On the mean and variance of the writhe of random polygons

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Abstract. In this paper, we study two issues concerning the writhe of a random polygon. Suppose that we are dealing with a set of random polygons with the same length and knot type (which could be the model of some circular DNA with the same topological property) and would like to know whether the corresponding knot type is chiral or not, then a simple way of detecting this is to compute the mean writhe of these polygons. A nonzero writhe would imply the chirality of the knot type of these polygons. However, how feasible is this method? If the mean writhe would decrease to zero as the length of the polygons increases, then this method would be limited in the case of long polygons. We conjecture that this is not the case and show the support of this conjecture through numerical studies. The second part of our study focuses on the variance of the writhe, a problem that has not received much attention in the past. In this case, we focused on the equilateral random polygons. We give numerical as well as analytical evidence that shows the variance of the writhe of equilateral random polygons (of length n) behaves as a linear function of the length of the equilateral random polygon.

AMS classification scheme numbers: Primary 57M25, secondary 92B99.

1. Introduction

Polymer scientists had long suspected that the topological entanglement of long polymer chains would play an important role in the physical sciences. They even conjectured that in long polymer chains knots would occur with almost sure certainty (the Frisch-Wasserman-Delbrück Conjecture [11, 20]). This conjecture was proved under several polymer models [13, 17, 34, 47] and verified experimentally on randomly circularized DNA chains [4, 30, 37, 40].

How a circular DNA molecule is knotted and to what extent it is topologically entangled is an important question in the study of the DNA because it helps characterize biochemical processes. Examples include the binding and action of site-specific recombinases (reviewed in [46]), the action of topoisomerases (e.g. [38, 49]), the packing of DNA in certain bacteriophages [3, 5, 31].

In theory, the knot type (and complexity) of a circular DNA can be rigorously determined [1, 8, 10, 26]. But in the case of DNA such information is sometimes not easy to retrieve. In particular if the circular DNA molecule is long. One thus turns to measures that can be obtained without such rigor (hence are easier to obtain experimentally) and yet still can be used to detect the average overall knot complexity of the circular DNA family being studied. For example, the mean average crossing number (ACN) is a measure that can be detected experimentally [29, 42, 48]and from which a number of theoretical properties are known [2, 14, 15, 18, 41]. In this paper, we are interested on a different measure , also motivated by biological problems, called the writhe.

The writhe is a measure of the chirality of the DNA molecule and is essential to the maintenance of the chromosome [36]. On unknotted plasmids the writhe is a direct measure of the degree of supercoiling of the molecule. The situation is less understood when the DNA is knotted nevertheless it is believed to be closely linked to the biological activity of certain enzymes such as condensins [24, 45] and topoisomerases [44] or to DNA packing [5]. The writhe of random polymer models has also been studied under different settings [16, 21, 22, 27, 28, 32, 33] and topological invariants to predict the writhe have ben proposed [9] . Mathematically speaking the writhe is similar to the ACN in terms of the definition and easiness of computation. Here one assigns each crossing in a knot projection diagram a ± 1 according to a right hand rule, and considers the summation of these signs averaged over all possible projections of the knot, the measure so obtained is defined as the writhe of the knot. So in some sense one could think of the writhe of a knot as the signed generalization of the ACN. Like the ACN, the writhe of a knot is not a knot invariant, but is a measure that reflects geometrical and topological aspects of the knot. However, in general, the writhe contains more topological information than the ACN. For example, the mean ACN of all polygons with the same knot type and length (which is likely to be a large positive number if the polygons are long) cannot tell us whether the polygons are knotted (much less how complicated the knots are), yet a nonzero mean writhe over an ensemble of polygons of the same length and knot type would indicate that the knot type of these polygons is nontrivial and is in fact chiral.

In this paper, we will focus on two issues regarding the writhe of random polygons that have not been addressed previously. One question concerns the behavior of the mean writhe as the function of the length of the polygons, when the random polygons are sampled from the ensemble of polygons of the same length and knot type. The motivation for studying this problem is the following. Assume that we are studying a sample of knotted DNA in which all molecules have the same unknown knot type. Then if one could estimate the population's writhe then it would be possible to estimate the knot type and its chirality provided that a correspondence between the writhe and the knot type has been established (knowing in advance that different knot populations may have the same writhe). Here we use computer simulations of random polygons to establish such correspondence between knots up to eight crossings and the mean write of such population. We conjecture that if the writhe of an "ideal knot" (with knot type $\mathcal{K}$) is a nonzero constant $w_{\mathcal{K}}$, then the mean writhe of the random polygons with knot type $\mathcal{K}$ and length n would approach to a constant that is close to $w_{\mathcal{K}}$ as n goes to infinity. The concept of ideal knot can be found in the various articles collected in [43]. However our definition of the ideal knot in this paper will be slightly different. To check the plausibility of this conjecture, one would need to be able to sample large random polygons of a given knot type effectively. Unfortunately this is not feasible for most random polygon models commonly used and our study of this problem is thus limited to the self-avoiding polygons on the cubic lattice, where such a random polygon generating algorithm already exists.

The second question that we address in this paper concerns the variance of the writhe (when the writhe of a random polygon is treated as a random variable). This problem is motivated by computer simulations of DNA packing in bacteriophages that suggest that the DNA molecule inside the baceriophage capsid is chirally organized [5]. In this and other studies [6, 7, 35] simulations of random polygons biased by the writhe were performed in order to establish the interplay between the values of the writhe and the knotting probability and distribution. However these simulations were performed without an estimation of the variance of the writhe. It is known that the mean writhe of all random polygons (regardless of which model is used, so long as the model is not biased toward any particular configuration) of the same length is zero (by way of a symmetry argument). In the case of lattice polygons, it has been shown in [22] that the mean absolute writhe is bounded below by $O(\sqrt{n})$ where n is the length of the polygons and similar observations have been made for the wormlike chain [25]. In the case of uniform random polygons bounded in a fixed volume, it has been shown that the mean squared writhe behaves as $O(n^2)$, where n is the number of edges of the random polygons [33]. However, there has not been any specific study on the variance of writhe in the case of equilateral random polygons. This is an important question since the equilateral random polygon is a useful model in many applications. For example, it is used to model a relaxed circular DNA and to model a ring polymer in dilute solution. In order to use the mean writhe of the equilateral polygons (with fixed knot type and length) to detect the chirality of these polygons, one needs to use sample data to make inference on these mean writhe values. Understanding the behavior of the variance of the writhe in general would certainly be helpful in making the inference more powerful.

The paper is organized as follows. In the next section (section 2), we give a brief introduction to key concepts and terms in knot theory. In Section 3, we present the results of our numerical study on the mean writhe of lattice polygons with fixed knot type. In Section 4, we discuss the equilateral random polygon. We formulate the variance of the writhe by treating the writhe as a random variable. We show that the variance of the writhe is equivalent to the mean squared writhe. Some analytical discussions will follow, from which we conjecture that the variance of the writhe (of all equilateral random polygons of length n) behaves as $O(n)$, where n is the length of the polygon. The paper is concluded in Section 5 with some discussions on the findings and some questions for future study.

2. Basic concepts and terminology of Knot Theory

Our discussion of basic knot theory in this section is quite informal (emphasizing intuition over rigor). If so wish, a reader may want to check out details and precise definitions in a standard text in knot theory, see for example [1, 8, 10].

Throughout this paper, a knot means a simple closed curve in the 3-dimensional space. Two knots K_1 and K_2 are topologically equivalent if one can be continuously deformed into the other without self intersection. The collection of all knots that are topologically equivalent is called a *knot type*.

For a fixed knot K, a knot diagram of K is the projection of K (as a space curve) onto a plane. Such a projection is regular if no more than two segments of K cross at any point in the projection. The number of self intersection points (crossing points) in a knot diagram is called the *crossing number* of that diagram. Apparently, such a number not only depends on the knot type of K, it also depends on the geometrical shape of K and the projection direction chosen. The minimal number of crossings in all regular projections of all simple closed curves having the same knot type as K is called the *crossing number* of the knot K and is denoted by $Cr(K)$. By this definition, if K_1 and K_2 are of the same knot type, then we have $Cr(K_1) = Cr(K_2)$. Furthermore, it may be the case that for a fixed embedding of K none of its regular projections has crossing number $Cr(K)$.

If we assign a fixed embedding K of knot type $\mathcal{K}$ an orientation, then this orientation allows us to assign a ± 1 at each crossing in a diagram D of K using the right hand rule as shown in Figure 1.

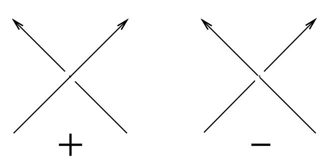

Figure 1. A positive and a negative crossing.

The *writhe* of the diagram D is the sum of these signed crossing numbers and is denoted by w_D. The average of w_D over all possible projections of K is defined as the *writhe* of K and will be written as $w(K)$. In general, the writhe of a knot K largely depends on the geometry of K and is not a knot invariant. However, if K is an alternating knot, then w_D is invariant among all reduced alternating diagrams having the same knot type as that of K (though that is a concept not needed in this paper). Note that the writhe of a knot diagram is independent of the orientation of the knot chosen. However, a knot diagram and its mirror image have opposite writhe, as one can tell by realizing that the mirror image of a crossing and the crossing itself are related as the two crossings shown in Figure 1.

Given a knot K as a space curve, one can estimates its writhe by taking various projections of K and average the writhes of these projections. Alternatively, one can use the following Gaussian integral formula to compute the writhe directly:

$$w(K) = \frac{1}{2\pi}\int_K\int_K \frac{(\dot\gamma(t), \dot\gamma(s), \gamma(t)-\gamma(s))}{|\gamma_1(t)-\gamma_2(s)|^3}\mathrm{d}t\mathrm{d}s, \quad (1)$$

where γ is the arclength parameterization of K and $(\dot\gamma(t), \dot\gamma(s), \gamma(t)-\gamma(s))$ is the triple scalar product of $\dot\gamma(t)$, $\dot\gamma(s)$, and $\gamma(t)-\gamma(s)$.

If a knot K is topologically equivalent to its mirror image, then K is said to be *achiral*. Otherwise we say that K is *chiral*. If K is chiral, then for any K' that is equivalent to K, K' is also chiral. The mean writhe is a good measure in detecting the chirality of the knot type of random polygons as stated in the following lemma.

Lemma 1 *Let $P(\mathcal{K}, n)$ be the set of all polygons of length n and of knot type $\mathcal{K}$, here the polygons can be the self-avoiding polygons on the simple cubic lattice, the equilateral random polygons, the Gaussian random polygons, the uniform random polygons or any other random polygons that do not favor any polygon over its mirror image. If the mean writhe of the polygons from $P(\mathcal{K}, n)$ is nonzero, then $\mathcal{K}$ is a nontrivial knot and is in fact chiral.*

Proof. This is rather obvious: if $\mathcal{K}$ is achiral (which would include the trivial knot), then for each realization of a nonzero writhe value by a polygon, there is a writhe value of the opposite sign by the mirror image of the polygon (since the mirror image of the polygon is also in $P(\mathcal{K}, n)$ given that $\mathcal{K}$ is achiral). Thus the mean writhe is zero. □

A key issue in knot theory (as well as in this paper) is how to identify different knots. In this paper we will use the various knot invariant polynomials for this purpose . A knot invariant polynomial can be computed from any knot projection and is invariant so long as the projections represent the same knot type. The Jones Polynomial, the Alexander polynomial and the HOMFLY polynomial are a few of the well known and commonly used knot polynomials. We will not go into the details about how these polynomials are defined and computed. The Interested reader may refer to a standard knot text such as [1, 8, 10]. Each of these polynomials has its own strength and weakness. For example, the Alexander polynomial is reasonably good at distinguishing knots and links while the HOMFLY polynomial unambiguously distinguishes most knots with 9 or fewer crossings.

3. The mean writhe of lattice polygons with fixed knot types

In this section, we explore the mean writhe of random polygons with a fixed knot type. In order to carry out a numerical study with significant results, we would need to generate large sample of random polygons with fixed knot types and of various lengths. Unfortunately, there are no known fast algorithms that would allow us to generate such data for the off lattice random polygons. Luckily, for the lattice polygons, there is a well known and fast algorithm called the BFACF algorithm [23].

The BFACF algorithm starts with a lattice polygon of any given knot type and then samples various lattice polygons without changing the knot type.

In this study we computed the mean writhe for all knot types up to 8 crossings and for polygons of lengths 75, 100, 150 and 200. For chiral knots, our numerical studies include the two knots that are mirror images of each other. For achiral knots, even though it is expected that the mean writhe is zero, we computed their mean writhe as well, so as to show how good our numerical estimates are in general. For each given knot type, we collected 5000 lattice polygons each with length 75, 100, 150 and 200. The results are summarized in Table 1, where the error bar is set at the 99% confidence level.

Table 1: The mean writhe of self-avoiding polygons on the cubic lattice of fixed knot types at lengths 75, 100, 150 and 200. A * indicates the mirror image of the corresponding knot type. A knot type without a corresponding mirror image counterpart implies that it is achiral.

K	75	100	150	200
3_1	3.45 ± 0.04	3.52 ± 0.05	3.45 ± 0.04	3.48 ± 0.07
3_1^*	-3.45 ± 0.04	-3.45 ± 0.05	-3.45 ± 0.04	-3.43 ± 0.07
4_1	0.006 ± 0.03	0.00 ± 0.04	0.01 ± 0.03	0.03 ± 0.07
5_1	6.32 ± 0.03	6.33 ± 0.04	6.32 ± 0.03	6.28 ± 0.07
5_1^*	-6.32 ± 0.03	-6.30 ± 0.04	-6.32 ± 0.03	-6.30 ± 0.07
5_2	4.57 ± 0.03	4.58 ± 0.04	4.57 ± 0.03	4.62 ± 0.07
5_2^*	-4.56 ± 0.03	-4.58 ± 0.04	-4.56 ± 0.03	-4.59 ± 0.07
6_1	1.17 ± 0.03	1.19 ± 0.04	1.17 ± 0.03	1.20 ± 0.07
6_1^*	-1.17 ± 0.03	-1.20 ± 0.04	-1.17 ± 0.03	-1.23 ± 0.07
6_2	2.89 ± 0.03	2.87 ± 0.04	2.89 ± 0.03	2.85 ± 0.07
6_2^*	-2.89 ± 0.03	-2.89 ± 0.04	-2.89 ± 0.03	-2.84 ± 0.07
6_3	-0.01 ± 0.03	-0.01 ± 0.04	-0.01 ± 0.03	0.03 ± 0.07
$6c_1$	6.96 ± 0.03	6.96 ± 0.04	6.96 ± 0.03	6.93 ± 0.07
$6c_1^*$	-6.96 ± 0.03	-6.95 ± 0.04	-6.96 ± 0.03	-6.89 ± 0.07
$6c_2$	-0.01 ± 0.03	0.02 ± 0.04	-0.01 ± 0.03	0.03 ± 0.07
7_1	9.16 ± 0.03	9.13 ± 0.04	9.16 ± 0.03	9.09 ± 0.06
7_1^*	-9.15 ± 0.03	-9.16 ± 0.04	-9.15 ± 0.03	-9.05 ± 0.06
7_2	5.77 ± 0.03	5.78 ± 0.04	5.77 ± 0.03	5.80 ± 0.06
7_2^*	-5.75 ± 0.03	-5.79 ± 0.04	-5.75 ± 0.03	-5.82 ± 0.06
7_3	7.40 ± 0.03	7.40 ± 0.04	7.40 ± 0.03	7.37 ± 0.06
7_3^*	-7.40 ± 0.03	-7.41 ± 0.04	-7.40 ± 0.03	-7.43 ± 0.06
7_4	5.67 ± 0.03	5.66 ± 0.04	5.67 ± 0.03	5.71 ± 0.06
7_4^*	-5.69 ± 0.03	-5.69 ± 0.04	-5.69 ± 0.03	-5.74 ± 0.06
7_5	7.47 ± 0.03	7.49 ± 0.04	7.47 ± 0.03	7.49 ± 0.06
7_5^*	-7.49 ± 0.03	-7.49 ± 0.04	-7.49 ± 0.03	-7.47 ± 0.06
7_6	3.40 ± 0.03	3.38 ± 0.04	3.40 ± 0.03	3.39 ± 0.06
7_6^*	-3.39 ± 0.03	-3.41 ± 0.04	-3.39 ± 0.03	-3.37 ± 0.06
7_7	0.54 ± 0.03	0.55 ± 0.04	0.54 ± 0.03	0.53 ± 0.06
7_7^*	-0.53 ± 0.03	-0.53 ± 0.04	-0.53 ± 0.03	-0.52 ± 0.06
$7c_1$	3.49 ± 0.03	3.48 ± 0.04	3.49 ± 0.03	3.46 ± 0.06

K	75	100	150	200
$7c_1^*$	-3.47 ± 0.03	-3.47 ± 0.04	-3.47 ± 0.03	-3.49 ± 0.06
8_1	2.34 ± 0.03	2.38 ± 0.03	2.34 ± 0.03	2.44 ± 0.06
8_1^*	-2.36 ± 0.03	-2.37 ± 0.04	-2.36 ± 0.03	-2.42 ± 0.06
8_2	5.70 ± 0.02	5.69 ± 0.04	5.70 ± 0.02	5.65 ± 0.06
8_2^*	-5.69 ± 0.03	-5.70 ± 0.03	-5.69 ± 0.03	-5.66 ± 0.06
8_3	0.00 ± 0.03	0.02 ± 0.03	0.00 ± 0.03	-0.01 ± 0.06
8_4	1.73 ± 0.02	1.71 ± 0.04	1.73 ± 0.02	1.67 ± 0.06
8_4^*	-1.73 ± 0.03	-1.72 ± 0.04	-1.73 ± 0.03	-1.69 ± 0.07
8_5	5.73 ± 0.03	5.75 ± 0.03	5.73 ± 0.03	5.76 ± 0.06
8_5^*	-5.74 ± 0.02	-5.74 ± 0.04	-5.74 ± 0.02	-5.76 ± 0.06
8_6	4.07 ± 0.03	4.07 ± 0.04	4.07 ± 0.03	4.12 ± 0.06
8_6^*	-4.07 ± 0.03	-4.11 ± 0.03	-4.07 ± 0.03	-4.09 ± 0.06
8_7	2.83 ± 0.03	2.83 ± 0.03	2.83 ± 0.03	2.78 ± 0.06
8_7^*	-2.83 ± 0.03	-2.83 ± 0.03	-2.83 ± 0.03	-2.78 ± 0.06
8_8	1.20 ± 0.03	1.21 ± 0.03	1.20 ± 0.03	1.18 ± 0.06
8_8^*	-1.20 ± 0.02	-1.20 ± 0.03	-1.20 ± 0.02	-1.25 ± 0.06
8_9	0.00 ± 0.02	0.00 ± 0.04	0.00 ± 0.02	0.00 ± 0.06
8_{10}	2.87 ± 0.03	2.87 ± 0.03	2.87 ± 0.03	2.88 ± 0.06
8_{10}^*	-2.88 ± 0.02	-2.86 ± 0.03	-2.88 ± 0.02	-2.82 ± 0.06
8_{11}	3.98 ± 0.03	3.98 ± 0.03	3.98 ± 0.03	4.00 ± 0.06
8_{11}^*	-3.97 ± 0.02	-3.95 ± 0.03	-3.97 ± 0.02	-3.99 ± 0.06
8_{12}	-0.01 ± 0.03	-0.02 ± 0.04	-0.01 ± 0.03	0.00 ± 0.06
8_{13}	1.12 ± 0.02	1.11 ± 0.03	1.12 ± 0.02	1.07 ± 0.06
8_{13}^*	-1.11 ± 0.02	-1.12 ± 0.04	-1.11 ± 0.02	-1.11 ± 0.06
8_{14}	4.06 ± 0.03	4.09 ± 0.03	4.06 ± 0.03	4.09 ± 0.06
8_{14}^*	-4.06 ± 0.03	-4.06 ± 0.03	-4.06 ± 0.03	-4.03 ± 0.06
8_{15}	8.00 ± 0.02	8.02 ± 0.03	8.00 ± 0.02	8.03 ± 0.06
8_{15}^*	-7.99 ± 0.02	-8.01 ± 0.03	-7.99 ± 0.02	-8.04 ± 0.06
8_{16}	2.83 ± 0.02	2.83 ± 0.03	2.83 ± 0.02	2.81 ± 0.06
8_{16}^*	-2.82 ± 0.02	-2.82 ± 0.03	-2.82 ± 0.02	-2.83 ± 0.06
8_{17}	-0.01 ± 0.03	0.02 ± 0.03	-0.01 ± 0.03	-0.07 ± 0.06
8_{18}	0.01 ± 0.03	-0.01 ± 0.03	0.01 ± 0.03	0.00 ± 0.06
8_{19}	8.81 ± 0.03	8.80 ± 0.04	8.81 ± 0.03	8.81 ± 0.07
8_{19}^*	-8.80 ± 0.03	-8.80 ± 0.04	-8.80 ± 0.03	-8.87 ± 0.07
8_{20}	1.92 ± 0.03	1.91 ± 0.04	1.92 ± 0.03	1.96 ± 0.07
8_{20}^*	-1.91 ± 0.03	-1.93 ± 0.04	-1.91 ± 0.03	-1.91 ± 0.06
8_{21}	4.68 ± 0.03	4.69 ± 0.04	4.68 ± 0.03	4.76 ± 0.06
8_{21}^*	-4.68 ± 0.03	-4.70 ± 0.04	-4.68 ± 0.03	-4.73 ± 0.07
$8c_1$	9.81 ± 0.03	9.78 ± 0.04	9.81 ± 0.03	9.80 ± 0.06
$8c_1^*$	-9.80 ± 0.03	-9.80 ± 0.03	-9.80 ± 0.03	-9.79 ± 0.06
$8c_2$	2.83 ± 0.03	2.86 ± 0.04	2.83 ± 0.03	2.80 ± 0.06
$8c_2^*$	-2.86 ± 0.03	-2.86 ± 0.03	-2.86 ± 0.03	-2.81 ± 0.07
$8c_3$	8.04 ± 0.02	8.07 ± 0.04	8.04 ± 0.02	8.06 ± 0.06
$8c_3^*$	-8.05 ± 0.03	-8.06 ± 0.04	-8.05 ± 0.03	-8.04 ± 0.06
$8c_4$	1.09 ± 0.03	1.10 ± 0.03	1.09 ± 0.03	1.13 ± 0.06
$8c_4^*$	-1.09 ± 0.03	-1.06 ± 0.03	-1.09 ± 0.03	-1.08 ± 0.06
$8c_5$	-0.01 ± 0.03	-0.02 ± 0.04	-0.01 ± 0.03	0.03 ± 0.07

It appears from our numerical study that the mean writhe values are rather stable in the sense that as the lengths of the polygons increase, the mean writhe values only fluctuate within a narrow interval that does not include zero in the case of the chiral knots in our study. These results suggest that the mean writhe of random polygons fluctuate around the mean writhe of some "ideal" shape. Since the random polygons studied in this section are self-avoiding polygons on the cubic lattice, it is natural for us to define an "ideal" shape for given knot type as the polygon with the shortest length for that given knot type. For example, an ideal shape for the trefoil knot has length 24 and there are 3328 such configurations (half of which are the right hand trefoils and the other half are the left hand ones) [12, 39]. We include the mean writhe of these "ideal" lattice polygons in Table 2 for comparison with Table 1. Comparison of both tables suggest that indeed the mean writhe fluctuates around the mean writhe of the knot with minimal number of steps.

Table 2: The mean writhes of ideal polygons on the cubic lattice of knot types up to 8 crossings. The data for a mirror image is not shown since it can be obtained by the symmetry argument.

K	mean writhe	# of polygons	chirality
0_1	$0.000000 \pm nan$	3	achiral
3_1	3.441707 ± 0.018019	1664	chiral
4_1	0.111842 ± 0.016440	1824	achiral
5_1	6.228417 ± 0.007563	3336	chiral
5_2	4.528091 ± 0.014957	57456	chiral
6_1	1.095703 ± 0.011326	3072	chiral
6_2	2.788743 ± 0.010422	16416	chiral
6_3	0.155405 ± 0.013357	1776	achiral
7_1	9.215548 ± 0.031597	16980	chiral
7_2	5.751980 ± 0.009182	168180	chiral
7_3	7.475000 ± 0.011296	240	chiral
7_4	5.571429 ± 0.012323	84	chiral
7_5	7.271574 ± 0.007981	4728	chiral
7_6	3.440762 ± 0.013264	17016	chiral
7_7	0.511905 ± 0.017055	252	chiral
8_1	2.411021 ± 0.013715	11868	chiral
8_2	5.544764 ± 0.009436	45840	chiral
8_3	$0.000000 \pm nan$	12	achiral
8_4	1.655216 ± 0.006650	23928	chiral
8_5	5.625000 ± 0.010979	576	chiral
8_6	4.007609 ± 0.008857	5520	chiral
8_7	$2.750000 \pm nan$	24	chiral
8_8	1.080769 ± 0.020181	1560	chiral
8_9	-0.007143 ± 0.009418	17640	achiral
8_{10}	3.007143 ± 0.008567	840	chiral
8_{11}	4.125000 ± 0.012758	96	chiral
8_{12}	0.328704 ± 0.009443	1296	achiral
8_{13}	1.183364 ± 0.022171	13056	chiral

K	mean writhe	# of polygons	chirality
8_{14}	3.983333 ± 0.008958	360	chiral
8_{15}	7.884800 ± 0.014484	40104	chiral
8_{16}	2.625000 ± 0.018042	48	chiral
8_{17}	-0.048962 ± 0.009660	26592	achiral
8_{18}	-0.270270 ± 0.007844	1776	achiral
8_{19}	8.759005 ± 0.009449	6996	chiral
8_{20}	2.100000 ± 0.011180	120	chiral
8_{21}	4.535118 ± 0.010979	28020	chiral

Figure 2 is a visualization of the comparison between the mean writhe values (of polygons with different lengths but fixed knot types) and that of the polygons that represent the ideal shapes of the same knot types (though the specific knot types are not shown in the figure).

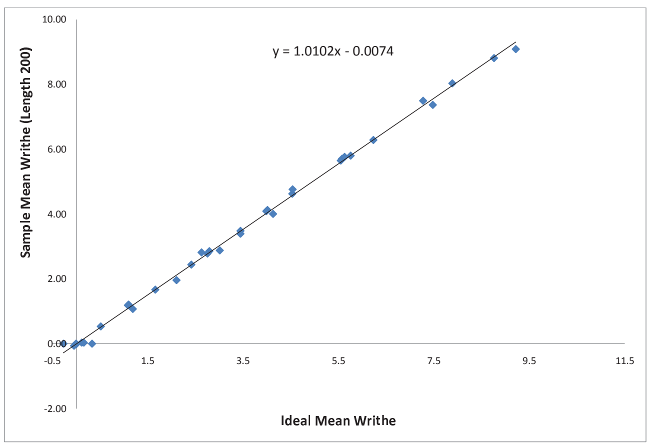

Figure 2. Comparison between overall mean writhe values and that of the ideal shape polygons (minimum length polygons).

Based on this observations one thus could conjecture that the following happens for most chiral knots: if the mean writhe of a chiral knot at some initial "ideal" shape is a non-zero number, then the mean writhe of a random polygon of the same knot type will stay in an interval containing this value, but not containing zero, as the length of the polygon increases. If this were true in general, then the mean writhe would indeed be a very useful tool in detecting chiral knots in random polygons with the same knot type. Furthermore we would like to propose that in that case the sign of the mean writhe would be a topological invariant of chiral knots and therefore provide a very useful method for knot identification. It is important to highlight that the ideal lattice knots are not easy to enumerate in general. Thus the ideal lattice polygons presented in Table 1 are obtained by computer searches and are not theoretically proven (except for the cases of 3_1, 4_1 and 5_1 [39]), nor is the list of all such ideal polygons proven to be exhaustive.

For off lattice knots in $\mathbb{R}^3$, it is difficult to generate large samples for each knot type. This is due to the fact that the commonly used crankshaft algorithm and the generalized hedgehog algorithm sample over the entire space of equilateral polygons. To generate a large sample of equilateral random polygons with a given knot type, one would have to take one of the following two approaches. The first one is simply generate an equilateral random polygon with the desired length and then use the knot polynomials to determine its knot type (and only keep the ones that match the desired knot type). The other approach is to start with an equilateral polygon with the given knot type and then apply local crankshaft moves that do not change the knot type. Both methods have severe drawbacks and are extremely time consuming. For example, when the length of the polygon is long, most polygons generated may have knot types that are more complicated than the knot polynomials can distinguish (and the polynomial computation time for such polygons will be very long too). As for the second method, it may require a very long run time to get an equilateral polygon that is sufficiently de-correlated to the starting polygon.

4. The variance of writhe of the equilateral random polygons

Let EP_n be an equilateral random polygon of n edges. In this section we discuss the variance of the writhe of EP_n. From now on we will denote the writhe of EP_n by $w(EP_n)$. We conjecture that the variance of $w(EP_n)$ behaves as $O(n \ln n)$, namely as the order of the mean average crossing number (mean ACN) of EP_n and provide some numerical evidence of this.

Let ℓ_1, ℓ_2, ..., ℓ_n be the consecutive edges of EP_n. So if we let X_0, X_1, ..., $X_n = X_0$ be the consecutive vertices of EP_n, then $\ell_k = \overline{X_{k-1}X_k}$ $(1 \le k \le n)$. If we let w_{ij} be the mean writhe between ℓ_i and ℓ_j, then the writhe of EP_n is simply the sum of the $e(\ell_i, \ell_j)$'s:

$$w(EP_n) = \sum_{1 \le i < j \le n} w_{ij} = \frac{1}{2} \sum_{1 \le i, j \le n} w_{ij},$$

and

$$E(w(EP_n)) = \sum_{1 \le i < j \le n} E(w_{ij}) = \frac{1}{2} \sum_{1 \le i, j \le n} E(w_{ij}).$$

By a simple symmetry argument, one has $E(w_{ij}) = 0$ (since ℓ_i and ℓ_j have equal chance to take the positions that are mirror image to each other which would produce opposite crossing signs as shown in Figure 1), therefore we must have $E(w(EP_n)) = 0$, where EP_n is taken over the entire ensemble of equilateral random polygons with length n, not some special ones with a fixed knot type. Figure 3 summarizes our numerical estimates of the mean writhe of equilateral random polygons of various lengths, which completely agrees with this theoretical observation.

It follows that the variance of $w(EP_n)$ is simply

$$\begin{aligned} & E((w(EP_n) - E(w(EP_n))^2) \\ &= E(w^2(EP_n)) \\ &= \frac{1}{4} E\Big(\sum_{1 \le i,j,m,k \le n} w_{ij} w_{mk}\Big) \\ &= \frac{1}{4} \sum_{1 \le i,j,m,k \le n} E(w_{ij} w_{mk}). \end{aligned}$$

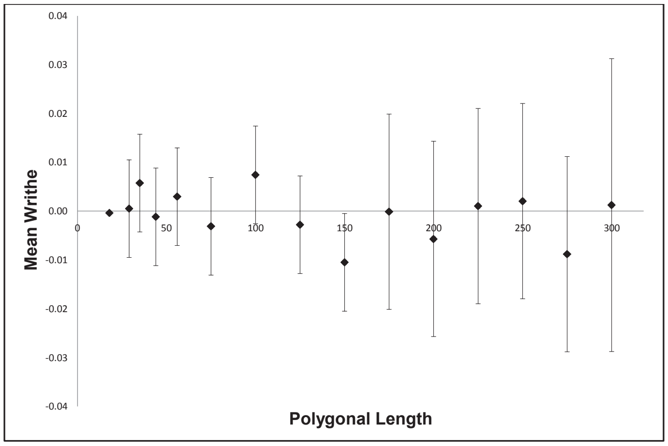

Figure 3. 99% confidence intervals for the mean writhe of equilateral polygons. The polygons are generated using the crankshaft algorithm. The sample size for each length is 500,000 and the error bars are at the 99% confidence level. The writhe is computed using the Gaussian formula given in (1).

In the case that $i = m$ and $j = k$, namely that w_{ij} and w_{mk} stand for the writhe of the same pair of edges ℓ_i and ℓ_j, then we should have $E(w_{ij}w_{mk}) \approx 0$. Although w_{ij} and w_{mk} are not independent and we cannot take the expected values of them separately, they are almost independent when the two pairs are reasonably far away from each other. And even when they are not, most configurations would have close counterparts that produce the opposite signs. Thus we suspect that the behavior of $E(w^2(EP_n))$ is dominated by the terms $E(w_{ij}^2)$ in the above. Since for each fixed pair of edge ℓ_i and ℓ_j, the sign of the crossing between them in any projection (where there is a crossing between them) is the same, it follows that $|w_{ij}| = a(\ell_i, \ell_j)$, where $a(\ell_i, \ell_j)$ is the average crossing number between ℓ_i and ℓ_j. Hence we have $w_{ij}^2 = a^2(\ell_i, \ell_j)$. In the following, we provide an analysis to show that $\sum_{1 \le i,j \le n} E(w_{ij}^2) = \sum_{1 \le i,j \le n} E(a^2(\ell_i, \ell_j))$ behaves as $O(n \ln n)$. For the convenience of our reader, we include some basic results about the density distribution functions of the vertices of an equilateral random polygon. More details can be found in [14].

Let X_k be the k-th vertex of an EP_n and let h_k be its density function, then

$$h_k(X_k) = \left(\sqrt{\frac{3}{2\pi\sigma_{nk}^2}}\right)^3 \exp\left(-\frac{3|X_k|^2}{2\sigma_{nk}^2}\right) + O\left(\frac{1}{k^{5/2}} + \frac{1}{(n-k)^{5/2}}\right), \quad (2)$$

where $\sigma_{nk}^2 = \frac{k(n-k)}{n}$. On the other hand, if X_1, X_{k+1} and X_{k+2} are the first, $(k+1)$-st and $(k+2)$-nd vertices of an EP_n; then their joint probability density function $h_k(X_1, X_{k+1}, X_{k+2})$ can be approximated by

$$\varphi(X_1)\varphi(X_{k+2} - X_{k+1}) \left(\frac{3}{2\pi\sigma_{nk}^2}\right)^{\frac{3}{2}} \exp\left(-\frac{3|X_{k+1}|^2}{2\sigma_{nk}^2}\right), \quad (3)$$

where $\sigma_{nk}^2 = \frac{k(n-k)}{n}$ and the error term is at most of order $O\left(\frac{1}{k^{5/2}} + \frac{1}{(n-k)^{5/2}}\right)$.

Let ℓ_1' and ℓ_2' be two random edges (of unit length) in $\mathbb{R}^3$ with one end points fixed (they are NOT two consecutive edges along a random polygon). Let us consider $a(\ell_1', \ell_2')$. Assume that P and P_1 are the end points of ℓ_1' and Q, Q_1 are the end points of ℓ_2' and let $r = |P - Q| \geq b$, where b is some rather arbitrary positive constant. For example we can just pick $b = 4$. If we assume that P_1 and Q_1 are uniformly distributed on the spheres centered at P and Q respectively, then we have

$$E(a^2(\ell_1', \ell_2')) = \frac{1}{18\pi^2 r^4} + O(\frac{1}{r^5}). \tag{4}$$

Let us outline a proof of this fact. Without loss of generality, let us assume that $P = O$ and Q is on the positive z-axis. Let θ_1 be the angle between $U_1 = \overrightarrow{PP_1}$ and the z-axis and θ_2 be the angle between $U_2 = \overrightarrow{QQ_1}$ and the z-axis. Furthermore, let ϕ be the angle between the projections of U_1 and U_2 on the xy-plane. See Figure 4.

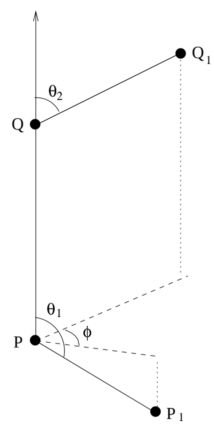

Figure 4. The relationship between two random edges ℓ_1' and ℓ_2'.

By [19], $a(\ell_1, \ell_2)$ is given by

$$\frac{1}{2\pi} \int_{\ell_1} \int_{\ell_2} \frac{|(\dot{\gamma}_1(t), \dot{\gamma}_2(s), \gamma_1(t) - \gamma_2(s))|}{|\gamma_1(t) - \gamma_2(s)|^3} \mathrm{d}t\mathrm{d}s, \tag{5}$$

where γ_1 and γ_2 are the arclength parameterizations of ℓ_1' and ℓ_2' respectively, and $(\dot{\gamma}_1(t), \dot{\gamma}_2(s), \gamma_1(t) - \gamma_2(s))$ is the triple scalar product of $\dot{\gamma}_1(t)$, $\dot{\gamma}_2(s)$, and $\gamma_1(t) - \gamma_2(s)$. Using this, it was derived in [14] that

$$a(\ell_1', \ell_2') = \frac{1}{2\pi r^2} \sin\phi \sin\theta_1 \sin\theta_2 + O(\frac{1}{r^3}).$$

It follows that

$$a^2(\ell_1', \ell_2') = \frac{1}{4\pi^2 r^4} \sin^2\phi \sin^2\theta_1 \sin^2\theta_2 + O(\frac{1}{r^5}).$$

It is known that ϕ is uniformly distributed over $[0, \pi]$ and that ϕ, θ_1, and θ_2 are independent; furthermore, the probability density functions for θ_1 and θ_2 are $\frac{1}{2}\sin\theta_1$ and $\frac{1}{2}\sin\theta_2$. Thus

$$E(a^2(\ell_1', \ell_2')) = \int\int a^2(\ell_1, \ell_2)\varphi(U_1)\varphi(U_2)\mathrm{d}U_1\mathrm{d}U_2$$

$$= \frac{1}{16\pi^3 r^4} \int_0^\pi \int_0^\pi \int_0^\pi \sin^2\phi \sin^3\theta_1 \sin^3\theta_2 \mathrm{d}\phi \mathrm{d}\theta_1 \mathrm{d}\theta_2 + O(\frac{1}{r^5})$$
$$= \frac{1}{18\pi^2 r^4} + O(\frac{1}{r^5}).$$

Let us now return to the estimation of $\sum_{1\le i,j\le n} E(w_{ij}^2) = \sum_{1\le i,j\le n} E(a^2(\ell_i, \ell_j))$. Observe that if ℓ_{i_1}, ℓ_{j_1}, ℓ_{i_2}, and ℓ_{j_2} are edges of an EP_n, then we have $E(a^2(\ell_{i_1}, \ell_{j_1})) = E(a^2(\ell_{i_2}, \ell_{j_2}))$ whenever $|j_1 - i_1| = |j_2 - i_2|$ or $|j_1 - i_1| = n - |j_2 - i_2|$ by symmetry. It follows that

$$\sum_{1\le i,j\le n} E(a^2(\ell_i, \ell_j)) = n \sum_{3\le j\le (n+1)/2} E(a^2(\ell_1, \ell_j)).$$

In the above summation, j starts at 3 since $a(\ell_1, \ell_2)$ is always 0. Let $r_j = |X_{j-1} - X_1|$. Since $a(\ell_1, \ell_j)$ depends only on X_1, X_{j-1} and X_j, by (3) and (4), we have

$$\begin{aligned}
& E(a^2(\ell_1, \ell_j)) \\
= & \int\int\int a^2(\ell_1, \ell_j) h_{j-2}(X_1, X_{j-1}, X_j) \mathrm{d}X_1 \mathrm{d}X_{j-1} \mathrm{d}X_j \\
= & \int\int a^2(\ell_1, \ell_j)\varphi(X_1)\varphi(X_j - X_{j-1}) \mathrm{d}X_1 \mathrm{d}X_j \cdot \\
& \int \left(\left(\sqrt{\frac{3}{2\pi\sigma^2_{n(j-2)}}} \right)^3 \exp\left(-\frac{3|X_{j-1}|^2}{2\sigma^2_{n(j-2)}} \right) + O\left(\frac{1}{j^{5/2}}\right) \right) \mathrm{d}X_{j-1} \\
= & \int\int a^2(\ell_1, \ell_j)\varphi(U_1)\varphi(U_2) \mathrm{d}U_1 \mathrm{d}U_2 \cdot \\
& \int_{r_j<4} \left(\left(\frac{3}{2\pi\sigma^2_{n(j-2)}} \right)^{\frac{3}{2}} \exp\left(-\frac{3|X_{j-1}|^2}{2\sigma^2_{n(j-2)}} \right) + O\left(\frac{1}{j^{5/2}}\right) \right) \mathrm{d}X_{j-1} \\
+ & \int\int a^2(\ell_1, \ell_j)\varphi(U_1)\varphi(U_2) \mathrm{d}U_1 \mathrm{d}U_2 \cdot \\
& \int_{r_j\ge 4} \left(\left(\frac{3}{2\pi\sigma^2_{n(j-2)}} \right)^{\frac{3}{2}} \exp\left(-\frac{3|X_{j-1}|^2}{2\sigma^2_{n(j-2)}} \right) + O\left(\frac{1}{j^{5/2}}\right) \right) \mathrm{d}X_{j-1} \\
= & O(\frac{1}{j^{\frac{3}{2}}}) + \frac{2}{9\pi} \int_4^{j-2} \left(\frac{1}{r_j^2} + O(\frac{1}{r_j^3}) \right) \cdot \\
& \left(\frac{3}{2\pi\sigma^2_{n(j-2)}} \right)^{\frac{3}{2}} \exp\left(-\frac{3r_j^2}{2\sigma^2_{n(j-2)}} \right) \mathrm{d}r_j \\
= & O(\frac{1}{j^{\frac{3}{2}}}),
\end{aligned}$$

where $U_1 = X_1$ and $U_2 = X_j - X_{j-1}$. Since $\sum_{3\le j\le n/2} \frac{1}{j^{\frac{3}{2}}}$ converges, it follows that $\sum_{1\le i,j\le n} E(a^2(\ell_i, \ell_j)) = n \sum_{3\le j\le (n+1)/2} E(a^2(\ell_1, \ell_j)) = O(n \sum_{3\le j\le (n+1)/2} \frac{1}{j^{\frac{3}{2}}}) = O(n)$.

Thus we conjecture that for equilateral random polygons of length n, the variance of the writhe behaves as $O(n)$. Table 3 shows the numerical estimate of the squared writhe for the chosen lengths of the polygons. Figure 5 is the corresponding plot of Table 3. A near perfect linear relation is rather obvious from the plot, which strongly support our conjecture.

Table 3: The plot of the estimated mean squared writhe.

polygon length	mean squared writhe	95% error bar
18	1.788483994	0.008070885
29	3.199573119	0.014280251
35	4.057503482	0.017950673
44	4.988473074	0.021343331
56	76.586347181	0.028147813
75	9.196751367	0.038991441
100	12.45734892	0.052380225
125	15.81068417	0.066056364
150	19.26239305	0.080204212
200	25.94806785	0.10663432
225	29.34655275	0.120589997

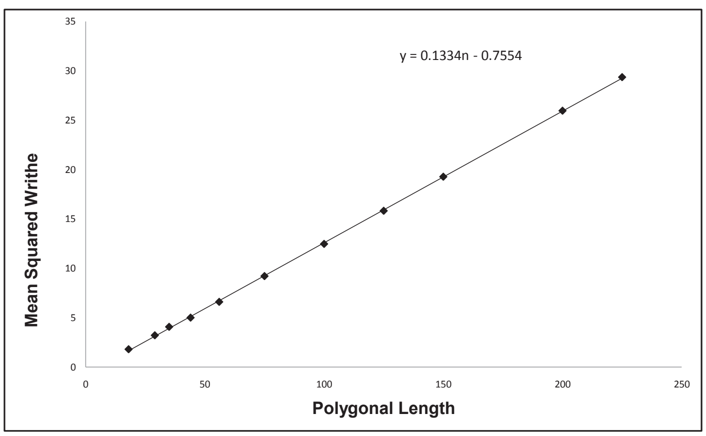

Figure 5. The estimated mean squared writhe values compared to their linear regression line.

5. Discussions and conclusions

DNA knots have been observed in a number of biological systems and in many of these studies it has been proposed a key role for the writhe of the molecule. This study was motivated by two questions. First can one distinguish the chirality of a knot population of the same knot type by its mean writhe? and second, what is the variance of the writhe? Our numerical results on section 3 strongly indicate that the mean writhe is an effective way of detecting the chirality of the polygons provided they have the same knot type. As the length n increases, it is clear that the mean writhe values vary only slightly, hence it is quite plausible that the signs of the mean writhe stays invariant. Indeed, a visual inspection of the confidence intervals for the mean writhe of each knot type generated using the BFACF algorithm shown in Table 1 shows no exception. Of course this does not mean that this will work for any chiral knots, since some chiral knots may have mean writhe values either equal to or very close to zero. Interestingly, these estimated mean writhe values are also close to the mean writhe values of the ideal polygons (of the corresponding knot types). Whether this is a general trend for knots with large crossing numbers remains unclear. For future studies, we plan to carry out larger scale numerical studies to cover more complicated knot types and also carry out more rigorous analysis.

In the case of equilateral random polygon, we had provided strong analytic and numerical evidence that the variance of the writhe of an equilateral random polygon behaves as a linear function of n, where n is the length of the polygon. This information is important if we are to carry out numerical studies to make inferences on the mean writhe of equilateral random polygons under various constraints (such as confined volume or fixed knot types). Though some technical challenges remain in proving this linear behavior rigorously. It is worthwhile to point out that one should not consider that $E(w^2(EP_n)) = O(n)$ as something intuitive or obvious. For example, recall that for the uniform random polygons confined in a volume, it has been shown that the mean squared writhe behaves as $O(n^2)$. We strongly suspect that this is also true for the equilateral random polygons confined in a fixed volume. On the other hand, it can be shown that the mean ACN of an equilateral random polygon of n edges confined in fixed volume behaves as $O(n^2)$ well. However, the mean ACN of an equilateral random polygon without confinement behaves as $O(n \ln n)$ instead. So if we were to use the mean ACN (since it behaves the same as the mean squared writhe in the confined case) as a reference, we would guess that the mean squared writhe should behaves as $O(n \ln n)$ instead. Another observation is that the determination of the maximum $w^2(EP_n)$ values is quite difficult. In fact, the maximum writhe of a polygon with n edges (in terms of n) is an open question. Without this, one does not even have a complete picture of the range of the distribution of $E(w^2(EP_n))$. This makes the prediction of $E(w^2(EP_n))$ difficult without further information. Recently, a study has been done on the mean squared writhe of random knot diagrams [16]. There it is observed that the mean squared writhe behaves as $O(n)$, where n is the number of crossings in the diagram. However, the knot diagrams studied there are mostly alternating (hence minimum) knot diagrams, which are very different from the knot diagrams obtained by projecting our random polygons. Hence a direct comparison cannot be made.

Acknowledgments

Part of this work (Y. Diao) was supported by an internal summer grant from UNC Charlotte in 2008-2009. Y. Diao is currently supported by NSF Grants DMS-0920880 and DMS-1016460. J. Arsuaga, R. Scharein and M. Vazquez are currently supported by NSF grant DMS-0920887. J. Portillo was supported by the NIH-RISE program (R25-Gm59298) and by a grant from the Genentech Foundation to Dr. F. Bayliss.

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