An Introduction to the Differential Geometry of DNA

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A very interesting application of differential geometry and topology to the study of DNA has recently emerged [1], [3], [5], [6], [7]. By approximating the topological structure of the DNA molecule by a ribbon, biologists have used quantities borrowed from topology and knot theory to describe DNA more precisely. This has enabled them to further understand the effects of enzymes (eg., topoisomerases and gyrases) on DNA, explain why additional twisting of DNA results in coiling, and quantitatively measure the changes which occur in recombinant DNA reactions. For anyone trying to acquaint themselves with such work, however, it is difficult to find an introductory paper which is both comprehensive and accessible to one not trained in biology and advanced mathematics.

Attempting to address this need, the aim of this paper is twofold. First, it will serve as an introduction to the differential geometry of ribbons (as applied to DNA) for biologists with a background in vector calculus. Second, an introduction to the molecular biology of DNA will be given for mathematicians interested in this field. The highpoint will be an elementary proof that the writhing number, a quantity which describes the coiling of DNA, depends solely on the molecule's axis.

In section 1, the properties, configuration, and components of DNA will be discussed. The subsequent sections up through 6 will introduce and explain the ribbon representation of DNA and the associated mathematical concepts of linking, twisting, and writhing, as well as the linking deficit. Mathematical proofs have been relegated to Section 7, and the bibliography has been annotated to facilitate further study.

1. DNA

Deoxyribonucleic acid (DNA) is the molecule upon which the genetic code is stored for nearly all organisms. An understanding of its chemical, geometric, and topological structure plays a key role in understanding its function. Here the topology and geometry of DNA will be emphasized, but
Fig. 1

Fig. 2

Fig. 3
not to the exclusion of its chemistry. Actually, studying the topological and geometric properties of DNA leads to insights into its chemistry.

DNA consists of two sugar-phosphate strands connected by nitrogenous bases through hydrogen bonding (figure 1). These strands run in opposite directions relative to each other, based on their chemistry. One strand is said to run from the 5’ carbon to the 3’ carbon while the other runs from the 3’ to the 5’. This structural feature is described in saying that the strands are antiparallel (figure 2). The subunits of these strands are called nucleotides, each consisting of a five carbon sugar, a phosphate group, and a nitrogenous base (figure 3). The natural conformation of DNA is that of an alpha-helix, which means that the double-stranded chain twists right-handedly. This property is independent of the direction of travel along the molecule (figure 4). Because DNA is helical and is composed of two strands, it is commonly referred to as a double helix. In the unstressed state of the alpha-helix, there are approximately 10.2 base pairs per turn of the helix. Being the configuration of minimum energy, any change in the molecule’s rate of twist will cause a corresponding increase in the potential energy of the molecule. Take, for example, the recombinant enzyme gyrase. Given an energy source, such as adenosine triphosphate (ATP), this enzyme increases DNA’s rate of twist. On the other hand, a dye called ethidium bromide causes a local decrease in the rate of twist [3].

Recent investigations have shown that DNA spends a significant amount of time as a closed loop (figure 5a) [ ]. The DNA molecule joins back on itself, with strands of like orientation bonded together. If we view the molecule as a ribbon-like surface whose edges are the sugar-phosphate strands, this is equivalent to saying that the surface is orientable and not a möbius strip.

One can imagine that if a DNA molecule closes while in a stressed state, there will be a net potential energy stored in the closed chain. Experience with tubes and telephone cords leads us to expect that a closed cord with a net potential energy forms coils to relieve the energy due to twisting. This is exactly the case with closed, circular DNA, which provides an explanation for why DNA is often observed in a highly condensed state (figure 5b) [ ], [ ]. More precisely, the molecule is said to be supercoiled, where the alpha-helix itself winds to form a helix of
Fig. 4

Fig. 5a

Fig. 5b
higher order (figure 5c). By representing the structure of closed, circular DNA by a ribbon, we can measure and predict the effect of recombinant enzymes on DNA and further understand its general properties.

2. **The Ribbon Representation and Knots**

To study the structure of DNA mathematically, it is convenient to construct a model in which the molecule is represented by a narrow, twisted ribbon of infinitesimal thickness. One's initial inclination would be to define the edges of the ribbon to be the antiparallel strands of the DNA molecule and its axis to be the line halfway between the strands, but doing so results in the ribbon's axis winding around the axis of the superhelix (recall figure 5a-c). For the purpose of studying DNA's structure, it is preferable to choose an axis which coincides with the axis of the superhelix itself.

Construction of such a ribbon model is achieved by drawing a line segment perpendicular to the superhelical axis from the superhelical axis to the line halfway between the antiparallel strands (figure 6). As the strands wind their way up the superhelical axis, one of the ribbon's edges is traced out. Extension of each line segment an equal distance in the opposite direction past the superhelical axis gives the other edge of the ribbon. Alternatively, we may imagine a right circular cylinder of diameter D (figure 7) where the alpha-helix winds up the cylinder's surface. Focus attention on the line halfway between the strands; the ribbon is defined at a particular point P by the diameter D of a thin cross section of the cylinder which has on its perimeter the point P. As the strands move up the cylinder, a ribbon is traced out.

Because the strands of DNA are antiparallel, we will assign to the edges of our ribbon opposite orientations. Note that there are two ways to assign an orientation to the ribbon, but our discussion will be independent of the choice. The ribbon model follows the same axis as the superhelix and twists as the two strands of the molecule twist around that axis. This approximation will suffice for our purposes. Also note that the ribbon's axis is often a closed loop, or, in mathematical language, a *knot*. The rest of our discussion will concern this ribbon model, although the assumption that it be closed is not always necessary.
Mathematically, a ribbon can be described as follows. Let the curve \( \mathbf{X} \) be the axis of the ribbon parameterized by a vector \( \mathbf{X}(t) \) in 3-space depending on \( t \), with \( 0 \leq t \leq L \). We assume that \( \mathbf{X} \) is smooth and simple (no self-intersections) and that the tangential velocity vector \( \mathbf{T}(t) = (d/dt)\mathbf{X} \) is of unit length, so that the unit tangent vector \( \mathbf{T}(t) = \mathbf{X}'(t) \) is everywhere defined along the curve. Now define a unit normal vector, \( \mathbf{U}(t) \), in the plane of the ribbon and perpendicular to \( \mathbf{T}(t) \) (figure 8). This vector \( \mathbf{U}(t) \) lies along the radius of the cylindrical cross section in figure 7. The ribbon can be parameterized by \( \mathbf{R}(s,t) = \mathbf{X}(t) + s\mathbf{U}(t) \), where \(-\varepsilon \leq s \leq \varepsilon \) (\( \varepsilon > 0 \) is a positive real number). For sufficiently small \( \varepsilon \) the curves \( \mathbf{X} \pm \varepsilon \mathbf{U} \) are disjoint simple curves from \( \mathbf{X}(t) \) and represent the edges of the ribbon.

The ribbon is closed when \( \mathbf{X}(0) = \mathbf{X}(L) \), \( \mathbf{X}^{(k)}(0) = \mathbf{X}^{(k)}(L) \), \( \mathbf{U}^{(k)}(0) = \mathbf{U}^{(k)}(L) \), and \( \mathbf{U}(0) = \mathbf{U}(L) \), for all \( k > 0 \). Each edge joins back with itself to form a knot, as does the axis.

Now that we have a ribbon model, let us look at two ways of describing how the edges of the ribbon wind around the central axis.

3. **The Linking Number**

Two disjoint, oriented, simple closed space curves are said to be *linked* if they cannot be separated without one curve passing through another, or by temporarily breaking one curve (figure 9). The *linking number* of two such curves, say \( L_1 \) and \( L_2 \), is an integer and will be denoted by \( \text{Lk}(L_1,L_2) \). For example, the edges of a closed ribbon are a pair of disjoint closed curves that may be linked. The linking number has been defined so that two unlinked closed curves, \( L_1 \) and \( L_2 \), satisfy \( \text{Lk}(L_1,L_2) = 0 \), those which pass through each other once have \( \text{Lk}(L_1,L_2) = 1 \), etc. (see below for sign convention). The linking number of two closed curves is a topological invariant, meaning that smooth a deformation of either curve does not alter their linking number.

The concept of the linking number of two closed curves is easily applied to the oriented edges of our ribbon model. The edges of an orientable closed ribbon consist of two distinct simple closed oriented curves \( L_1 \), \( L_2 \). Therefore we can define their linking number \( \text{Lk}(L_1,L_2) = \text{Lk}(\mathbf{X} \pm \varepsilon \mathbf{U}) \). By the negative \(-L\) of \( L \) we mean the curve \( L \) with opposite orientation. The properties of the linking number are such that its value remains unchanged
Fig. 11

Fig. 12

Fig. 13
if the orientation of both linked curves are reversed, as its value is changed by a factor of -1 when the orientation of one curve is reversed. That is, $\text{Lk}(-L_1, -L_2) = \text{Lk}(L_1, L_2)$ because $\text{Lk}(-L_1, L_2) = - \text{Lk}(L_1, L_2)$ and $\text{Lk}(L_1, L_2) = \text{Lk}(L_2, L_1)$.

There are two algorithms for calculating the linking number of two closed space curves which are particularly useful in the present context.

For the first, we need the concept of a regular projection of a link onto a plane. Given a plane with normal vector $n$, and two closed space curves $L_1(t)$ and $L_2(t)$, we want to project these two curves onto the plane such that $L_1'(t)$ and $L_2'(t)$ are never parallel to $n$ (figure 10), meaning that the velocity vectors of the projected curves are never zero. The plane can be chosen specifically to accommodate this requirement and to satisfy the additional requirement that the projected curves always have normal crossings (i.e., if $f(t_1) = f(t_2)$, then $f'(t_1)$ and $f'(t_2)$ are not parallel).

The first method, which we will call the projection method, is implemented by first taking a regular projection of the curves onto a plane and requiring that all crossings be normal. Under these conditions, the projections are smooth curves in the plane, which have distinct tangent lines where they intersect. Each of the intersection points of the two projected curves is assigned a +1 or -1 index value, dependent upon the orientation of the top curve relative to the bottom curve (figure 11). In practice it is helpful to color each line differently, say: one red and the other blue. We only consider red/blue intersections, not self-intersections (i.e., red/red or blue/blue). Summation of the index values and dividing by 2 (the number of linked curves) gives the value of the linking number, $\text{Lk}(L_1(t), L_2(t))$ (example 1).

The first step of the second method is to find an orientable surface $R$ such that $\partial R = L_1$ and such that $L_2$ makes normal intersections with $R$. The surface $R$ must be smooth everywhere except possibly at a finite number of points $F$; $L_2$ must not intersect $R$ at the singular points $F$; and $L_2$ must not be tangent to $R$ at the points of intersection. Such a surface $R$ always exists. The initial spacial arrangement of the two curves may make the visualization of $R$ difficult, but recalling that $\text{Lk}(L_1, L_2)$ is a topological invariant, and therefore unchanged by smooth deformations, we can simply deform the curves (without passing them through each other) to facilitate the computation. The surface $R$ is assigned a normal vector $\mu$ in
accordance with its orientation (figure 12). Note that L2 will pass through the surface R a finite number of times, sometimes in the same direction as \( \mu \) and sometimes in the opposite direction. Passage in the same direction is assigned a -1, and passage in the opposite direction is assigned a +1. The linking number \( \text{Lk}(L_1, L_2) \) is obtained by summing the index values (example 2). Note that in this method the sum is not divided by 2.

The linking number has been defined here so that \( \text{Lk}(X \pm \varepsilon U) \) of the DNA alpha-helix will be positive. This convention is the opposite of the usual convention used in topology. As an example, a relaxed, closed circular DNA 5,000 base pairs long, with 10 base pairs for each turn of the helix, would have a linking number of +500.

One should be aware that there exist physically linked circles with linking number equal to zero (figure 13).

Now let us analyze the ribbon model of DNA from a different perspective. Instead of looking at the relationship between its edges as we have with the linking number, we now look at the way the ribbon twists around its axis.

4. The Twisting Number

The twisting number of a ribbon \( R(s,t) = X(t) + sU(t) \), with axis \( X \) and normal vector field \( U \), is a real number that will be denoted by \( \text{Tw}(X,U) \). This quantity is a geometric invariant of the ribbon, meaning that it remains unchanged under rigid motion yet may change under continuous deformation. Note that the definition of \( \text{Tw}(X,U) \), in contrast to the linking number, will not require that the ribbon be closed.

The concept of a ribbon's twist is most easily understood for ribbons whose axis lies in a plane. Let \( X \) be a smooth curve in a plane \( P \). Define a vector field \( \beta(t) \) such \( \beta(t) \) is normal to \( X(t) \) and lies in the plane \( P \). The twisting number of a ribbon \( X(t) + sU(t) \) is simply a measurement of the net angular deviation of \( U \) from \( \beta \). If the ribbon is closed, the twisting number will always be an integer, since \( U(0) = U(L) \). Following our convention, a right-handed turn about the axis is assigned a value of +1, and a left-handed turn is assigned a value of -1 (figure 14).
Fig. 14

Fig. 15

Fig. 16
For a relaxed piece of DNA 5,000 base pairs long (10 base pairs per turn), the vector \( \mathbf{U}(t) \) makes one complete rotation around the axis for every turn of the double helix. So the twisting number equals +500, being positive because the double helix is right-handed. Note that in this simple case in which the ribbon's axis is planar, \( \text{Lk}(\mathbf{X} \pm \varepsilon \mathbf{U}) = \text{Tw}(\mathbf{X}, \mathbf{U}) \).

Definition of the twisting number for the general case where \( \mathbf{X}(t) \) is a space curve poses a more difficult problem, but it is still geometrically intuitive. In order to measure the twisting number of \( \mathbf{U} \) about its axis \( \mathbf{X} \), we need a vector field \( \mathbf{B} \) such that \( \mathbf{B} \) does not twist about \( \mathbf{X} \), thereby establishing a reference frame from which to measure the rotation of \( \mathbf{U} \) about \( \mathbf{X} \). The vector field \( \mathbf{B}(t) \) is defined so that \( ||\mathbf{B}|| = 1, \mathbf{B}(t) \cdot \mathbf{X}(t) = 0, \) and \( \mathbf{B}'(t) = c(t) \mathbf{X}'(t) \). The first two properties of \( \mathbf{B} \) ensure that it is of unit length and normal to \( \mathbf{X} \). The third property signifies that the component of \( \mathbf{B}'s \) velocity normal to \( \mathbf{X} \) vanishes, so that \( \mathbf{B} \) does not rotate about \( \mathbf{X} \). A vector field defined in this manner is said to be a parallel normal field of \( \mathbf{X} \). A proof of the existence and uniqueness (up to a rotation) of parallel normal fields is given in Section 7.

One can intuitively understand the significance of a parallel normal field by imagining the curve \( \mathbf{X} \) to be a rollercoaster track and \( \mathbf{B} \) to point upward through the cart. As the track travels through space, its cart does not twist around the track but rather twists with it.

Now let \( \phi(t) \) equal the angle between \( \mathbf{U}(t) \) and \( \mathbf{B}(t) \). The twisting number is defined by:

\[
\text{Tw}(\mathbf{X}, \mathbf{U}) = \frac{1}{2\pi} \left[ \phi(L) - \phi(0) \right],
\]

where angular displacement is positive for a right-handed turn. Equivalently,

\[
\text{Tw}(\mathbf{X}, \mathbf{U}) = \frac{1}{2\pi} \int_{0}^{L} \phi'(t) \, dt.
\]

In general, the value of the twisting number will be a real number, in contrast to the linking number, which is always an integer.
To illustrate the significance of the twisting number and its properties, consider figure 15. The figure on the left has twisting number equal to zero and linking number equal to -1. Deforming the figure into the figure on the right decreases the twisting number to -1, but the linking number remains equal to -1, illustrating that $Tw(X, U)$ can change under smooth deformation, while $Lk(X \pm \epsilon U)$ remains unchanged.

Having described the linking number and the twisting number, quantities which are properties of the ribbon, let us now use them to define a quantity which is solely dependent upon the axis.

5. **The Writhing Number**

Define a new quantity, the *writhing number* of a closed ribbon $R(s, t) = X(t) + sU(t)$, as the difference

$$Wr(X, U) = Lk(X \pm \epsilon U) - Tw(X, U)$$

between the ribbon's linking and twisting numbers. Since the linking number is an integer and the twisting number is generally a real number, the writhing number will be a real number in general. When the axis $X$ lies in a plane, $Tw(X, U)$ is an integer and therefore the writhing number of such a ribbon is also an integer.

The writhing number measures the extent to which coiling of the central curve $X$ has relieved potential energy due to local twisting of the ribbon. Experience with cords and hoses leads one to recall that when additional twist is introduced into a closed cord or hose, coils are formed. Likewise, when coiling a garden hose or rope it is necessary to insert twists to prevent the hose from writhing.

Recalling that the linking number of two closed curves is a topological invariant, any change in the twisting number of the ribbon will be completely transferred (neglecting thermal dissipation) to its writhing number. As $Tw(X, U)$ becomes more positive, $Wr(X, U)$ becomes more negative.

The simplest method for calculating the writhing number of a ribbon is to calculate its linking and twisting numbers, then take their difference. Observe again figure 15. The figure on the left has $Wr(X, U) = -1$, while
that on the right has $\text{Wr}(\mathbf{X}, \mathbf{U}) = 0$. Notice that the figure with non-zero writhing number is "coiled," while the other contains a twist. By coiling into the figure onto the left, the potential energy due to twisting has been partially relieved, while the linking number remains constant.

The final and most profound property of the writhing number of a ribbon we shall refer to as the Writhing theorem:

Given a closed curve $\mathbf{X}$ defined by a three dimensional vector $\mathbf{X}(t)$ depending continuously of a parameter $t$, $0 \leq t \leq L$, such that $\mathbf{X}(0) = \mathbf{X}(L)$; and given two normal vector fields $\mathbf{U}_1(t)$ and $\mathbf{U}_2(t)$, $\mathbf{U}_1(t) \neq \mathbf{U}_2(t)$ along $\mathbf{X}$ satisfies $\mathbf{U}_1(0) = \mathbf{U}_1(L)$; the two ribbons determined by $\mathbf{X} \pm \epsilon \mathbf{U}_1$ and $\mathbf{X} \pm \epsilon \mathbf{U}_2$ have equal writhing numbers. This means that the writhing numbers of two different ribbons with the same axis are equal. That is, the writhing number of a ribbon depends solely on its axis.

A proof of this theorem is left for section 7. In light of this property, it is more accurate for us to refer to the writhing number of a closed space curve $\mathbf{X}$, since its value does not actually depend on $\mathbf{U}$, and to denote $\text{Wr}(\mathbf{X}, \mathbf{U})$ by $\text{Wr}(\mathbf{X})$. One can also calculate the writhing number of a knot $\mathbf{X}$ directly by using a Gauss integral [2], [4].

In the case of a simple planar ribbon this theorem is geometrically clear. The writhing number is always zero because the linking and twisting numbers are always equal. No matter how one alters the ribbon by inserting or removing turns, keeping the axis planar and maintaining the same axis $\mathbf{X}$, the linking and twisting numbers will change by the same amount. Their difference, the writhing number, is therefore constant. When the axis is a space curve, the situation is more complicated and we defer further treatment until the last section.

With the preliminary discussion of the differential geometry of DNA completed, now let us focus our attention on one of its fundamental applications.

6. **Supercoiling and DNA**

Recall that supercoiling occurs when a helix itself winds in a helical manner. Observations made concerning the polyoma-virus DNA, a virus
which causes tumors in mice, lead to a way to define supercoiling. This DNA can be separated using sedimentation techniques into three components: I and II, which are circular, and III, which is linear. The average linking number for a population of relaxed (II, III) circular molecules is about +500, while for a population of closed circular, supercoiled molecules (I) the average linking number is +475. The fact that closed circular DNA is present in an underwound form suggests a way to define supercoiling [ ], [ ].

Define the linking deficit, $\Delta L_k$, of a closed molecule as the difference between the linking number of a molecule in the natural, closed supercoiled state ($L_{kn}$) and the linking number of the same molecule in the relaxed closed circular state ($L_{kr}$) [ ]. (The relaxed state is achieved by a process called "nicking" in which one strand of the DNA molecule is temporarily cut, allowed to unwind to relieve stress, and then reattached. Well-known enzymes which can accomplish this amazing feat are in common use in molecular biology [3]). Therefore, $\Delta L_k = L_{kn} - L_{kr}$, and for the polyoma-virus DNA example, $\Delta L_k = -25$.

This quantity describes the entire DNA molecule, but DNA frequently has length above 5,000 base pairs, and an additional twist does not change the extent of supercoiling as much as in a smaller molecule. We suggest the definition of a different quantity, the average linking deficit $\Delta L_k^*$, to describe the supercoiling of closed DNA per unit length. Its value is given by $\Delta L_k^* = (L_{kn} - L_{kr})/\text{length}$, where the length is the number of base pairs. Recalling our ribbon model, $W_r(X)$ gets more positive as $T_w(X, U)$ gets more negative. Underwound, closed DNA, the naturally occurring configuration [ ], can therefore reduce its deformation energy due to twist by writhing.

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This brief introduction to the study of supercoiled DNA will hopefully serve as a springboard into further study. The bibliography has been annotated to facilitate the location of particular topics of interest, and the next section will elaborate on the mathematics surrounding DNA's differential geometry.
7. Mathematical Background

7.1 Frenet Formulas

We begin our discussion with a review of the Frenet formulas for a space curve \([\cdot]\). Let \(X(t)\) be a smooth, space curve parameterized by \(t\), with \(X'(t)\) of unit length for all \(t\) in \([a,b]\). A curve so defined will be referred to as "well-behaved." Let \(T(t)\) be a unit tangent vector in the direction of \(X'(t)\), so that \(X'(t) = T(t)\). The curvature \(k(t)\) is defined to be the length \(||T'(t)||\) of \(T'(t)\). In this section we are assuming that the curvature \(k(t)\) is never zero. The principal normal vector \(N(t)\) is defined by \(N(t) = T'(t)/k(t)\). Note that \(N(t)\) is also of unit length (figure 16).

7.1.1 Proposition: For all \(t\), \(T(t) \cdot N(t) = 0\)

**Proof:** Since \(T(t)\) is of unit length, \(T \cdot T = 1\). Differentiating, we obtain \(2T \cdot T' = 0\). Recalling that \(T'(t) = k(t) N(t)\), we see that \(2k(t) T \cdot N(t) = 0\), or equivalently, \(T \cdot N = 0\). The vectors \(T\) and \(N\) are therefore perpendicular to each other.  

Next define the binormal vector \(B(t)\) by \(B(t) = T(t) \times N(t)\). Because \(T\) and \(N\) are of unit length and perpendicular to each other, \(B\) will also be of unit length. Now observe that \(T, N,\) and \(B\) form a right-handed, orthonormal set of vectors.

7.1.2 Proposition: There exists a smooth, scalar function \(\tau(t)\) such that \(B'(t) = \tau(t) N(t)\) for all \(t\).

**Proof:** Differentiating \(B = T \times N\), we see that \(B' = T \times N' + T' \times N\). Since \(T' = kN\),

\[
B' = T \times N' + kN \times N = T \times N',
\]

from which it follows that \(B'\) is perpendicular to \(T\). By an argument similar to that used in 7.1.1, \(B'\) is perpendicular to \(B\). Therefore, \(B'\) is a multiple of \(N = B \times T\). That is, \(B' = \tau N\).

This quantity \(\tau(t)\) is called the torsion of \(X(t)\). We shall see that it measures the rate at which \(X\) itself twists.

7.1.3 Proposition: For all \(t\), \(N'(t) = -\tau B(t) - kT(t)\).
Proof: Since $N = B \times T$, and since $T' = kN$, and $B' = \tau N$, 
$N' = B' \times T + B \times T' = \tau N \times T + kB \times N = -\tau B - kT$. ■

We summarize these results in the following theorem.

7.1.4 Theorem: For all $t$, the vectors $T(t)$, $N(t)$, and $B(t)$ form a set of 
right-handed orthonormal vectors satisfying 

a) $T' = kN$  
b) $B' = \tau N$  
c) $N' = -\tau B - kT$. ■

7.2 Parallel Normal Fields

Now we can address the problem of proving the existence of parallel normal fields, as required in the definition of the twisting number.

7.2.1 Definition: Suppose $X(t)$ is a well-behaved curve (cf. 7.1). A 
vector field $U(t)$ along $X(t)$ is:

a) *normal* if $U(t) \cdot T(t) = 0$ for all $t$

b) *parallel normal* if it is normal and:
i) $U'(t) = c(t) \ T(t)$

ii) $\| U(t) \| = \text{constant}$

To analyze the DNA double helix in its ribbon representation, we are interested in vectors $U(t)$ perpendicular to $X(t)$ which define the ribbon. Under what conditions, if any, does the normal vector field $U(t)$ become a parallel normal vector field?

7.2.2 Theorem: If $X(t)$ is well-behaved with $a \leq t \leq b$ and $V_a$ is a vector 
normal to $T(a)$, then there exists a unique parallel normal field $U(t)$ along $X$ and through $V_a$. Moreover, if $k(t) \neq 0$ for 
t near some constant, then $U(t)$ can be represented by 
$U(t) = \cos \varphi(t) \ N(t) + \sin \varphi(t) \ B(t)$, $0 \leq \varphi \leq 2\pi$, and

$$\varphi(t) = \int_{c}^{t} \tau(u) \ du + \varphi(c), \text{ or } \varphi'(t) = \tau(t)$$

Proof: We will prove the theorem under the assumption that $k(t) \neq 0$. 
Visualize the situation by looking down the axis of the ribbon (figure 17).

Now, for $U(t)$ to be parallel normal, it must be perpendicular to $T(t)$ 
and of constant length; both of which have already been established.
Furthermore, its derivative must have a component only in the direction of \( T(t) \). We must find the conditions, if any, under which this is true.

Let \( U(t) = \cos\phi(t) N(t) + \sin\phi(t) B(t) \) be a normal vector along \( X \). Then,

\[
U'(t) = \cos\phi N' - \sin\phi \frac{d\phi}{dt} N \sin\phi B' + \cos\phi \left( \frac{d\phi}{dt} \right) B
\]

Since \( N' = -\tau B - kT \) and \( B' = \tau N \), we have

\[
U'(t) = \cos\phi \left( -\tau B - kT \right) - \sin\phi \left( \frac{d\phi}{dt} \right) N \sin\phi \tau N + \cos\phi \left( \frac{d\phi}{dt} \right) B
\]

\[
= \left( \tau - \frac{d\phi}{dt} \right) \sin\phi N + \left( \frac{d\phi}{dt} - \tau \right) \cos\phi B - k\cos\phi T.
\]

For \( U(t) \) to be parallel normal, the quantity in brackets must equal zero, so that \( U'(t) = c(t) T(t) \), where \( c(t) = -k\cos\phi \). The vectors \( N \) and \( B \) are linearly independent by definition, and therefore the above equation forces the two coefficients to equal zero for all \( \phi \). Noting that \( \sin\phi \) and \( \cos\phi \) do not both vanish at the same \( \phi \), we have

\[
\tau - \frac{d\phi}{dt} = \frac{d\phi}{dt} - \tau = 0. \quad \text{That is } \frac{d\phi}{dt} = \tau. \quad \blacksquare
\]

So, for \( U(t) \) to be parallel normal to \( X(t) \), the angular rate of change of \( U(t) \), \( \frac{d\phi}{dt} \), must equal the rate at which \( X(t) \) twists, \( \tau(t) \), which is its torsion. The vector field \( B(t) \) described in Section 4 does exist and provides a reference from which to measure the twist of the ribbon about its axis.

7.2.3 Proposition: If \( U_1 \) and \( U_2 \) are parallel normal vector fields of \( X(t) \), then the angle between them remains constant for all \( t \).

Proof: Consider figure 18. Let \( \Omega(t) \) be the angle between \( U_1(t) \) and \( U_2(t) \). Then, since \( U_1 \) and \( U_2 \) are of unit length,

\[
U_1 \cdot U_2 = ||U_1|| ||U_2|| \cos\Omega = \cos\Omega.
\]

Differentiating, we see that

\[
-\sin\Omega \frac{d\Omega}{dt} = U_1' \cdot U_2 + U_1 \cdot U_2' = c_1(t) T(t) \cdot U_2 + c_2(t) T(t) \cdot U_1 = 0,
\]

as \( U_1 \) and \( U_2 \) are parallel normal vectors of \( X \). Therefore, \( d\Omega/dt = 0. \quad \blacksquare \)
7.3 Writhing Theorem

We begin by restating the writhing theorem as proposed in Section 5.

7.3.1 Theorem: Given a closed curve \( X \) defined by a three dimensional vector \( X(t) \) depending continuously of a parameter \( t, 0 \leq t \leq L \), such that \( X^{(k)}(0) = X^{(k)}(L), \ k \geq 0; \) and given two normal vector fields \( U_1(t) \) and \( U_2(t) \), \( U_1(t) \neq U_2(t); \) the two ribbons determined by \( X(t) + sU_1(t) \) and \( X(t) + sU_2(t) \), \( -\varepsilon \leq s \leq \varepsilon \), have equal writhing numbers.

Proof: A ribbon is constructed from a knot by finding some normal vector \( U(t) \) (note that this vector is not necessarily parallel) such that \( U(0) = U(L) \), where \( 0 \leq t \leq L \). As discussed previously, there are two invariants we can associate to such a ribbon:

- Linking number \( \text{Lk}(X \pm \varepsilon U) \): an integer and a topological invariant
- Twisting number \( \text{Tw}(X, U) \): a real number and a geometric invariant

We then defined a third quantity, the writhing number \( \text{Wr}(X, U) \), as the difference between the linking and twisting numbers:

\[ \text{Wr}(X, U) = \text{Lk}(X \pm \varepsilon U) - \text{Tw}(X, U). \]

The aim here is to show that the writhing number depends only on the axis \( X(t) \) and not on the choice of \( U(t) \).

Our strategy will be to first show that the writhing numbers of two ribbons \( X \pm \varepsilon U_0 \) and \( X \pm \varepsilon U_1 \) about the fixed axis \( X \) are equivalent, given the assumption that the normal vector fields \( U_0 \) and \( U_1 \) can be deformed continuously and smoothly into each other. Then we address the case in which arbitrary \( U_0 \) and \( U_1 \) are chosen, showing that the writhing number of a closed, fixed axis \( X \) is independent of the ribbon which winds about it.

Case 1

Given a fixed axis \( X(t) \) and two normal vector fields \( U_0 \) and \( U_1 \) as defined above, assume that \( U_1 \) can be continuously deformed into \( U_0 \) without breaking the ribbon defined by \( U_1 \). By the topological invariance of the linking number, we see that the linking numbers \( \text{Lk}(X \pm \varepsilon U_0) \) and
Lk(X ± εU_1) are equal. Our aim is to show that the writhing number
Wr(X, U_0) of X ± εU_0 is equal to the writhing number Wr(X, U_1) of X ± εU_1.

See that under these conditions U_1(t) is equal to some rotation of
U_0 (t) for all t, modulo 2π, and that a function θ can be defined such that

\[ U_1(t) = T_{θ(t)} U_0(t), \]

where θ maps t, 0 ≤ t ≤ L, into the real numbers so that θ: [0, L] → ℝ.
Because U_1 can be continuously deformed into U_0 without breaking and
therefore Lk(X ± εU_0) = Lk(X ± εU_1), it follows that θ(0) = θ(L).

We previously defined ω_i = ω_i(t) to be the angular velocity of U_i(t)
about X, where ω_i(t) is the angular deviation of U_i from the parallel normal
vector field B(t) (Section 4). Since θ(t) measures the angle between U_0
and U_1, we see that

\[ ω_1(t) = ω_0(t) + θ(t). \]

so that,

\[ ω_1'(t) = ω_0'(t) + θ'(t). \]

Recall from Section 4 that the twisting number of U_i about X is given by

\[ 2π Tw(X, U_i) = \int_0^L ω_i'(t) \, dt. \]

Substituting our expression for ω_1'(t), we have

\[ 2π Tw(X, U_1) = \int_0^L ω_0'(t) \, dt + \int_0^L θ'(t) \, dt, \]

which by the fundamental theorem of calculus yields

\[ 2π Tw(X, U_1) = 2π Tw(X, U_0) + θ(L) - θ(0). \]
Because \( \theta(0) = \theta(L) \), we see that \( Tw(X, U_1) = Tw(X, U_0) \). That is, the twisting number is unchanged by continuous deformations of \( U \). Recall that \( Lk(X \pm \varepsilon U_0) = Lk(X \pm \varepsilon U_1) \) by our assumption that \( U_1 \) can be continuously deformed into \( U_0 \) without breaking. Therefore, we see that the writhing numbers \( Wr(X, U_1) \) and \( Wr(X, U_2) \) are equal. The writhing number of a fixed curve \( X \) and normal vector field \( U_i \) is therefore constant under smooth deformation of \( U_i \).

**Case 2**

Turn now to the general case in which \( U_0 \) and \( U_1 \) are arbitrary, so that their linking numbers are not necessarily equal. Suppose that \( Lk(X \pm \varepsilon U_0) = n \) and that \( Lk(X \pm \varepsilon U_1) = n + k \), where \( k \geq 0 \). If \( k = 0 \), then we are in the previous case and need go no further. If \( k > 0 \), construct a new ribbon \( X \pm \varepsilon U_1^* \) from \( X \pm \varepsilon U_1 \) by temporarily cutting one of its edges and unwinding it \( k \) times (if \( k < 0 \), simply reverse the roles of \( U_0 \) and \( U_1 \)).

By Case 1, \( Wr(X, U_0) = Wr(X, U_1^*) \). Our aim is to determine the value of \( Wr(X, U_1) = Lk(X \pm \varepsilon U_1) - Tw(X, U_1) \). Because we have removed \( k \) twists from the ribbon \( X \pm \varepsilon U_1 \), and because the twisting number is unchanged by deformations of \( U \), we see that

\[
Lk(X \pm \varepsilon U_1) = Lk(X \pm \varepsilon U_1^*) + k
\]

and

\[
Tw(X, U_1) = Tw(X, U_1^*) + k,
\]

recalling that the linking and twisting numbers are positive for an alpha-double helix (edges oriented oppositely) and a right-handed turn, respectively. We therefore have

\[
Wr(X, U_0) = Wr(X, U_1^*) = Lk(X \pm \varepsilon U_1^*) - Tw(X, U_1^*)
\]

and

\[
Wr(X, U_1) = [Lk(X \pm \varepsilon U_1^*) + k] - [Tw(X, U_1^*) + k]
\]

\[
= Lk(X \pm \varepsilon U_1^*) - Tw(X, U_1^*)
\]

\[
= Wr(X, U_0).
\]
So, we see that the writhing number of a normal vector field \( \mathbf{U}_i \) about a closed axis \( \mathbf{X} \) is independent of the choice of \( \mathbf{U}_i \) (given the assumptions stated in the theorem) and depends solely on \( \mathbf{X} \).

* * *

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**BIBLIOGRAPHY**


**The Writhing Number of a Space Curve:** DNA structure is approximated by a closed ribbon, then geometrically described by its linking number, twisting number, and writhing number. The writhing number is defined as the difference between the linking number and the twisting number, claiming that the writhing number is a geometric invariant, dependent solely on the closed space curve which is the DNA axis. It is shown quantitatively how the elastic energy due to local twisting of DNA may be reduced if the central curve of the rod forms coils, thereby increasing the writhing number.


**The Self-Linking Number of a Closed Space Curve:** An amplification and thorough explanation of G. Calugareanu's work, which presents an integer invariant for a single, simple closed space curve, later to be called the writhing number. This article requires an understanding of differential geometry, advanced calculus, and modern algebra.


**Supercoiled DNA:** An excellent, comprehensive introduction to the topic of supercoiled DNA. Although most treatment is qualitative, this paper serves as a good starting point for someone from any background. Topics covered range from the mathematical description of DNA to current advances toward a more complete understanding of DNA structure.

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