

Untangling Knots Through Curve Repulsion



Department of Mathematics
University of Oxford
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Abstract

Curves are one of the fundamental objects in geometry and engineering, yet most analysis of curves often disregard their physical characteristics such as their spatial volume or uncrossability. One common situation that such physical characteristics become significant is when one attempts to untangle a knot. An approach to achieve this is to assign an “energy” to a curve such that this energy would increase when two points on “different sides” of a curve are closer, then one continuously deforms the curve to reduce this energy, the expectation being that the curve that achieves minimal energy must be the untangled knot. This dissertation explores numerical methods of achieving this.

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1 Introduction

Shape optimisation is an important idea in engineering, relevant in anywhere from aircraft designs to packaging ramen noodle. One of the simplest and most fundamental shapes to consider is a curve. While curves are simple objects in theory, they prove to be quite difficult to analyse in practice with realistic physics. Even in absence of other objects, one must consider resilience to bending, stretching, and especially, impenetrability against itself. With these physical factors in mind, untangling a knot like the one shown (Figure 1) becomes a very complicated process, especially in a computer simulation. In this dissertation, we explore numerical methods to achieve this.

The main idea is to *assign energy that penalises “physical entanglement”*. Given a parameterised curve $\gamma : M \rightarrow \mathbb{R}^3$ (M being the domain of the parameter, often



Figure 1: A complicated knot in \mathbb{R}^3

an interval), one defines some *curve energy* \mathcal{E} of the form:

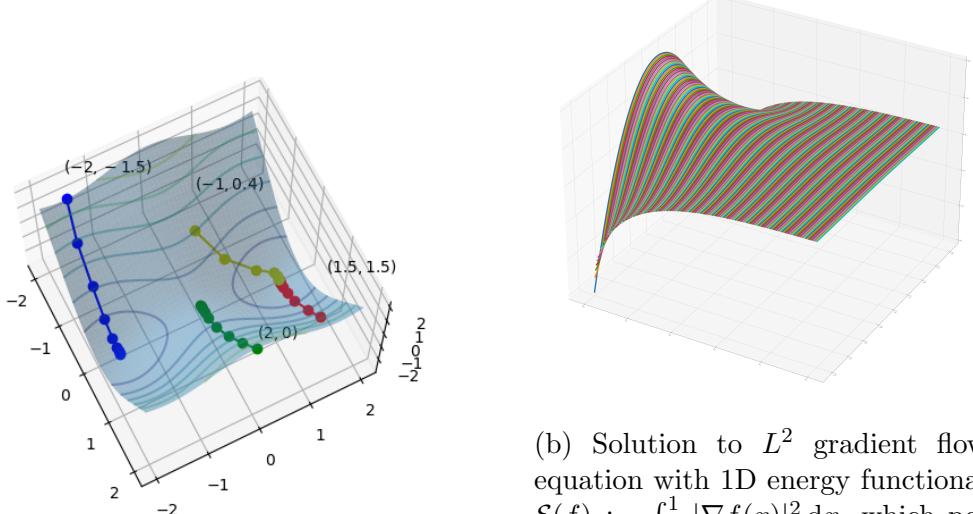
$$\mathcal{E}(\gamma) := \iint_{M^2} k(\gamma_x, \gamma_y) d\gamma_x d\gamma_y \quad (1)$$

where $k(\gamma_1, \gamma_2) \geq 0$ is the *curve energy kernel* such that $k \rightarrow +\infty$ as $|\gamma_1 - \gamma_2| \rightarrow 0^+$.

A naïve choice of k satisfying this condition is $k_S(\gamma_1, \gamma_2) := \frac{1}{|\gamma_1 - \gamma_2|}$. However, it turns out that $k_S \sim O\left(\frac{1}{|\gamma_1 - \gamma_2|}\right)$ as $|\gamma_1 - \gamma_2| \rightarrow 0$ (consider neighbouring points), meaning the \mathcal{E} diverges all continuous curves γ of nonzero measure. This seemingly ill-defined energy, however, may not be the end of story in terms of numerics, and will be explored later.

A more analytically sensible choice of k would be the tangent-point kernel introduced in a paper by Buck and Orloff[1] and later generalised by Yu, Schumacher, and Crane[3].

The next part of the idea is to *reduce \mathcal{E} by continuously deforming the curve* based on a descent method until it reaches a stationary curve, at which, we expect it to be the “unknot” of the original curve. Note that by construction of \mathcal{E} , if the curve is to self-intersect, \mathcal{E} increases, and the descent method encourages the curve to repel, preventing the self-intersection.



(a) SDM applied to $f(x, y) = -3 \cos x + \cos^2 y$ at different initial points.

(b) Solution to L^2 gradient flow equation with 1D energy functional $\mathcal{E}(f) := \int_{-1}^1 |\nabla f(x)|^2 dx$, which penalises variation in function. Note that the solution converges to a function with no variation.

Figure 2: Gradient flow can be understood as a continuous analogue of steepest descent.

2 Curve Energy Reduction via Gradient Flow

Since we pose the problem as continuous reduction of some functional, we need an applicable framework which fits our intention. In our case, **gradient flow equation** seems to be appropriate.

2.1 Motivation of Gradient Flow Equation

For minimising a differentiable function $f : E \subset \mathbb{R}^n \rightarrow \mathbb{R}$, there is a well-known method known as **steepest descent method** (SDM)[2].

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \alpha_k \nabla f(\mathbf{x}^k) \quad (2)$$

Starting from the initial input point \mathbf{x}^0 , at each iteration, input points $\{\mathbf{x}^k\}$ move in the direction of “steepest” decrease, with specified step size $\alpha_k > 0$, reducing the value at evaluation of f . Note that in general, this method is not guaranteed to find the minimiser as shown in Figure (2a). On the other hand, convergence is guaranteed under certain assumptions, for example, convexity and L -smoothness¹ with a certain choice of step size α_k .

Analogously, differential equation known describing the reduction process of a functional $F : \mathcal{X} \rightarrow \mathbb{R}$ (where \mathcal{X} is an inner product function space) can be moti-

¹ $||\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})|| \leq L ||\mathbf{x} - \mathbf{y}||$ for some constant $L > 0$

vated. Starting from (2), replacing \mathbf{x}^k by f_k and $\nabla f(\mathbf{x}^k)$ by $\text{grad}_{\mathcal{X}} F(f_k)$

$$f_{k+1} = f_k - \alpha_k \text{grad}_{\mathcal{X}} F(f_k) \quad (3)$$

Now think of f_k as “snapshots” at certain time $t = t_k$. Without loss of generality, let $\alpha_k \equiv 1$.² Dividing (3) by time step $\Delta t := t_{k+1} - t_k$, and taking the limit as $\Delta t \rightarrow 0$, we acquire the **gradient flow equation**[3].

$$\frac{\partial f}{\partial t} = - \text{grad}_{\mathcal{X}} F(f) \quad (4)$$

where index k transforms to “time” variable t .

Note that grad of a functional is not defined yet. This depends on the inner product function space \mathcal{X} (eg. L^2 , H^1 , …) of interest.

2.2 Gradient of Functional

Gradient of a function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ characterises the first-order variation in a certain direction, that is,

$$\forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^n \quad \nabla f(\mathbf{x}) \cdot \mathbf{y} = \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} f(\mathbf{x} + \epsilon \mathbf{y}) \quad (5)$$

While this is not a conventional definition of function gradient, it is an appropriate definition.

One could analogously construct the definition of gradient of a functional.

Definition (Gradient of Functional). For a functional $F : \mathcal{X} \rightarrow \mathbb{R}$, define functional gradient $\text{grad}_{\mathcal{X}} F(f)$ as:

$$\langle \text{grad}_{\mathcal{X}} F(f), g \rangle_{\mathcal{X}} = \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} F(f + \epsilon g) \quad (6)$$

where \mathcal{X} is an inner product space.

3 Tangent-Point Energy

Given a curve $\gamma : M \rightarrow \mathbb{R}^3$, a sensible choice of curve energy is the tangent-point energy[3].

Definition (Tangent-Point Energy). For a continuously differentiable parameterised curve $\gamma : M \rightarrow \mathbb{R}^3$, define **tangent-point energy** as:

$$\mathcal{E}_{\beta}^{\alpha}(\gamma) := \iint_{M^2} k_{\beta}^{\alpha}(\gamma_x, \gamma_y, \mathbf{T}_x) d\gamma_x d\gamma_y \quad (7)$$

²This is justified by taking a different time scale; essentially nondimensionalisation. Also $\alpha_k \sim O(1)$ as $k \rightarrow \infty$ (eg. $\alpha = L^{-1}$ for L -smooth optimisation) is in fact a realistic choice.

where $\mathbf{T}_x := \frac{d\gamma_x}{dt} / | \frac{d\gamma_x}{dt} |$ is the unit tangent vector at γ_x along the curve, and **tangent-point kernel** is given as:

$$k_\beta^\alpha(\mathbf{p}, \mathbf{q}, \mathbf{T}) := \frac{|\mathbf{T} \wedge (\mathbf{p} - \mathbf{q})|^\alpha}{|\mathbf{p} - \mathbf{q}|^\beta} \quad (8)$$

α and β are parameters one could choose, but for tangent-point energy to be well-defined, one may choose them to satisfy $\alpha > 1$ and $\beta \in [\alpha + 2, 2\alpha + 1]$.

Note that choosing $\alpha = 2$ and $\beta = 4$ results in the original tangent-point energy by Buck and Orloff[1].

The choice of parameters α and β changes the behaviour of the tangent-point energy as stated in the following lemma.

Lemma 1. *Tangent-point energy \mathcal{E}_β^α defined as (7) is scale invariant with respect to the curve if and only if $\beta = \alpha + 2$. Moreover, if $\beta > \alpha + 2$, then \mathcal{E}_β^α scales inversely with the curve.*

Proof. Take a parameterised curve $\gamma : M \rightarrow \mathbb{R}^3$ and $\Gamma := c\gamma$, a curve scaled by factor $c > 0$ of γ . Note that the unit tangent vector is identical for γ and Γ , that is, $\mathbf{T}_x := \frac{d\gamma_x}{dt} / | \frac{d\gamma_x}{dt} | = \frac{d\Gamma_x}{dt} / | \frac{d\Gamma_x}{dt} |$

Then,

$$\frac{k_\beta^\alpha(\gamma_x, \gamma_y, \mathbf{T}_x)}{k_\beta^\alpha(\Gamma_x, \Gamma_y, \mathbf{T}_x)} = \frac{|\gamma_x - \gamma_y|^\alpha}{|\Gamma_x - \Gamma_y|^\beta} = c^{\beta-\alpha} \quad (9)$$

Also note that

$$d\Gamma = c d\gamma \quad (10)$$

So, we deduce from (7),

$$\mathcal{E}_\beta^\alpha(\Gamma) = c^{\alpha-\beta+2} \mathcal{E}_\beta^\alpha(\gamma) \quad (11)$$

Hence, \mathcal{E}_β^α is scale invariant with respect to the curve if and only if $\alpha - \beta + 2 = 0$, and if $\beta > \alpha + 2$, \mathcal{E}_β^α scales at the rate of $O(\frac{1}{c^{\beta-(\alpha+2)}})$ as $c \rightarrow \infty$. \blacksquare

4 Functional Reduction to Function Reduction

5 Fourier Series

For a continuous 2π -periodic 1D function $f : \mathbb{R} \rightarrow \mathbb{R}$ (where one only needs to define f on $[0, 2\pi)$), there exists a Fourier series representation:

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} (a_n \cos(nx) + b_n \sin(nx)) \quad (12)$$

$$= \sum_{n=-\infty}^{\infty} c_n e^{inx} \quad (13)$$

where the two representations are equivalent. The coefficients are given by

$$a_n = \frac{1}{\pi} \int_0^{2\pi} f(x) \cos(nx) dx \in \mathbb{R} \quad (14)$$

$$b_n = \frac{1}{\pi} \int_0^{2\pi} f(x) \sin(nx) dx \in \mathbb{R} \quad (15)$$

$$c_n = \frac{1}{2\pi} \int_0^{2\pi} f(x) e^{-inx} dx \in \mathbb{C} \quad (16)$$

One may justify the use of Fourier series representation by the following theorem:

Theorem 2 (Fourier Convergence Theorem). *Lorem ipsum dolor sit amet, consecetuer adipiscing elit. Ut purus elit, vestibulum ut, placerat ac, adipiscing vitae, felis. Curabitur dictum gravida mauris. Nam arcu libero, nonummy eget, consectetuer id, vulputate a, magna. Donec vehicula augue eu neque. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas. Mauris ut leo. Cras viverra metus rhoncus sem. Nulla et lectus vestibulum urna fringilla ultrices. Phasellus eu tellus sit amet tortor gravida placerat. Integer sapien est, iaculis in, pretium quis, viverra ac, nunc. Praesent eget sem vel leo ultrices bibendum. Aenean faucibus. Morbi dolor nulla, malesuada eu, pulvinar at, mollis ac, nulla. Curabitur auctor semper nulla. Donec varius orci eget risus. Duis nibh mi, congue eu, accumsan eleifend, sagittis quis, diam. Duis eget orci sit amet orci dignissim rutrum.*

Now, for a vector-valued function such as a parameterised curve $\gamma : \mathbb{R} \rightarrow \mathbb{R}^3$, one could write 3D Fourier series, one for each coordinate:

$$\mathbf{f}(x) = \frac{1}{2} \begin{pmatrix} a_{1,0} \\ a_{2,0} \\ a_{3,0} \end{pmatrix} + \sum_{n=1}^{\infty} \begin{pmatrix} a_{1,n} & b_{1,n} \\ a_{2,n} & b_{2,n} \\ a_{3,n} & b_{N,n} \end{pmatrix} \begin{pmatrix} \cos(nx) \\ \sin(nx) \end{pmatrix} \quad (17)$$

$$= \sum_{n=-\infty}^{\infty} \begin{pmatrix} c_{1,n} \\ c_{2,n} \\ c_{3,n} \end{pmatrix} e^{-inx} \quad (18)$$

where the coefficients $\{a_{i,n}\}$, $\{b_{i,n}\}$, $\{c_{i,n}\}$ are given by

$$a_{i,n} = \frac{1}{\pi} \int_0^{2\pi} f_i(x) \cos(nx) dx \in \mathbb{R} \quad (19)$$

$$b_{i,n} = \frac{1}{\pi} \int_0^{2\pi} f_i(x) \sin(nx) dx \in \mathbb{R} \quad (20)$$

$$c_{i,n} = \frac{1}{2\pi} \int_0^{2\pi} f_i(x) e^{-inx} dx \in \mathbb{C} \quad (21)$$

for $i = 1, 2, 3$.

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