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Topological subtleties for molecular movies

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ABSTRACT

Synchronous movies permit visual analysis of shape perturbation during molecular simulations. The molecule is conceptualized as a knot and modeled as a spline curve. As the molecule writhes, the graphics approximation in each frame should display an ambient isotopic image of the perturbing spline. These graphics approximations raise subtleties for correctly rendering the embedding. A cautionary example was discovered through visualization experiments and the relevant characteristics are formally proved.

1. Introduction

For a molecular movie, a piecewise linear (PL) curve is created as an ambient isotopic approximation of an initial static spline. The frames of the movie are then based upon this PL approximation. Topological artifacts could be introduced. Consider the spline curve **c** depicted in Fig. 1(a) and its PL approximation, **k** of Fig. 1(b). Both **c** and **k** are the knot 4_1 and are defined by the same set of vertices, $\mathcal{P}$. In this example, a vertex of $\mathcal{P}$ is translated to produce $\mathbf{k}^*$, which is still 4_1, as shown in Fig. 1(c). However, the spline defined by these perturbed vertices is the unknot $\mathbf{c}^*$ of Fig. 1(d). A molecular movie using the incorrect embedding of Fig. 1(c) could mislead the viewer.[2]

During development of computer animations, attention to the appropriate embedding can be overlooked. For performance reasons, it is common to assume that an initial PL approximation suffices for all subsequent movements of the spline. Sufficient conditions have been given [14] where this prevails, but we provide a cautionary example outside those limits. Particularly poignant about this example is that the change of

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[2] The images of Figs. 1(c) and 1(d) were taken under slightly different projections than those of Figs. 1(a) and 1(b) to more clearly show the embeddings.

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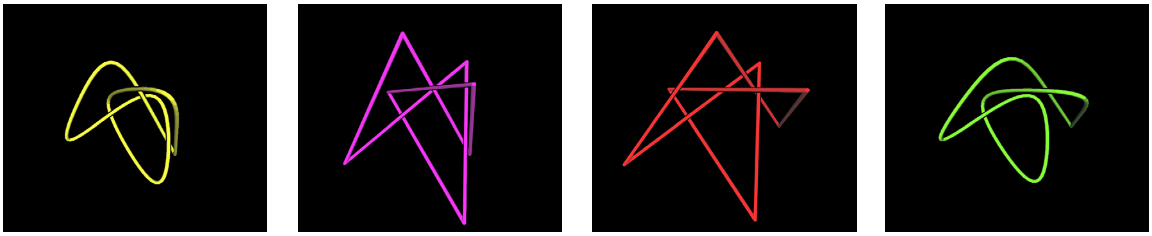

(a) Spline 4_1, $\mathbf{c}$ (b) PL 4_1, $\mathbf{k}$ (c) PL 4_1, $\mathbf{k}^*$ (d) Spline Unknot $\mathbf{c}^*$

Fig. 1. Comparing embedded spline curves to their approximated images.

embedding does not occur for the PL approximations, only the splines, so that the viewer could be misled, since only the PL approximations are rendered.

2. Related work

The term 'molecular movies' includes "... molecular animations ..." [22]. A contemporary treatment of knots and molecules [26] provided motivation for the visualization software [21] used here to explore topologically correct computer animation of knots.

The preservation of topological characteristics in computational applications is of contemporary interest [1–3,8,9,12–15,17,20]. Sufficient conditions for a homeomorphism between a Bézier curve and its control polygon have been studied [24], while topological differences have also been shown [5,18,25]. Sufficient conditions were given to insure that perturbations of the control points maintain isotopic equivalence of the perturbed splines [4]. There is an example of a PL structure that becomes self-intersecting while the associated Bézier curve remains simple [7].

The standard definition for a Bézier curve [25] of degree n is expressed by $\mathcal{B}(t)$, with control points $P_m \in \mathbb{R}^3$ with

$$\mathcal{B}(t) = \sum_{m=0}^{n} \binom{n}{m} t^m (1-t)^{n-m} P_m, t \in [0,1].$$

The curve formed by PL interpolation on $\mathcal{P} = \{P_0, P_1, \ldots, P_n\}$ is called the *control polygon*.

3. The defining data for the example

Consider the points $v_0, v_1, \ldots, v_7$, listed cyclically as (with $v_7 = v_0$):

$$(1.3076, -3.3320, -2.5072), (-1.3841, 4.6826, 0.9135), (-3.2983, -4.0567, 2.6862),$$
$$(-0.1233, 2.7683, -2.4636), (3.9080, -4.5334, 1.2264), (-3.9360, -0.4383, -0.9834),$$
$$(3.2182, 4.2961, 2.1125).$$

Let $\mathcal{P} = \{v_0, v_1, \ldots, v_7\}$ be the set of control points defining a closed Bézier curve. We iteratively inserted new control points as midpoints of this initial control polygon and observed that the generated Bézier curves approached the initial control polygon. Note that this process preserves the embedding of the initial control polygon. This strategy was motivated by experimental evidence that low degree curves were unlikely to display the expected artifact, while also wishing to minimize the number of relevant edges. Fig. 1(a) shows the 112 degree Bézier curve created after 4 iterations of inserting midpoints, with the associated control point, $\mathbf{k}$ shown in Fig. 1(b).

A linear perturbation of v_0 produces an embedding artifact. The vertex v_0 is translated to (1.9817, −1.7646, −4.5897), denoted by v_0', while vertices $v_1, \ldots v_6$ remain fixed, as shown by $\mathbf{k}^*$ in Fig. 1(c). The PL knots remain ambient isotopic, but the spline $\mathbf{c}$ is changed from the knot 4_1 to the unknot, $\mathbf{c}^*$, depicted in Fig. 1(d), with a proof in Section 4.

4. Topological comparisons

The following three subsections show that

- the initial and perturbed PL curves are both ambient isotopic to the knot 4_1,
- the initial Bézier curve is ambient isotopic to the knot 4_1,
- the perturbed Bézier curve is ambient isotopic to the trivial knot.

4.1. PL curves and ambient isotopy

Simplicity of $\mathbf{k}$ is a necessary condition for $\mathbf{k}$ to be a knot and can be shown by elementary calculations on each pair of line segments.[3] It is sufficient to consider merely the vertices of $\mathcal{P}$, since all added control points are on the edges of $\mathcal{P}$. Considering the regular projection [19] shown in Fig. 1(b), Reidemeister moves of Type 2b [19] were invoked to establish $\mathbf{k} = 4_1$ [19]. The simplicity of $\mathbf{k}^*$ follows from a trivial geometric argument showing that no self-intersections are introduced by the translation of v_0 to v_0'.

4.2. Nontrivial knot

For the nontrivial knottedness of $\mathbf{c}$, we start from a projection obtained by taking each z-coordinate to be zero. We used the simplex search method [16] and Horner's method to find pairs to find 4 crossings:

$$(-0.13, 0.93, -0.69), (-0.13, 0.93, -1.29) \ \& \ (-0.44, 1.82, -0.29), (-0.44, 1.82, 0.52)$$
$$(-1.87, -1.0, 0.43), (-1.87, -1.0, -0.34) \ \& \ (1.88, -1.06, -0.52), (1.88, -1.06, -1.13).$$

Visual inspection of the knot diagram led to identification of the knot 4_1.

4.3. Resultant trivial knot

For the unknottedness[4] of $\mathbf{c}^*$, again project onto the plane $z = 0$ and compute crossings:

$$(0.83, 0.44, -2.71), (0.83, 0.44, -1.21) \ \& \ (-0.04, 2.09, -1.28), (-0.04, 2.09, 0.68);$$
$$(-1.87, -1.0, 0.43), (-1.87, -1.0, -0.34) \ \& \ (2.05, -1.41, -0.35), (2.05, -1.41, -4.19).$$

The two consecutive under crossings, followed by two consecutive over crossings, imply that $\mathbf{c}^*$ is simple and unknotted.

5. Visual experiments by inserting midpoints

Hundreds of visual experiments were conducted to produce the example in Section 3. Fig. 2 shows the visual evidence suggesting convergence from iteratively inserting midpoints as new control points. This

[3] Some computational efficiency is gained by tests with oriented line segments [11] These calculations were independently verified by graphics students, as is acknowledged, with appreciation.
[4] Calculation of the instantaneous time for the change of knot type follows from previous results on self-intersections of splines [3] and can be solved with standard numerical algorithms.

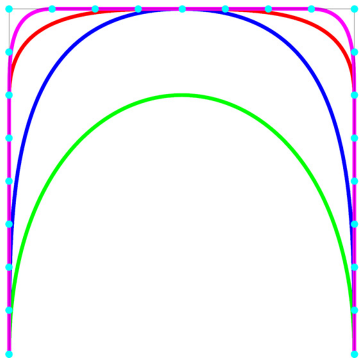

Fig. 2. Midpoint insertions.

convergence is formally proved as it is expected to be of interest in drawing rigorous conclusions from the graphics displays of future experiments.

The initial objective was to create a PL trefoil of only 6 edges defining a non-trivially knotted spline. All these attempts failed. When the number of edges was increased to 7, non-trivially knotted splines were generated. A similar example with only 6 edges is not precluded. Any example with more than 7 edges would require analysis beyond the scope of this work. Generating these examples is very time consuming, with most attempts being failures. In summary, the choice of 7 edge is an experimental balance. It is noted that 7 edges is minimal to create a PL instance of 4_1 [6].

6. Convergence theorem

The technique of iteratively adding midpoints as new control points starts with a given PL curve ℓ and generates a sequence of spline curves $\mathbf{b}^{(n)}$, which is shown to converge to ℓ. This proof is prompted by recognition of the pervasive interest in computer graphics on convergence properties between an object and its PL approximation [25]. Let $\mathbf{N}$ denote the natural numbers $\{1, 2, 3, \ldots\}$.

For $k \in \mathbf{N}$, consider the central binomial coefficient [10],

$$\binom{2k}{k}.$$

Lemma 6.1. *For $k \in \mathbf{N}$,*

$$\binom{2k}{k} \leq \frac{4^k}{\sqrt{2k+1}}.$$

Proof. The proof is by induction, by a relation informally attributed to P. Erdos [10]. □

The following notation has previously appeared [23] and is central to the convergence result that follows. For $k \in N$, let

$$N_1(2k) = \binom{2k}{k} \frac{2k}{2^{2k+2}}.$$

Lemma 6.2. *For $k \in N$,*

$$N_1(2k) < \frac{k}{2\sqrt{2k+1}}.$$

Proof. Invoke Lemma 6.1 on

$$N_1(2k) = \binom{2k}{k} \frac{2k}{2^{2k+2}} < \frac{4^k}{\sqrt{2k+1}} \frac{2k}{4^{k+1}} = \frac{k}{2\sqrt{2k+1}}. \qquad \square$$

Let b_i, with $i = 0, 1, \ldots d$ denote the control points of a degree d Bézier curve $\mathbf{b}$ and $b_i^{(n)}$ denote the control points for the curve $\mathbf{b}^{(n)}$, created after the n-th insertion of midpoints, with indexing $i = 1, 2, \ldots, d * 2^n$, with $n \in \{0\} \cup \mathbf{N}$. The notation employed here of $\Delta_2 \mathbf{b} = b_{i-1} - 2b_i + b_{i+1}$ has previously appeared [23].

Lemma 6.3. *For $n \in \{0\} \cup N$,*

$$\|\Delta_2 \mathbf{b}^{(n)}\|_1 \leq 2^{-n} \|\Delta_2 \mathbf{b}\|_1.$$

Proof. There are 2 cases to consider.

Case 1: For any newly added point $\mathbf{b}^{(n)}$ that is a midpoint,

$$b_{i-1}^{(n)} - 2b_i^{(n)} + b_{i+1}^{(n)} = 0,$$

so that these terms can be ignored in the computation of $\|\Delta_2 \mathbf{b}\|_1$.

Case 2: For any point, $b_i^{(n)}$ of $\mathbf{b}^{(n)}$ that is an original control point of $\mathbf{b}$, it suffices to consider each component separately. In each component, the distance between its preceding point and subsequent point have been reduced by a factor of 2^{-n} from the corresponding distance in the original control polygon. $\square$

Theorem 6.1. *For iterative insertion of midpoints, the distance between the control polygon and the generated Bézier curves converges to zero.*

Proof. Consider the published result [23] giving an upper bound for the distance between a univariate Bézier curve p of degree d and its control polygon ℓ of

$$\|p(t) - \ell(t)\|_{\infty,[0,1]} \leq N_1(d) \|\Delta_2 \mathbf{b}\|_1. \tag{1}$$

For n subdivisions, evaluate Inequality (1) for degree $d * 2^n$ and $\mathbf{b}^{(n)}$, apply Lemmas 6.2 and 6.3 and take the limit as $n \to \infty$. $\square$

7. Conclusion and future work

For synchronous visualizations of writhing molecules, a cautionary example is presented of different knot types between a polynomial curve and its rendering. The experimentally generated example relies upon a sequence of Bézier curves that converge to a given PL curve, with the convergence formally proven for possible further graphics applications. Concepts from knot theory are fundamental to the results. Questions persist as to whether 'more natural' examples could be generated with fewer control points and lower degree.

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