### Untangling Knots Through Curve Repulsion



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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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#### Part I

#### Introduction

Shape optimisation is an important idea in engineering, use 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 resiliance 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.

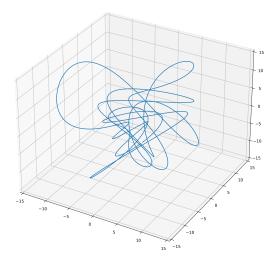


Figure 1: A complicated knot in  $\mathbb{R}^3$ 

The main idea is to assign energy that penalises "physical entanglement". Given a parameterised curve  $\gamma: M \to \mathbb{R}^3$  (M being the domain of the parameter), one defines some curve energy  $\mathcal{E}$  of the form:

$$\mathcal{E}(\boldsymbol{\gamma}) := \iint_{M^2} k\left(\boldsymbol{\gamma}_x, \boldsymbol{\gamma}_y\right) \, \mathrm{d}\gamma_x \, \mathrm{d}\gamma_y \tag{1}$$

where  $k(\gamma_1, \gamma_2) \geq 0$  is the curve energy kernel such that  $k \to +\infty$  as  $|\gamma_1 - \gamma_2| \to 0^+$ . 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  $|\gamma_1 - \gamma_2| \to 0$  (consider neighbouring points), meaning the  $\mathcal{E}$  diverges all continuous curves  $\gamma$  of nonzero measure.<sup>1</sup>

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.

<sup>&</sup>lt;sup>1</sup>This seemingly ill-defined energy, however, will be explored later.

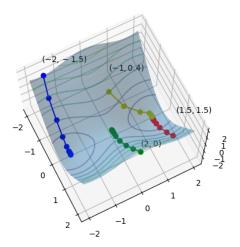


Figure 2: SDM applied to  $f(x,y) = -3\cos x + \cos^2 y$  at different initial points.

#### 1 Preamble

#### 1.1 Steepest Descent to Gradient Flow Equation

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

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

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. On the other hand, convergence is guaranteed under certain assumptions, for example, convexity and L-smoothness with a certain choice of step size  $\alpha_k$ .

Analogously, differential equation known describing the reduction process of a functional  $F: \mathcal{F} \to \mathbb{R}$  (where  $\mathcal{F}$  is some set of functions) can be motivated. Starting from (2), replacing  $\mathbf{x}^k$  to  $f_k$  and  $\nabla f(\mathbf{x}^k)$  to  $\operatorname{grad}_X F(f_k)$ 

$$f_{k+1} = f_k - \alpha_k \operatorname{grad}_X F(f_k)$$
(3)

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

$$\frac{\partial F}{\partial t} = -\operatorname{grad}_X F \tag{4}$$

where index k transforms to "time" variable t.

Note that grad of a functional is not defined yet. This depends on the function space X (eg.  $L^2$ ,  $H^1$ , ...) of interest.

<sup>&</sup>lt;sup>2</sup>This is justified by taking a different time scale; essentially nondimensionalisation.

# Part II Curve Energy Reduction via Gradient Flow

#### Part III

## Functional Reduction to Function Reduction

#### References

- [1] Gregory Buck and Jeremey Orloff. "A simple energy function for knots". In: *Topology and its Applications* 61.3 (Feb. 1995), pp. 205–214. DOI: 10.1016/0166-8641(94)00024-w.
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