Untangling Knots Through Curve Repulsion

Joo-Hyun Paul Kim

March 2, 2023

What the curious folks ponder about

Introduction

A Cool Knot

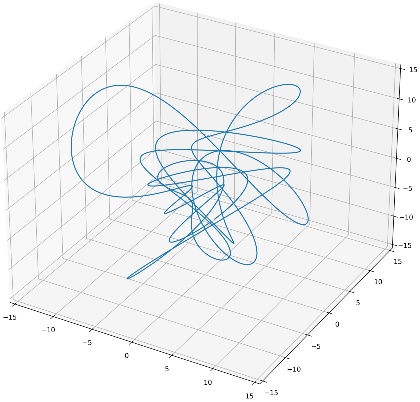

Figure: Imagine your earphones getting tangled like this…

Aim

- Finding a "homotopy" from a knot to an unknot.

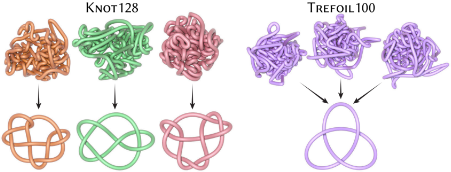

Figure: Unknots of test knots.[3]

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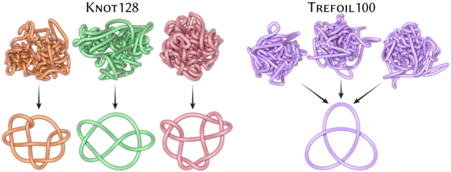

Figure: Unknots of test knots.[3]

- “Avoiding self-intersection”

General Strategy

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2. Attempt to decrease the curve energy by continuously deforming the curve.
   - We evolve the curve according to the gradient flow equation.
   - There is a freedom in choosing the "gradient" here.
3. We expect the stationary state to be the "unknot"
   - Or at least a simpler state...

Tangent-Point Energy

Defining Curve Energy

Given an (arc-length parameterised) curve $\gamma : M \to \mathbb{R}^3$, we wish to assign energy of the form:

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

such that

- $\mathcal{E}$ is very high when two non-neighbouring points are very close.

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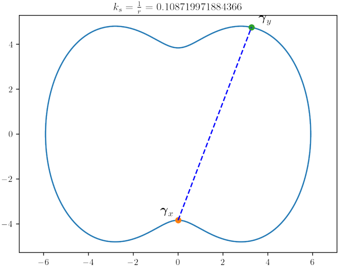
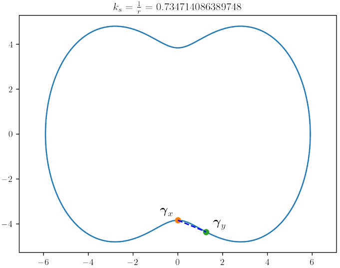
A naïve choice is $k\left(\gamma_x, \gamma_y\right) := \frac{1}{||\gamma_x - \gamma_y||}$

Pitfall of the “Simple Energy”

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





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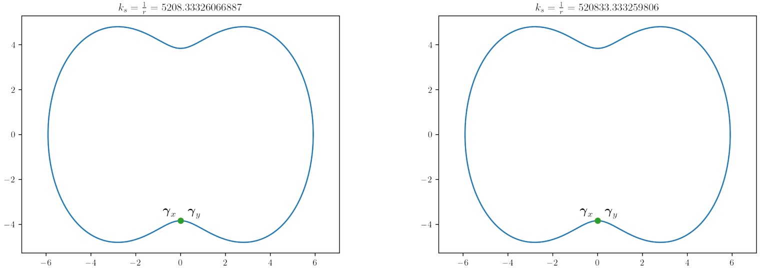

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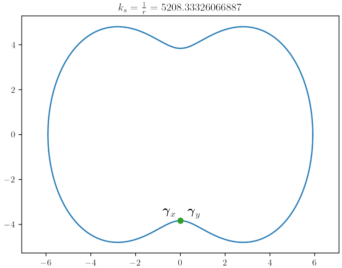

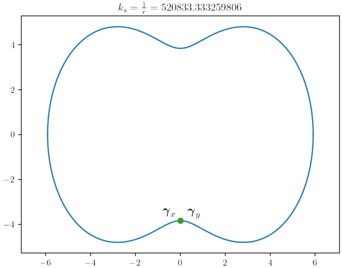

This energy is not well-defined for a lot of curves!

Buck-Orloff Tangent-Point Energy

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Definition (Buck-Orloff Tangent-Point Energy)

For a smooth curve γ, define

$$\mathcal{E}(\gamma) := \iint_{M^2} k_4^2\left(\gamma_x, \gamma_y, \mathbf{T}_x\right)\, \mathrm{d}\gamma_x\, \mathrm{d}\gamma_y$$

where $\mathbf{T}_x$ is the unit tangent vector at γ_x, with the kernel defined as

$$k_4^2(\mathbf{p}, \mathbf{q}, \mathbf{T}) := \frac{||\mathbf{T} \wedge (\mathbf{p} - \mathbf{q})||^2}{||\mathbf{p} - \mathbf{q}||^4}$$

as **Buck-Orloff Tangent-Point Energy**.[1]

Intuition

What is the intuition behind the kernel $k_4^2(\mathbf{p}, \mathbf{q}, \mathbf{T}) := \frac{||\mathbf{T} \wedge (\mathbf{p}-\mathbf{q})||^2}{||\mathbf{p}-\mathbf{q}||^4}$?

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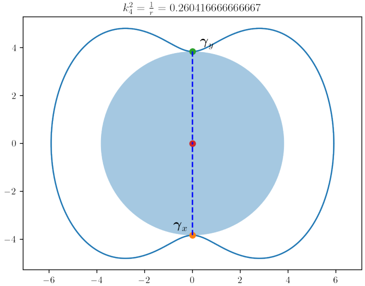

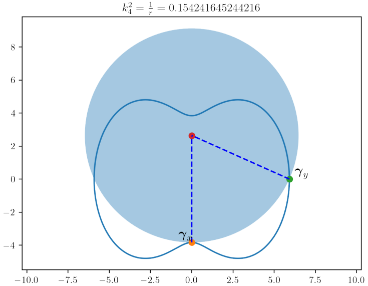

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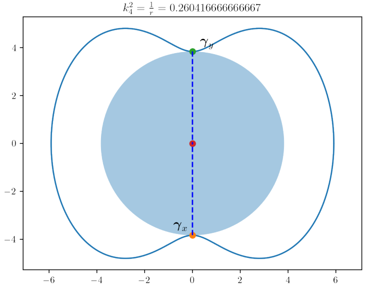

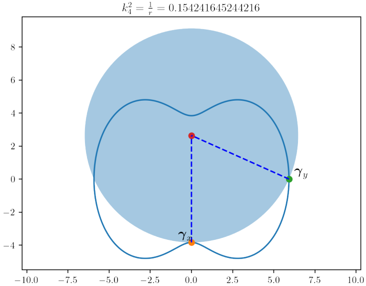

Remark

Note that closer does not necessarily mean the kernel is larger.

Intuition

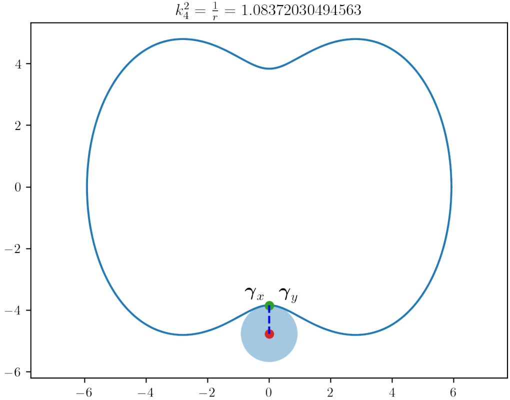

Figure: When two points are very close, the kernel converges to the curvature of the curve.

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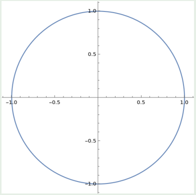

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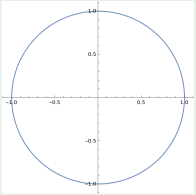

Then write:

$$\begin{cases} \gamma_x(\theta) = (\cos\theta, \sin\theta, 0) \\ \gamma_y(\phi) = (\cos\phi, \sin\phi, 0) \\ \mathbf{T}_x(\theta) = (-\sin\theta, \cos\theta, 0) \end{cases}$$

Example (Cont.)

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Substituting to Buck-Orloff Tangent-Point energy formula:

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Using a few identities:

$$\mathcal{E}(\gamma) = \int_{\theta=0}^{2\pi} \int_{\phi=0}^{2\pi} \frac{||\mathbf{T}_x||^2 ||\gamma_x - \gamma_y||^2 - \left(\mathbf{T}_x \cdot (\gamma_x - \gamma_y)\right)^2}{||\gamma_x - \gamma_y||^4} \, d\theta \, d\phi$$

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$$= \int_{\theta=0}^{2\pi}\int_{\phi=0}^{2\pi} \frac{\sin^2\frac{\theta-\phi}{2}}{(-1+\cos(\theta-\phi))^2}\,\mathrm{d}\theta\,\mathrm{d}\phi \tag{3}$$

$$= \int_{\theta=0}^{2\pi}\int_{\phi=0}^{2\pi} \frac{\sin^2\frac{\theta-\phi}{2}}{\sin^4\frac{\theta-\phi}{2}}\,\mathrm{d}\theta\,\mathrm{d}\phi \tag{4}$$

$$= \pi^2 \tag{5}$$

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Remark

Note that (4) suggests the order at "singularity" is inverse-square.

General Tangent-Point Energy

A more general form of tangent-point energy comes from Yu, Schumacher, and Crane [3]:

Definition (Generalised Tangent-Point Energy)

$$\mathcal{E}_\beta^\alpha(\gamma) := \iint_{M^2} \frac{||\mathbf{T}_x \wedge (\gamma_x - \gamma_y)||^\alpha}{||\gamma_x - \gamma_y||^\beta} \, \mathrm{d}\gamma_x \, \mathrm{d}\gamma_y$$

where $\alpha > 1$ and $\beta \in [\alpha + 2, 2\alpha + 1)$

Remark

When $\alpha = 2$ and $\beta = 4$, we are back to Buck-Orloff.

Gradient Flow

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Remark

cf) For minimising a function $f : \mathbb{R}^n \to \mathbb{R}$, one may consider

$$\frac{\partial \mathbf{x}}{\partial t} = -\nabla f(\mathbf{x})$$

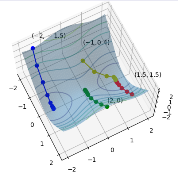

Figure: Steepest Descent [2]

Gradient in Space of Function?

(Gradient of Function)
$\nabla f(\mathbf{x})$ is such that for all $\mathbf{y} \in \mathbb{R}^n$

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$\mathrm{grad}_X E(f)$ is such that for all $g \in X$,

$$\langle\langle \mathrm{grad}_X E, g \rangle\rangle_X = \frac{\partial}{\partial \epsilon} E(f + \epsilon g) \Big|_{\epsilon=0}$$

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Remark

For $X = L^2$, $(\operatorname{grad}_X E)(f)$ is the first order variation from f with respect to ϵ.

Example: Dirichlet Energy in 1D

Definition (1D Dirichlet Energy)

For a differentiable function $f : \mathcal{I} \to \mathbb{R}$, define **1D Dirichlet energy**

$$E_D(f) := \int_{\mathcal{I}} |\nabla f(x)|^2 \, \mathrm{d}x = \int_{\mathcal{I}} |f'(x)|^2 \, \mathrm{d}x$$

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Remark

Dirichlet energy is high for function f that varies a lot, and minimised by any constant function.

Example: L^2 Gradient Flow of Dirichlet Energy

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(for suitable boundary condition if finite interval)

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Lemma (L^2 Gradient of Dirichlet Energy)

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(for suitable boundary condition if finite interval)

Then the gradient flow equation for Dirichlet energy becomes:

$$\frac{\partial f}{\partial t} = \Delta f \tag{6}$$

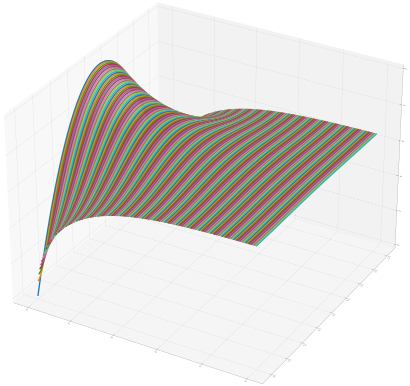

Figure: Solution to L^2 Gradient Flow Equation for Dirichlet Energy (AKA Heat Equation)

Dirichlet Gradient Flow in Other Function Space

Definition (Famous Inner Product Function Spaces)

- $L^p = \left\{ f \middle| \left(\int |f|^p \, \mathrm{d}x \right)^{1/p} < \infty \right\}$
  - $\langle\langle f, g \rangle\rangle_{L^2} = \int fg \, \mathrm{d}x$
- $p = 2$ Sobolev Space $H^k = \left\{ f \middle| \sum_{i=0}^{k} \int \left| \mathcal{D}^{(i)} f \right|^2 \, \mathrm{d}x < \infty \right\}$
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- $L^2 = H^0$: $\frac{\partial f}{\partial t} = -\Delta f$
- H^1: $\frac{\partial f}{\partial t} = -f$
- H^{-1}: $\frac{\partial f}{\partial t} = -\Delta^2 f$
  - $\langle\langle f, g \rangle\rangle_{H^{-1}} = \langle\langle \Delta^{-1} f, \Delta^{-1} g \rangle\rangle_{H^1}$
- H^2: $\frac{\partial f}{\partial t} = \Delta^{-1} f$

Curve Repulsion

Gradient Flow on Tangent-Point Energy

We now take the tangent-point energy and gradient flow together:

$$\frac{\partial \gamma}{\partial t} = -\operatorname{grad}_{L^2} \mathcal{E} \tag{7}$$

with $\gamma\big|_{t=0}$ is the tangled curve.

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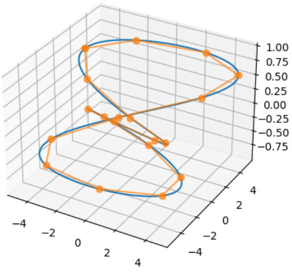

Figure: Discretised Curve

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For numerical solution, one discretises the curve. Enumerate each point as $\mathbf{x}_0, \mathbf{x}_1, \cdots, \mathbf{x}_{J-1}$, and write $\mathbf{\Gamma}$ for the resulting polygonal curve.

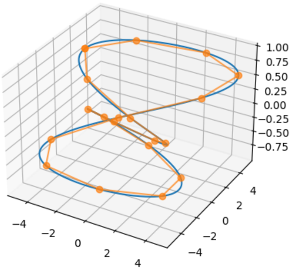

Figure: Discretised Curve

Subtlety

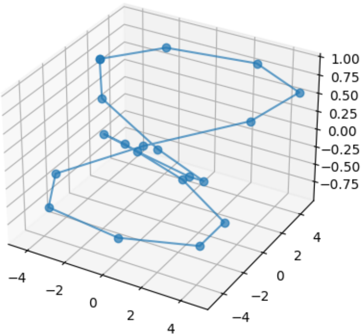

Figure: Tangent-point energy is not well-defined for polygonal curves.

Energy Discretisation

Note the form of tangent-point energy:

$$\mathcal{E}_{\beta}^{\alpha}(\gamma) := \iint_{M^2} k_{\beta}^{\alpha}\left(\gamma_x, \gamma_y, \mathbf{T}_x\right) \, \mathrm{d}\gamma_x \, \mathrm{d}\gamma_y \tag{8}$$

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Definition (Discretised Energy)

Given a closed curve with discretised points $\mathbf{x}_0, \mathbf{x}_1, \cdots, \mathbf{x}_{J-1}$, define **discretised energy** E as:

$$E(\boldsymbol{\Gamma}) := \sum_{\substack{i,j \in \{0,1,\cdots,J-1\} \\ \mathrm{dist}_{\mathrm{geodesic}}(\boldsymbol{\Gamma}(i),\boldsymbol{\Gamma}(j))>1}} k_{i,j} ||\mathbf{x}_{i+1} - \mathbf{x}_i|| \, ||\mathbf{x}_{j+1} - \mathbf{x}_j||$$

where the discretised kernel $k_{i,j}$ is given by:

$$\frac{1}{4}\left(k_\beta^\alpha\left(x_i, x_j, T_i\right) + k_\beta^\alpha\left(x_i, x_{j+1}, T_i\right) + k_\beta^\alpha\left(x_{i+1}, x_j, T_i\right) + k_\beta^\alpha\left(x_{i+1}, x_{j+1}, T_i\right)\right)$$

Bibliography

[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.

[2] "Chapter 8: Primal and Dual Projected Subgradient Methods". In: *First-Order Methods in Optimization*, pp. 195–245. DOI: 10.1137/1.9781611974997.ch8. eprint: https://epubs.siam.org/doi/pdf/10.1137/1.9781611974997.ch8. URL: https://epubs.siam.org/doi/abs/10.1137/1.9781611974997.ch8.

[3] Chris Yu, Henrik Schumacher, and Keenan Crane. "Repulsive Curves". In: *ACM Transactions on Graphics* 40.2 (Apr. 2021), pp. 1–21. DOI: 10.1145/3439429.