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The projection graph of the augmented ribbon model is unique

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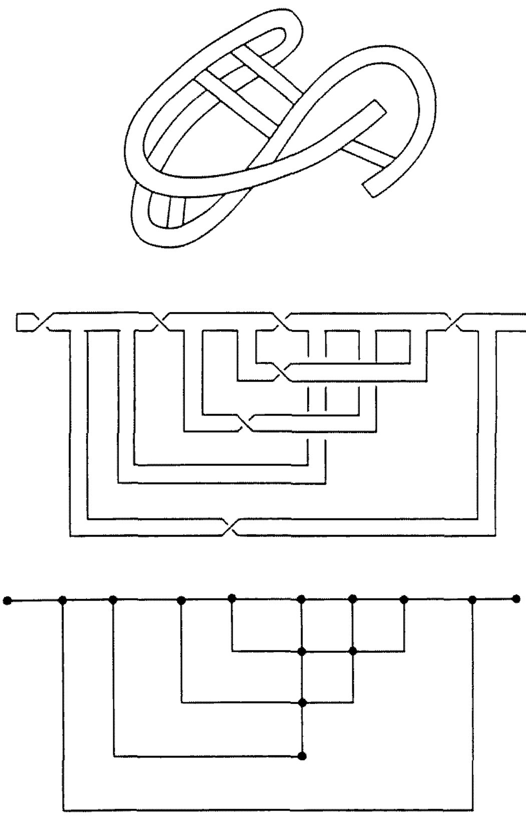
The augmented ribbon model of a protein provides a way of describing features of its primary, secondary, and super-secondary structure. Associated with the model is a graph obtained by an ambient isotopy in space followed by a projection into the plane. This projection graph is shown to be independent of the ambient isotopy.

1. Introduction

An augmented ribbon model (ARM) of protein structure was introduced in ref. [1]. The model is constructed from a topological cell complex, referred to as a twisted surface, embedded in three-dimensional space. An example of a twisted surface is shown in fig. 1(a). A twisted surface is the union of twisted strips. The backbone strip corresponds to the backbone of the protein. The backbone strip is augmented by additional strips called connections, which are attached along the edges of the backbone strip. Connections can represent disulfide bridges or hydrogen bonds between alpha carbons in close proximity.

An important feature of the twisted surface is its graph which lies along the center of the surface. In this paper, a graph is regarded as a topological one-dimensional cell complex and may have multiple edges. Here, we are interested in a graph defined by a family of subintervals of the unit interval $I = [0, 1]$. An *arc-with-chords* is a directed graph $G = (V, E)$ whose vertex set V consists of a sequence of distinct points $0 = v_1 < \ldots < v_{2n+2} = 1$ in I, and whose edge set E consists of the edges $v_j v_{j+1}, j = 1, \ldots, 2n+1$ and edges $E_i = a_i b_i$, where V can also be expressed as $V = \{0, 1\} \cup \{a_1, \ldots, a_n, b_1, \ldots, b_n\}$, where $0 < a_1 < \ldots < a_n < 1$ and $a_i < b_i$, $i = 1, \ldots, n$. An arc-with-chords is said to be *closed* if it has an additional edge E_0 with $a_0 = 0$ and $b_0 = 1$. The union of the edges in I is the *arc* of G and the edges E_i are called *chords*. The *graph* of a twisted surface is the arc-with-chords whose arc lies along the center of the backbone strip and whose chords are defined by the connections. The arc is directed in the same sense as the backbone of the protein, from N-terminus to C-terminus. The connection chords are directed so that their initial endpoint precedes their terminal endpoint along the arc.



(a)

(b)

(c)

Fig. 1. (a) An example of a twisted surface. (b) The same surface after being moved by an ambient isotopy to standard position. (c) The projection graph of the graph of the twisted surface.

An *embedding* of a graph G in R^3 is a particular configuration (or placement) of G in R^3; that is, an embedding is a 1–1 continuous function $g: G \to R^3$. We visualize an embedding by a picture of the graph produced by projecting the graph into a plane. It is convenient to place a condition on such projections. Suppose G is a graph in R^3. Let P be any plane and $p : R^3 \to P$ the orthogonal projection. Say that p is a *regular* projection of G provided every $p^{-1}(x)$, $x \in P$, intersects G in 0, 1 or 2 points and, if 2, neither of them is a vertex of G. It is known that any projection can be adjusted to a regular projection by an arbitrarily small adjustment of the graph or the plane.

An *ambient isotopy* of R^3 is a continuous one-parameter family of homeomorphisms $h_t: R^3 \to R^3$, $0 \le t \le 1$, with h_0 the identity function. An ambient isotopy defines a continuous movement of an object and its surrounding space in a way that preserves topological properties. The condition that the initial function ($t = 0$) be the identity prevents a reversal of orientation which can occur when Euclidean space is mapped onto its mirror image. If the ends of the twisted surface shown in fig. 1(a) are pulled outward so that the backbone straightens, the surface can be moved to the position illustrated in fig. 1(b). This position is referred to as the standard position. Suppose G is an arc-with-chords in R^3 and the orthogonal projection $p: R^3 \to R^2$ is a regular projection of G into the xy-plane. Let $P_i = p(E_i)$, $i = 1, \ldots, n$, be the *projected chords*. We say that G is in *standard position* if (1) the arc of G lies in the x-axis and with the same direction, (2) each P_i is an arc in the bottom half of the xy-plane, (3) any pair of P_i intersects in at most one point, (4) no P_i meets the arc at an interior point of P_i, (5) if P_i meets P_j and P_k with $i < j < k$, then P_i first crosses P_j and then crosses P_k. In the following, we assume that the graph of each twisted surface is ambient isotopic to one in standard position.

Suppose G is an arc-with-chords, $g: G \to R^3$ in any embedding of G such that $g(G)$ is in standard position, and $p: R^3 \to R^2$ is a regular projection of $g(G)$. We define the *projection graph* of G to be the graph $G' = p(g(G))$ whose vertices are the images of the projected vertices together with the points where the projected chords cross. The projection graph of the surface in fig. 1(b) is shown in fig. 1(c).

2. Uniqueness of the projection graph

We claim that the projection graph of an arc-with-chords G is a well-defined graph uniquely embedded in the plane. Suppose h_t is an ambient isotopy carrying any embedding of G in R^3 to $h_1(G)$ which is in standard position. The vertices of the projection graph of degree 3 occur where the projected chords meet the arc. By condition (4) for standard position, the projected chords do not cross the arc in the x-axis. Hence, the vertices of degree 4 arise at crossings of the projected chords. Since two projected chords can cross at most once by (3), two chords cross if and only if exactly one endpoint of one lies between the two endpoints of the other on the x-axis. Also the order of the crossings along a projected chord is determined by condition (5). Thus, the vertices and edges of the projection graph are determined, making the projection graph well defined.

If a graph is embedded on an orientable surface, the clockwise order of the vertices adjacent to a given vertex is defined up to a cyclic permutation of these vertices. The rotational embedding scheme theorem [3] provides a converse. That is, if the embedding of the graph on the surface has the property that the closure of each region is a 2-cell, then the embedding is determined by these permutations. The plane is an orientable surface and the regions of the projection graph are 2-cells by the Schonflies theorem [3].

The ordering of the vertices of the projection graph along the x-axis is determined by condition (1), which requires the order of the arc to match that of the x-axis. Since the projected chords meet the x-axis from below, the clockwise order of the vertices adjacent to each vertex with degree 3 is determined. The clockwise order of the vertices adjacent to a vertex of degree 4 is determined by the ordering of the endpoints of the projected chords along the x-axis. Thus, the embedding of the projection graph is unique.

The graph of a twisted surface is determined by the ordering of the backbone of the protein and the connections. The projection graph is determined by the graph of the surface. The projection graph is independent of the embedding and the ambient isotopy used to move the graph into standard position.

3. Crossings

The ARM of a protein can be represented by a labeled digraph which is similar to a chemical graph. The ARM is obtained by modifying the graph of the twisted surface. Edges labeled Ov and Un denote over or under crossings of connections, respectively. Vertices are inserted to make these edges. This serves to encode the embedding of the graph of the twisted surface in three-dimensional space in the ARM.

The conditions on the standard position of an arc-with-chords prevent much of the possible pathology of embedded graphs. An embedding of a circle is called a *knot*, and an embedding of two or more circles is called a *link*. A link or knot is said to be trivial (or unlinked and unknotted, respectively) if there is an ambient isotopy that carries it into the plane. Nontrivial links can occur in large proteins if proximity connections are used [4]. Small nontrivial knots are unknown in proteins.

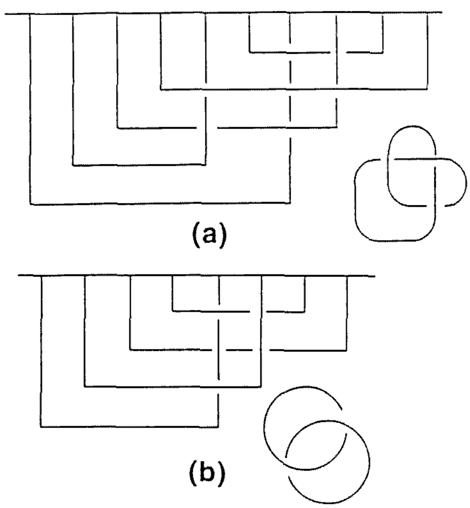


Fig. 2. (a) An arc-with-chords in standard position that contains a knot. (b) An arc-with-chords in standard position that contains a link.

A cycle in the graph of a twisted surface can form a nontrivial knot by using several connections. An arc-with-chords in standard position containing a nontrivial knot is shown in fig. 2(a). Number the vertices along the x-axis in the figure by

$0 = v_1 < \ldots < v_{12} = 1$. The endpoints v_1 and v_{12} have degree one. The order in which the vertices are encountered in following along the knot is 2, 3, 6, 7, 10, 11, 5, 4, 9, 8, 2. A nontrivial link in an arc-with-chords in standard position is shown in fig. 2(b). Number the vertices along the x-axis in the figure by $0 = v_1 < \ldots < v_{10} = 1$. The endpoints v_1 and v_{10} have degree 1. One component of the link has vertices with subscripts 2, 3, 7, 6, 2 and the other 4, 5, 8, 9, 4.

4. Twisting

Two types of twists arise in the ARM, fixed and free twists. Fixed twists arise from the torsional angles along the backbone of the protein. Free twists occur because of the three-dimensional structure of the protein. Each of the strips in the twisted surface shown in fig. 1(a) appears flat. In fig. 1(b), there are a number of twists. These are free twists.

The movement of the twisted surface by ambient isotopy to a standard position may introduce extra twists. For example, fig. 3 shows a "flipped connection" obtained by flipping a connection around the backbone and over the top. A requirement that the backbone have minimal twisting may remove these extra twists.

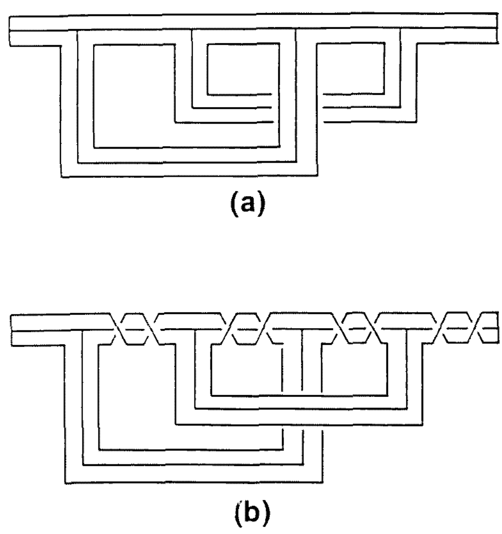


Fig. 3. (a) A twisted surface with two conditions. (b) The same surface with one connection flipped over the backbone.

The uniqueness of the projection graph means that it will remain invariant under changes in crossings and twists. The example of a "flipped connection" shows that crossings and twists are related and cannot independently be shown to be invariant.

References

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