure 5 for an example. Note that, since at each step we only move underpasses down and overpasses up, we cannot create new scenarios in which underpasses are located above their respective overpasses (and vice-versa), and thus the process of creating $rt(K)$ will terminate after at most $2n$ steps.

Lemma 3.1: $\ell(t(K)) \geq \ell(rt(K))$.

Proof.

We will show that, in each step in the creation of $rt(K)$, the length of the diagram is not increased. We will show the proof for the translating of underpasses, the case for overpasses is proved similarly.

Case 1: $h(q_i)$ is redefined to be u_i.

Then the change in the length of the diagram is clearly 0.

Case 2: $h(q_i)$ is redefined to be o_j or o_k.

WOLOG, assume $h(q_i)$ is redefined to be o_j. Then the change in the length of the diagram is equal to new lengths of the two edges hitting q_i minus the old lengths of those edges. This equals $(o_k - o_j) - ((u_i - o_j) + |o_k - u_i|) = o_k - u_i - |o_k - u_i| \leq 0$.

Therefore, at each step in the creation of $rt(K)$ the length of the diagram is not increased, it follows that $\ell(t(K)) \geq \ell(rt(K))$.

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Lemma 3.2: $\ell(rt(K)) = 2(\sum_{i=1}^{n} o_i - \sum_{i=1}^{n} u_i)$ (where the o_i and u_i are the new heights of the vertices in $rt(K)$).

Proof.

We know that $\ell(rt(K)) = \sum_{i=1}^{n} |o_i - u_i| + \sum_{i=1}^{n} |o_{i+1} - u_i|$, where the subscripts are modulo n. But by the definition of $rt(K)$, each $o_i - u_i$ and $o_{i+1} - u_i$ is positive. Each o_i and u_i appears in each of the two sums on the right hand side of the above equation exactly once, and so we have
$\ell(rt(K)) = 2(\sum_{i=1}^{n} o_i - \sum_{i=1}^{n} u_i)$.

■

Theorem 3.1: Given the CIG of a knot diagram of a reduced conformation K, let z be the infimum of the lengths of all reduced taut diagrams that fit the constraints of the CIG (i.e. if p_i and q_j are connected by an edge in the CIG, then $o_j - u_i \geq 2$). Then $Rop(K) \geq z$.

Proof.

Combining previous results, we have $Rop(K) \geq \ell(h(K)) \geq \ell(t(K)) \geq \ell(rt(K)) \geq z$.

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4 Linear Programming and the Simplex Algorithm

Here, we give an overview of the theory of linear programming and the simplex algorithm; a more detailed account can be found in [3]. In order to remain consistent with the notation of [3], we will momentarily redefine m, n, and c as in the following definition.

Definition 4.1: Let A be an $m \times n$ matrix, where $m \geq n$, with rows a_i. Let M and $\overline{M}$ be the sets of row indices corresponding to equality and inequality constraints respectively, and let N be the set of column indices corresponding to constrained variables respectively. Let $x \in \mathbb{R}^n$. Then an **instance of the general LP** is defined by:

$$min\ c \cdot x$$

$$a_i \cdot x = b_i\ for\ i \in M$$

$$a_i \cdot x \geq b_i\ for\ i \in \overline{M}$$

$$x_j \geq 0\ for\ j \in N$$

where $b \in \mathbb{R}^m$ and $c \in \mathbb{R}^n$ (c will be referred to as the cost vector). Any LP of the form

$$min\ c \cdot x$$

$$Ax = b$$

$$x_j \geq 0\ \forall j \in \{1, \ldots, n\}$$

is said to be in standard form.

It is shown in [3] that any LP can be written in standard form through the replacement of inequality constraints and unconstrained variables by equality constraints and constrained variables (respectively); this is done by introducing extra variables. Because of this, we will assume that any given LP is in standard form. As in [3], we will assume that A is of rank m, which in our case will turn out to be nonrestrictive.

Definition 4.2: A **basis** of A is a linearly indepenedent collection of columns $\mathcal{B} = \{A_{j_1}, \ldots, A_{j_m}\}$. Let B be an $m \times m$ matrix whose columns are the vectors (with subscripts in increasing order) of a given basis of A. The **basic solution** corresponding to $\mathcal{B}$ is a vector $x \in \mathbb{R}^n$ with

$$x_j = 0 \; for \; A_j \notin \mathcal{B}$$

$$x_{j_k} = the \; kth \; component \; of \; B^{-1}b \; for \; k = 1, \ldots, m.$$

If a basic solution satisfies all constraints of the LP, it is said to be a **basic feasible solution** (bfs).

Assuming the set of feasible points F (the set of points satisfying all constraints of the LP) is nonempty, it can be shown that, for any given LP, at least one bfs exists. One final assumption made by [3], which is again nonrestrictive in our case, is that the set $\{c \cdot x \mid x \in F\}$ is bounded from below (otherwise the LP would have no optimal solution). We now define the terminology necessary for the description of the simplex algorithm.

Definition 4.3: Given an LP in standard form with $m \times n$ matrix A, $b \in \mathbb{R}^m$ and cost vector $c \in \mathbb{R}^n$, we define the **original tableau** O of the LP to be the $(m+1) \times (n+1)$ matrix illustrated in Figure 6.
We will find it convenient to call the row and column adjoined to A as row and column 0. Any $(m+1) \times (n+1)$ matrix derived from the original tableau of the LP through elementary row operations is said to be a **tableau** T of the LP. The lower-right $m \times n$ block of T (which is derived from A through elementary row operations) will be called the **principal matrix** P of T. A will also be called the **original principal matrix** of the LP.
Definition 4.4: Suppose we have a tableau T of an LP whose principal matrix P has as a basis the columns of a subidentity matrix $[P_{j_1}, \ldots, P_{j_m}]$ (that is to say, P_{j_i} is the standard m-vector e_i), and that $T_{0j_i} = 0$ for $i = 1, \ldots, m$. Furthermore, suppose that l is the first column from the left, excluding column 0, such that $T_{0l} < 0$, and that k is the first row from the top such that $T_{kl} > 0$ and $\frac{T_{k0}}{T_{kl}} = min_{i \in R}(\frac{T_{i0}}{T_{il}})$, where $R = \{i \mid i > 0 \; and \; T_{il} > 0\}$. Then we define the action of **pivoting** on T_{kl} as adding appropriate multiples of row k to the other rows so that $P_l = e_k$ and $T_{0l} = 0$. In this, the basis loses the vector P_{j_k} and gains the vector P_l.

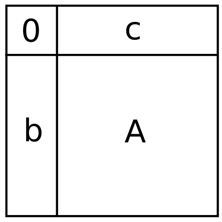

Figure 6: The original tableau of an LP

Note that it may not always be the case that any such k exists. However, it can be shown that, throughout the simplex algorithm, if any such k exists, then such an l must exist, as a consequence of our assuming that $\{c \cdot x \mid x \in F\}$ is bounded from below [3]. For convenience, our definition of pivoting on an entry of T is slightly different than that of [3] in that it also defines which row k and column l to choose (the first ones, excluding row and column 0) if more than one fit the other constraints, so that it is only possible to pivot on at most one entry of T. [3] includes this “tiebreaker” in the definition of the simplex algorithm, and the the simplex algorithm proceeds the same way in each case.

Definition 4.5: Given an LP with original tableau O, we define the simplex algorithm as follows: first, determine a basis $\{A_{j_1}, \ldots, A_{j_m}\}$ of A which will yield a bfs. Then, perform row operations on O so that $P_{j_i} = e_i$ and $T_{0j_i} = 0$ for $i = 1, \ldots, m$. Then pivot on entries of T (the tableau derived from O) until no k (as defined above) exists (that is to say, all the entries of T which were originally occupied by the components of c are non-negative).

It is shown in [2] that this form of the simplex algorithm must terminate after a finite number of steps.

Theorem 4.1: Suppose we are given an LP that has tableau T after performing the simplex algorithm on the original tableau O. Then $min(c \cdot x) = -T_{00}$. Furthermore, if we let the final basis of P be $\{P_{j_1}, \ldots, P_{j_m}\}$ (where $P_{j_i} = e_i \; \forall i$), then a vector x which yields this solution is given by:

$$x_k = T_{i0} \; if \; k = j_i \; for \; some \; i$$

$$x_k = 0 \; otherwise.$$

Figure 7 gives an example of the original tableau and simplex algorithm when applied to the following LP:

$$min \; x_1 + x_2 + x_3 + x_4 + x_5$$

0	1	1	1	1	1
1	1	2	1	0	0
3	2	1	1	1	0
4	2	5	1	0	1

$\longrightarrow$

-6	-2	-3	0	0	0
1	①	2	1	0	0
2	1	-1	0	1	0
3	1	3	0	0	1

$\longrightarrow$

-4	0	1	2	0	0
1	1	2	1	0	0
1	0	-3	-1	1	0
2	0	1	-1	0	1

Figure 7: An example of the original tableau and simplex algorithm

$$x_1 + 2x_2 + x_3 = 1$$
$$2x_1 + x_2 + x_3 + x_4 = 3$$
$$2x_1 + 5x_2 + x_3 + x_5 = 4$$
$$x_i \geq 0 \; for \; i = 1, \ldots, 5$$

The first tableau is the original, and the second tableau is after row operations have been performed to create a subidentity matrix in columns 3, 4, and 5 (which constitute the basis), as well as to get 0's in the 0th row of these three columns. This corresponds to the basic solution $(0, 0, 1, 2, 3)$, which is a bfs. The entry on which we perform the pivot at each step of the simplex algorithm is circled. For example, the first entry on which we pivot is the 1 in the first row, since the first column in the 0th row (excluding column 0) in which a negative entry is found is column 1, and the minimum of $\frac{1}{1}$, $\frac{2}{1}$ and $\frac{3}{1}$ (obtained from dividing entries in the 0th column by corresponding positive entries in column 1) is 1. After the first pivot (during which column 1 is transformed into a standard vector and enters the basis, while column 3 leaves the basis), all entries in the 0th row (excluding column 0) are non-negative, and thus the optimal value of 4 is given by the bfs (1,0,0,1,2).

5 Calculating the Lower Bound for Ropelength through Linear Programming

We now wish to apply the simplex algorithm to the minimalization of $\ell(rt(K))$. In order to do this, we need to ensure that the assumptions of [3] are met, and we need to supply a set of linearly independent columns that will result in a bfs. The assumptions requiring that $c \cdot x$ have a minimum value and that $Ax = b$ be consistent are automatic; to ensure that $rank(A)$ is maximal we make the following definition.

Definition 5.1: Given a knot diagram with set of crossings C, define the set of basic crossings $S \subseteq C$ such that $|S|$ is maximal and no two elements of S involve the same overpass and underpass. The number of basic crossings is invariant of how S is chosen, call $c' = |S|$ the **basic crossing number**.

Definition 5.2: Given an ordering $\{v_1, \ldots, v_{2n}\}$ of the maximal overpasses and underpasses of a knot diagram of a reduced conformation K, we define a total ordering on the basic crossings of the knot diagram as follows: let basic crossing c_1 be between overpass v_{i_1} and underpass v_{j_1}, and basic crossing c_2 be between overpass v_{i_2} and underpass v_{j_2}. Then we say $c_1 < c_2$ if $i_1 < i_2$, or if $i_1 = i_2$ and $j_1 < j_2$.

Based on how we defined z in the last section, we have the following theorem.

Theorem 5.1: Let $\{c_k\}$ be the totally ordered set of basic crossings of a knot diagram of a reduced conformation K, such that $c_i < c_j$ iff $i < j$. Let z be as defined in Theorem 3.1, then z is the solution to the LP:

$$min \sum_{i=1}^{n} 2o_i - \sum_{i=1}^{n} 2u_i$$

$$\forall k \in \{1, \ldots, c'\},\ h(v_{i_k}) - h(v_{j_k}) \geq 2$$

$$\forall j \in \{1, \ldots, n\},\ o_j - u_j \geq 0 \; and \; o_j - u_{j+1} \geq 0$$

$$o_i, u_i \geq 0 \; \forall i$$

where v_{i_k} and v_{j_k} are the overpass and underpass (respectively) corresponding to crossing c_k. We will find it more convenient to express the constraints requiring that overpasses be above their adjacent underpasses by: $\forall j \in \{1, \ldots, n\}$, $u_j - o_j \leq 0$ and $u_{j+1} - o_j \leq 0$.

Thus, z is actually the minimum of the lengths of all reduced taut diagrams satifsfying the constraints of the LP (it was originally defined as the infimum). In order to solve this LP, we first need to put it into standard form. We do this by introducing surplus variables $s_1, \ldots, s_{c'}$ corresponding to the constraints for each crossing, as well as introducing slack variables $t_1, \ldots, t_{2n}$ corresponding to the constraints for pairs of consecutive vertices of $rt(K)$. So the above LP is equivalent to the following LP:

$$min \sum_{i=1}^{n} 2o_i - \sum_{i=1}^{n} 2u_i$$

$$\forall k \in \{1, \ldots, c'\},\ h(v_{i_k}) - h(v_{j_k}) - s_k = 2$$

$$\forall j \in \{1, \ldots, n\},\ u_j - o_j + t_{2j-1} = 0 \; and \; u_{j+1} - o_j + t_{2j} = 0$$

$$o_i, u_i, t_j, s_k \geq 0 \; \forall i, j, k$$

We order the t_j in this way so that, beginning at the pair of consecutive vertices v_1 and v_2, the t_j appear in order in the equations corresponding to the pairs of consecutive vertices of $rt(K)$, ending with t_{2n} corresponding to the arcs v_{2n} and v_1. Thus, t_j can be thought of as the absolute value of the vertical distance one has to travel to get from v_j to v_{j+1}.

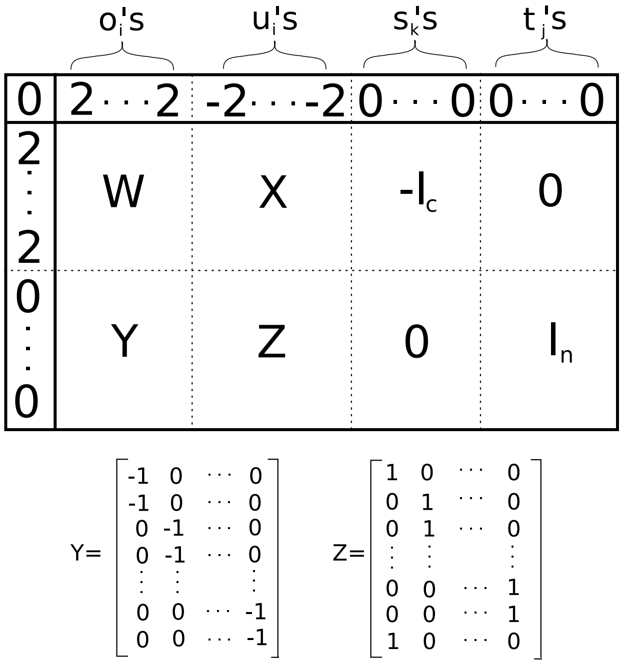

Figure 8: The form of the original tableau for any LP corresponding to the minimizing of $\ell(rt(K))$

We intend to solve this LP via the simplex algorithm, so we must first start with the original tableau. Because of the strict ordering we have imposed on the appearance of the variables in the constraint equations, the original tableau for any LP fitting the above description carries a great deal of structure, which is illustrated in Figure 8. W is a $c' \times n$ matrix which has a single 1 in each row (all other entries are 0), and each column of W has at least one 1. In addition, the 1 in each row of W (other than the first row) is at least as far to the right as the 1 in the preceding row. X is a $c' \times n$ matrix which has a single -1 in each row (all other entries are 0), and each column of X has at least one -1. See Figure 8 for the forms of Y and Z, which are both $2n \times n$ matrices.

Before giving a basic solution which will be a bfs for any LP corresponding to the minimizing of $\ell(rt(K))$, we present in Figure 9 an example of the process of creating the subidentity matrix and getting 0's above the basic columns, which are marked with a dot above them. The original tableau is derived from the CIG of Figure 3. We first multiply rows 4, 6, and 8 by -1. We then add row 3 to row 4, add row 5 to row 6, and add row 7 to row 8. Next, we add row 1 to rows 9 and 10, add row 2 to rows 11 and 12, add row 3 to rows 13 and 14, add row 5 to rows 15 and 16, and add row 7 to rows 17 and 18. Finally, we add -2 times each of rows 1, 2, 3, 5, and 7 to row 0, resulting in the bottom matrix of

Figure 9. Note that, in this case, our initial bfs is actually optimal, and that it agrees with [1]. Now we present a basic solution which is feasible for any LP fitting the above description.

Theorem 5.2: For any LP of the form above, let $\mathcal{A} \subseteq \{1, \ldots, c'\}$ with $|\mathcal{A}| = n$ and $\forall k, l \in \mathcal{A}, v_{i_k} = v_{i_l}$ iff $k = l$. That is, $\mathcal{A}$ corresponds to a set of n rows in the submatrix W in the original tableau, all of which have 1's in different columns. Then the set of columns of A corresponding to the variables in $\mathcal{B} = \{o_i \mid i \in \{1, \ldots, n\}\} \cup \{s_k \mid k \notin \mathcal{A}\} \cup \{t_j \mid j \in \{1, \ldots, 2n\}\}$ is a basis which will yield a bfs. Furthermore, the values of the o_i will all be 2, the values of the s_k will all be 0, and the values of the t_j will all be 2. This will correspond to the reduced taut diagram where the underpasses are all at height 0, and the overpasses are all at height 2.

Proof.

It is easy to see that the columns corresponding to the elements of $\mathcal{B}$ are linearly independent. Each column corresponding to a t_j is already a standard vector. Each column corresponding to an s_k is equal to -1 times a standard vector, so we multiply each row k by -1. Each column corresponding to an o_i contains a 1 in exactly one row, and all of the other columns corresponding to elements of $\mathcal{B}$ have a zero in that row. Since for each row corresponding to a constraint equation for c_k we have that either $k \in \mathcal{A}$ (resulting in the selection of an o_i) or $k \notin \mathcal{A}$ (resulting in the selection of an s_k), we have that the number of o_i's plus the number of s_k's equals c'. Therefore $|\mathcal{B}| = c' + 2n$ (since there are $2n$ t_j's; n is the bridge number), which is the required rank of the principal matrix. Thus, in order to get a subidentity matrix we just need to perform elementary row operations to transform all columns corresponding to o_i's into standard vectors. This is possible, since the only spots underneath the first 1 in any such column where anything other than a 1 could occur would be in the rows of the submatrix W corresponding to c_k with $k \in \mathcal{A}$, as well as in the submatrix Y (in fact, such an entry in both cases must be equal to -1). We can then add the row containing the selected 1 to these other rows, and the other basic columns will remain standard vectors since they have a 0 entry in that row. Therefore the columns corresponding to the elements of $\mathcal{B}$ are linearly independent and form a basis.

We now find the basic solution corresponding to this basis by examining the values of the entries in the 0th column of T after the row operations have been performed. First, note that, in the original tableau, in the first c' rows (excluding the 0th row) we find the entry 2 in the 0th column, in the subsequent $2n$ rows we find a 0 in the 0th column. As a reminder, we obtained a subidentity matrix from the basis by first multiplying each row k corresponding to an s_k by -1, and then adding rows containing the 1 of a basic column corresponding to an o_i (there is only one such 1 in each column) to rows beneath it in order to obtain a standard vector in that column. After the multiplication of each row k by -1, the value in the 0th column becomes a -2. However, since these rows contain undesired non-zero entries in a basic column corresponding to an o_i, the row containing the 1 of the basic vector will be added to it, and the entry in the 0th column of such a row must be a 2. Thus, each row k will end up

	·	·	·	·	·									·		·		·	·	·	·	·	·	·	·	·	·	·
0	2	2	2	2	2	-2	-2	-2	-2	-2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	1	0	0	0	0	0	0	0	0	-1	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	0	1	0	0	0	0	0	0	-1	0	0	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	0	0	1	0	0	0	-1	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	0	0	1	0	0	0	0	0	0	-1	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	0	0	0	1	0	-1	0	0	0	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	0	0	0
2	0	0	0	1	0	0	0	-1	0	0	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	0	0
2	0	0	0	0	1	0	0	-1	0	0	0	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	0
2	0	0	0	0	1	0	0	0	-1	0	0	0	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0
0	-1	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
0	-1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
0	0	-1	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
0	0	-1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
0	0	0	-1	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
0	0	0	-1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
0	0	0	0	-1	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
0	0	0	0	-1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
0	0	0	0	0	-1	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
0	0	0	0	0	-1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1

↓

	·	·	·	·	·									·		·		·	·	·	·	·	·	·	·	·	·	·
-20	0	0	0	0	0	0	0	0	0	0	2	2	2	0	2	0	2	0	0	0	0	0	0	0	0	0	0	0
2	1	0	0	0	0	0	0	0	0	-1	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	0	1	0	0	0	0	0	0	-1	0	0	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	0	0	1	0	0	0	-1	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	-1	0	0	1	0	0	-1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	0	0	0	1	0	-1	0	0	0	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	-1	0	1	0	0	0	0	0	0	-1	1	0	0	0	0	0	0	0	0	0	0	0	0
2	0	0	0	0	1	0	0	-1	0	0	0	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	-1	1	0	0	0	0	0	0	0	-1	1	0	0	0	0	0	0	0	0	0	0
2	0	0	0	0	0	1	0	0	0	-1	-1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
2	0	0	0	0	0	0	1	0	0	-1	-1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
2	0	0	0	0	0	0	1	0	-1	0	0	-1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0	1	-1	0	0	-1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
2	0	0	0	0	0	0	-1	1	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
2	0	0	0	0	0	0	-1	0	1	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
2	0	0	0	0	0	-1	0	0	1	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	1	0	0	0
2	0	0	0	0	0	-1	0	0	0	1	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	1	0	0
2	0	0	0	0	0	0	0	-1	0	1	0	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	1	0
2	0	0	0	0	0	1	0	-1	0	0	0	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	1

Figure 9: The original tableau for the constraints given by the CIG of Figure 3, followed by the matrix formed after creating the subidentity matrix and getting 0's above the basic columns, which have a dot above them.

with a 0 in the 0th column. Because of the structure of the submatrix Y, each of the bottom $2n$ rows will have a row with a 2 in the 0th column added to it exactly once, resulting in each of the bottom $2n$ rows ending up with a 2 in the 0th column. Keeping in mind that each of the variables not corresponding to a basic column will have value 0, we have that each of the o_i's has value 2, each of the u_i's has value 0, each of the s_k's has value 0, and each of the t_j's has value 2; this is easily seen to be a bfs.

■

Approaching the problem of minimizing the length of a taut diagram through the simplex algorithm allows us to easily prove the results of [1] and [4].

Theorem 5.3: Let K be a conformation that admits a reduced, paired diagram. Then $Rop(K) \geq 4n$.

Proof.

Suppose we are given a diagram with some pairing. We can assume that each crossing included in the pairing is a basic crossing, since taking two edges connecting the same two vertices of the CIG would contradict the fact that these crossings are in a pairing. We will let $\mathcal{A}$ be the set of all k such that c_k is included in the given pairing. We shall prove that the bfs corresponding to $\mathcal{A}$ found in the previous theorem (which results in the reduced taut diagram having length $4n$) is optimal. Recall that a bfs is optimal if all the entries in the 0th row of the tableau (excluding the 0th column) are nonnegative after the subidentity matrix is formed and the entries above the basic columns are equal to zero. In the original tableau, as well as in the tableau resulting from the creation of the subidentity matrix as in the preceding theorem, we have that the entries in the 0th row are 2 in the columns corresponding to the o_i's, -2 in the columns corresponding to the u_i's and 0 in the columns corresponding to the s_k's and t_j's. Thus, in order to get a 0 in the 0th row of each basic column, we need to add -2 $\cdot$ (each row corresponding to c_k with $k \in \mathcal{A}$) to the 0th row. Each such row corresponding to c_k has a 2 in the 0th column, a 1 in the column corresponding to the overpass of the crossing, a -1 in the column corresponding to the underpass of the crossing, a -1 in the column corresponding to s_k, and 0's everywhere else. Furthermore, since these crossings constitute a pairing, every column corresponding to an o_i has exactly one of the aforementioned 1's below it, and every column corresponding to a u_i has exactly one of the aforementioned -1's below it. Thus, when -2 times each of the chosen n rows is added to the zeroth row, the entries in the 0th row of all the columns corresponding to the o_i's and u_i's will become 0's. In the columns corresponding to the s_k with $k \in \mathcal{A}$, the entry in the 0th row will increase to 2; it will remain at 0 in the columns corresponding to s_k with $k \notin \mathcal{A}$. Finally, each of the entries in the 0th row of the columns corresponding to the t_j will remain at 0. Therefore all the entries in the 0th row of the tableau (excluding the 0th column) are nonnegative, and our initial bfs is optimal. Since each of rows added to the 0th row has a 2 in the 0th column, $T_{00} = n \cdot (-2 \cdot 2) = -4n$, and the optimal value is $4n$, as expected. So we have $Rop(K) \geq 4n$.

■

We now have the ability to find a lower bound for the ropelength of any conformation that admits a reduced diagram, given we have the (preferrably machine) power to carry out the simplex algorithm. We now move in the direction of finding this lower bound without directly appealing to the simplex algorithm.

6 The Geometry of the Simplex Algorithm, and an Application

Again, we begin by giving an overview of the material presented in [3]. For any d, an **affine subspace** of $\mathbb{R}^d$ is a subspace S translated by a vector u: $A = \{u + x \mid x \in S\}$. The **dimension** of A is that of S. Equivalently, an affine subspace A of $\mathbb{R}^d$ is the set of all points satisfying a set of inhomogeneous equations $A = \{x \in \mathbb{R}^d \mid a_{j1}x_1 + \ldots + a_{jd}x_d = b_j;\ j = 1, \ldots, m\}$. The **dimension of any subset** of $\mathbb{R}^d$ is the smallest dimension of any affine subspace which contains it. An affine subspace of $\mathbb{R}^d$ that has dimension $d - 1$ is called a **hyperplane**. Alternately, a hyperplane $H = \{x \in \mathbb{R}^d \mid a \cdot x = b\}$, where $a \in \mathbb{R}^d$, $a \neq 0$ and $b \in \mathbb{R}$. A hyperplane defines two **halfspaces**, which are the sets of points satisfying $a \cdot x \leq b$ and $a \cdot x \geq b$, respectively. The bounded and nonempty intersection of a finite number of halfspaces is called a **convex polytope**, or simply a **polytope**. As the name suggests, a convex polytope is convex, meaning that any two points in the polytope can be joined with a line lying entirely in the polytope. A **face** is the nonempty intersection of a hyperplane with the boundary of a polytope, subject to the condition that the hyperplane does not intersect the interior of the polytope. For a polytope of dimension d, there are three kinds of faces: a facet (of dimension $d-1$), an edge (of dimension 1), and a vertex (of dimension 0).

For any set of feasible points F of an LP with original principal matrix A, there exists a corresponding convex polytope P in $\mathbb{R}^d$, where $d =$ (number of columns in A) - (number of rows in A). In our case, $d = (c+4n)-(c+2n) = 2n$. Each point $(x_1, \ldots, x_\delta)$ in F is mapped to the point $(x_1, \ldots, x_d)$ in P (by simply projecting onto the first d coordinates). In our case, the first d coordinates are equal to the heights of the overpasses and underpasses in the reduced taut diagram. This map can be reversed, as the dimension of the polytope ensures that, given the values of d variables, we can solve the constraint equations to determine the necessary values of the rest. In this mapping, bfs's in F correspond to the vertices of P, and the movement from bfs to bfs during the simplex algorithm corresponds to the movement from vertex to vertex along the edges of F. We first prove an important lemma.

Lemma 6.1: Let $v \in \mathbb{R}^{2n}$ be in a convex polytope P; assume $dim(P) > 1$. Suppose there exists a non-zero vector $y \in \mathbb{R}^{2n}$ such that, for positive scalars $\alpha, \beta, v - \alpha y, v + \beta y \in P$. Then v is not a vertex in P.

Proof.

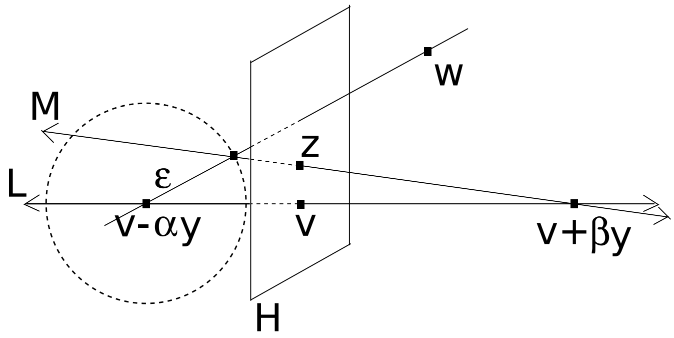

Figure 10: Illustration of the proof of Lemma 6.1

Refer to Figure 10. Let H be any hyperplane in $\mathbb{R}^{2n}$ that contains v; we will prove that H must contain some other point in P. Let H be defined by the equation $a \cdot x = b$ for some nonzero vector $a \in \mathbb{R}^{2n}$ and some $b \in \mathbb{R}$. If $v - \alpha y$ or $v + \beta y \in H$, then we are done. Otherwise, consider the function $f : [0,1] \times \mathbb{R}^{2n} \to \mathbb{R}$ by $f(\lambda, u) = \lambda(a \cdot (v + \beta y)) + (1 - \lambda)(a \cdot (v - \alpha y + u)) - b$. Then f is obviously continuous, and linear in λ. Since $f(0,0)$ is non-zero and $f(\frac{\alpha}{\alpha+\beta}, 0) = a \cdot v - b = 0$, we have that $\frac{df}{d\lambda} \neq 0$. We prove the case where $\frac{df}{d\lambda} > 0$, the other case is similar. Then we have $f(0,0) = a \cdot (v - \alpha y) - b < 0$ and $f(1,0) = a \cdot (v + \beta y) - b > 0$. Let the line $L = \{v + cy \mid c \in \mathbb{R}\}$. Since $dim(P) > 1$, $\exists w \in P - L$. Let $\epsilon > 0$ be small enough so that $f(0, \epsilon(w - (v - \alpha y))) < 0$. Then we have that $f(1, \epsilon(w - (v - \alpha y))) = f(1,0) > 0$, and since f is continuous, $\exists \lambda_0$ such that $f(\lambda_0, \epsilon(w - (v - \alpha y))) = 0$. Let the line $M = \{v + \beta y + d(\beta y + \alpha y - \epsilon(w - (v - \alpha y))) \mid d \in \mathbb{R}\}$; it follows (through algebra) that $L \cap M = \{v + \beta y\}$. We have $f(\lambda_0, \epsilon(w - (v - \alpha y))) =$

$$= \lambda_0(a \cdot (v + \beta y)) + (1 - \lambda_0)(a \cdot (v - \alpha y + \epsilon(w - (v - \alpha y)))) - b$$

$$= a \cdot (\lambda_0 v + \lambda_0 \beta y + v - \alpha y + \epsilon(w - (v - \alpha y)) - \lambda_0 v + \lambda_0 \alpha y - \lambda_0 \epsilon(w - (v - \alpha y))) - b$$

$$= a \cdot (v + \beta y + (\lambda_0 - 1)(\beta y - \alpha y - \epsilon(w - (v - \alpha y)))) - b = 0.$$

Let $z = v + \beta y + (\lambda_0 - 1)(\beta y + \alpha y - \epsilon(w - (v - \alpha y)))$. Then $z \in H$. But clearly $z \in M \subseteq P$ (since P is convex and $v + \beta y, v - \alpha y + \epsilon(w - (v - \alpha y)) \in M \cap P$), and assuming $z \in L$ produces (through algebra) $\lambda_0 = 1$, a contradiction. Therefore $z \in H \cap P$ with $z \neq v$, and v is not a vertex of P.

■

Theorem 6.1: Suppose that, for an LP corresponding to the minimizing of the length of a reduced taut diagram, we have a feasible solution in which there exists a vertex v_i in the reduced taut diagram such that $h(v_i) \neq 2q \; \forall q \in \mathbb{Z}^+ = \{0, 1, 2, \ldots\}$. Then this feasible solution is not a bfs.

Proof.

We shall show that the corresponding point $v = (h(v_1), \dots, h(v_{2n})) \in P$ is not a vertex of P. We split into two cases.

Case 1: There exist v_i, v_j such that $|h(v_i) - h(v_j)| \neq 2q \; \forall q \in \mathbb{Z}^+$.

WOLOG, assume $h(v_i) \neq 2q$ for any $q \in \mathbb{Z}^+$. Let $S = \{k \in \{1, \dots, 2n\} \mid |h(v_i) - h(v_k)| = 2q_k \; for \; some \; q_k \in \mathbb{Z}^+\}$. For any $l \in S$, consider the effect that increasing the height of v_l (along with the other vertices corresponding to elements of S) would have on the feasibility of the current arrangement. The only way in which v_l could be involved in a violation of the constraint equations of the LP would be if it was moved to within 2 of a vertex connected to it, or if it was an underpass and was moved above a consecutive overpass. But since we are moving all vertices a distance of 0 or 2 away from v_l along with v_l, $\exists \beta_l > 0$ such that increasing the height of all v_k with $k \in S$ by β_l will not result in a violation of any constraint equations involving v_l. Then $\exists \beta = min_{k \in S}(\beta_k) > 0$ such that increasing the height of all v_k with $k \in S$ by β will still result in a feasible solution. Similarly, $\exists \alpha > 0$ such that decreasing the height of all v_k with $k \in S$ by α will still result in a feasible solution (we will also have to consider the constraint that we not move vertices below zero, but this again results in our being able to decrease the $h(v_k)$ by some positive distance, since $h(v_i) \neq 2q$ for any $q \in \mathbb{Z}^+$). Let $y \in \mathbb{R}^{2n}$ be defined by:

$$y_k = 1 \; for \; k \in S$$

$$y_k = 0 \; otherwise$$

Then $v, v - \alpha y, v + \beta y \in P$, and by the previous lemma v is not a vertex of P.

Case 2: There exists $r \in \mathbb{R}$ such that $\forall i, h(v_i) = 2q_i + r$ for some $q_i \in \mathbb{Z}^+$.

Let $\alpha = min_i(h(v_i))$, $y = (1, 1, \dots, 1)$. Then clearly $v, v - \alpha y, v + \alpha y \in P$, and again by the previous lemma v is not a vertex of P.

Therefore, by [3], the corresponding feasible solution is not a bfs.

■

Corollary 6.1: There exists an arrangement of the reduced taut diagram with minimal length in which $\forall i \; h(v_i) = 2q_i$ for some $q_i \in \mathbb{Z}^+$.

7 Future Research

While we have successfully found an algorithm which will give a lower bound on the ropelength of any reduced conformation, there is much to be done in determining what this lower bound actually is. Ultimately, it would be nice to relate this lower bound back to properties of the knot and CIG, so that one does not have to resort to using the simplex algorithm every time one wants to find a lower bound. In addition, finding a simple formula for such lower bounds may allow us to make general statements about a lower bound for the ropelength of a knot. However, in order to do this, we also need to remove the constraint that the conformation be reduced, which is another possible direction for research.

The fact that there exists an arrangement of the taut diagram with minimum length in which each vertex is at a height of 2 greatly reduces the number of arrangements one has to consider when finding one with minimum length. Now that we have narrowed the minimalization of the length of the taut diagram to the "discrete" case, we may be in a position to develop an entirely new algorithm which is better tailored to this specific problem.

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