

# Untangling Knots Through Curve Repulsion

Joo-Hyun Paul Kim

March 5, 2023



# What the curious folks ponder about

1 Introduction

2 Tangent-Point Energy

3 Gradient Flow

4 Curve Repulsion

# Introduction

# A Cool Knot

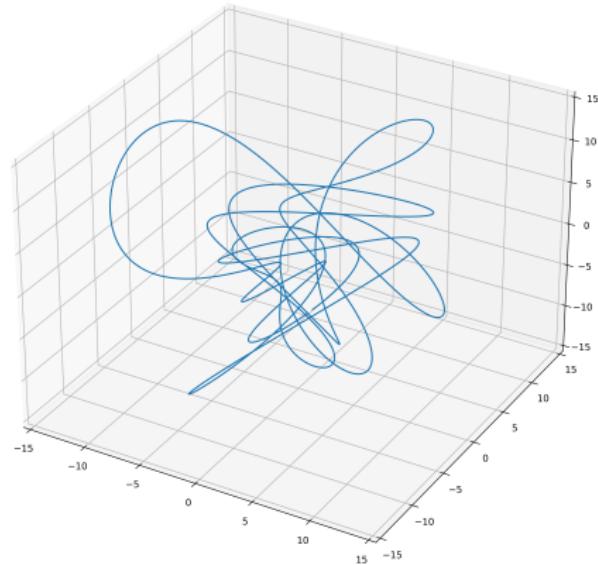


Figure: Imagine your earphones getting tangled like this...

# Aim

- Finding a “homotopy” from a knot to an unknot.

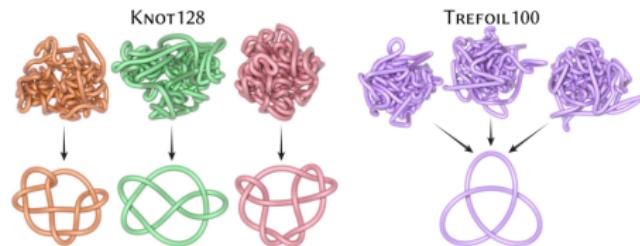


Figure: Unknots of test knots.[3]

# Aim

- Finding a “homotopy” from a knot to an unknot.

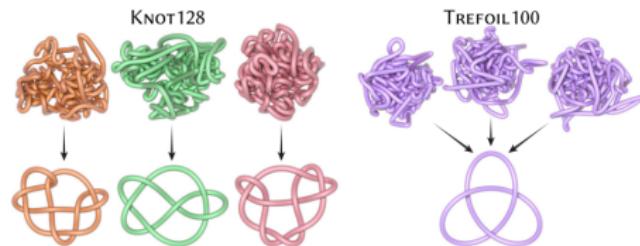


Figure: Unknots of test knots.[3]

- “Avoiding self-intersection”

# General Strategy

- ① Define curve energy; penalizing the closeness of points on a curve.
  - Extreme-closeness of points on curve is a natural characteristic of a tangled curve.

# General Strategy

- ① Define curve energy; penalizing the closeness of points on a curve.
  - Extreme-closeness of points on curve is a natural characteristic of a tangled curve.
- 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.

# General Strategy

- ① Define curve energy; penalizing the closeness of points on a curve.
  - Extreme-closeness of points on curve is a natural characteristic of a tangled curve.
- 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  $\gamma : M \rightarrow \mathbb{R}^3$ , we wish to assign energy of the form:

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

such that

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

# Defining Curve Energy

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

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

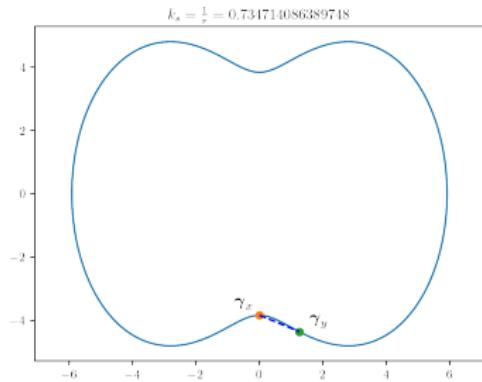
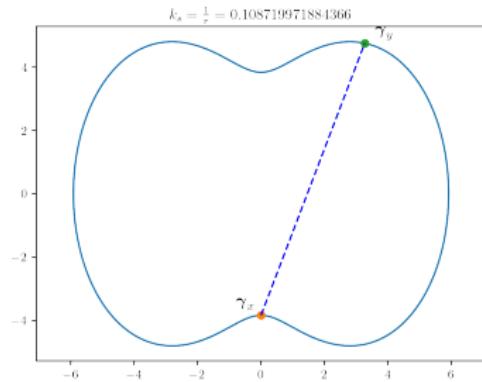
such that

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

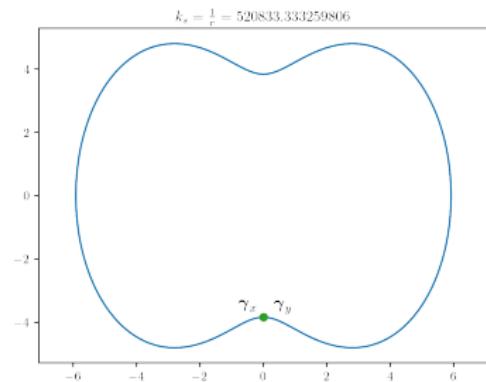
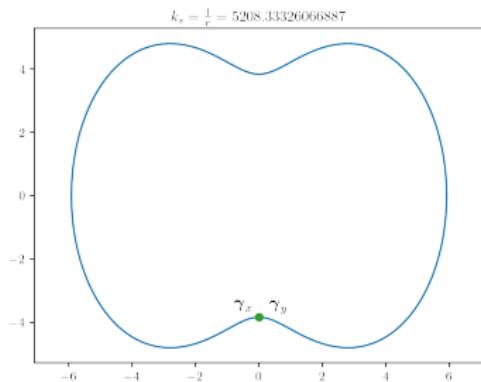
A naïve choice is  $k(\gamma_x, \gamma_y) := \frac{1}{\|\gamma_x - \gamma_y\|}$

# Pitfall of the “Simple Energy”

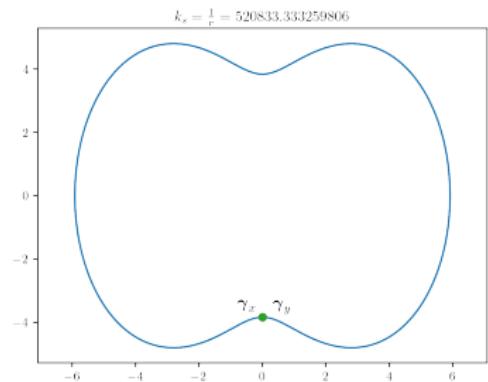
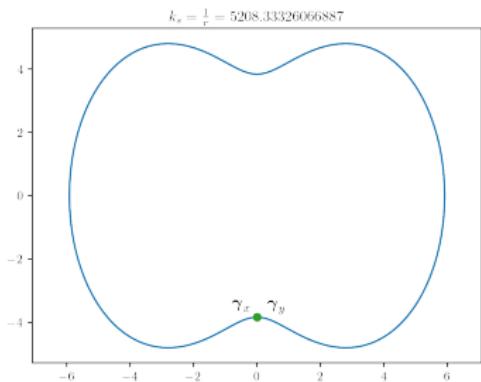
$$\mathcal{E}(\gamma) := \iint_{M^2} \frac{1}{||\gamma_x - \gamma_y||} d\gamma_x d\gamma_y$$



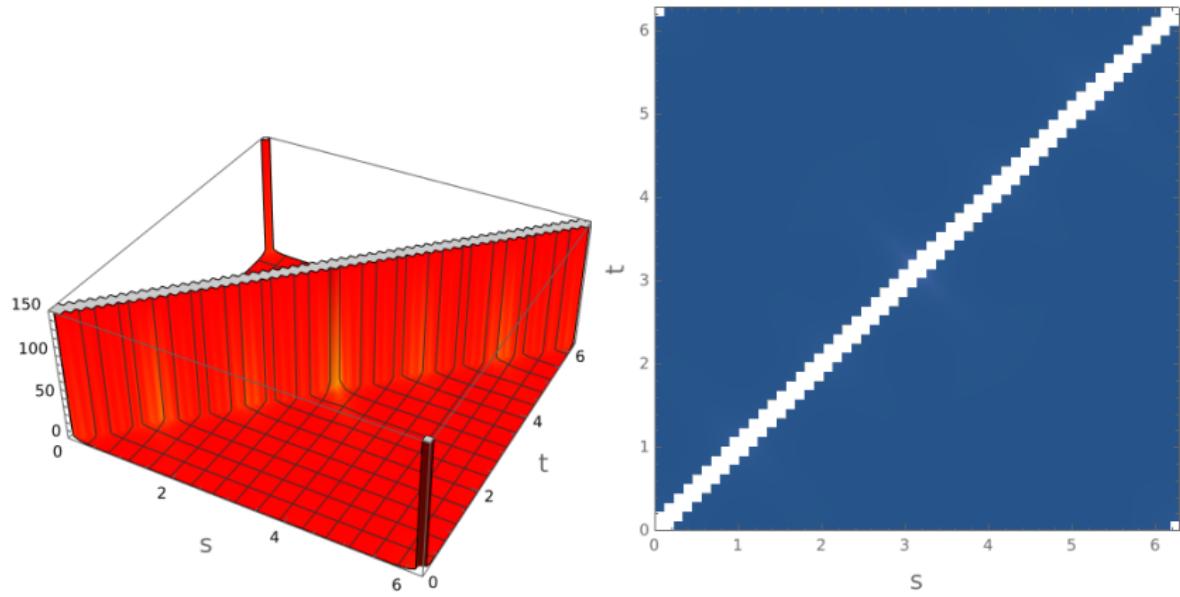
$$\mathcal{E}(\gamma) := \iint_{M^2} \frac{1}{\|\gamma_x - \gamma_y\|} d\gamma_x d\gamma_y$$



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



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



**Figure:** Simple Kernel Heat Map

# Buck-Orloff Tangent-Point Energy

- From the simple energy, need a way to suppress the infinite contribution of the “singularity”.

# Buck-Orloff Tangent-Point Energy

- From the simple energy, need a way to suppress the infinite contribution of the “singularity”.

## Definition (Buck-Orloff Tangent-Point Energy)

For a smooth curve  $\gamma$ , define

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

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

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

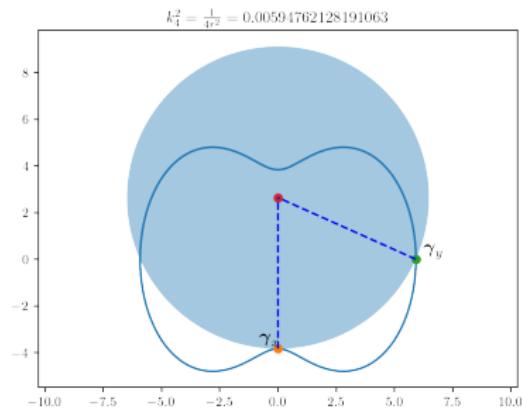
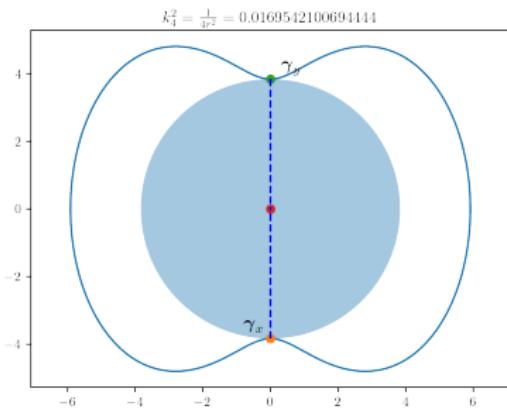
as **Buck-Orloff Tangent-Point Energy**.[1]

# Intuition

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

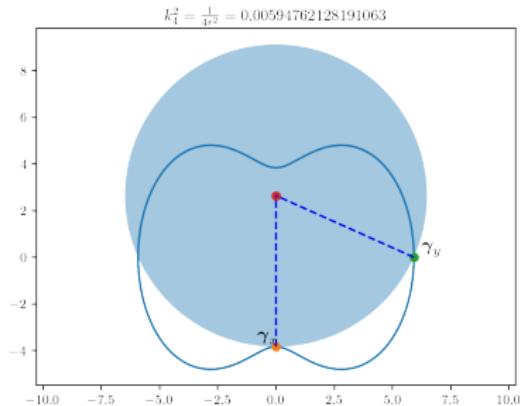
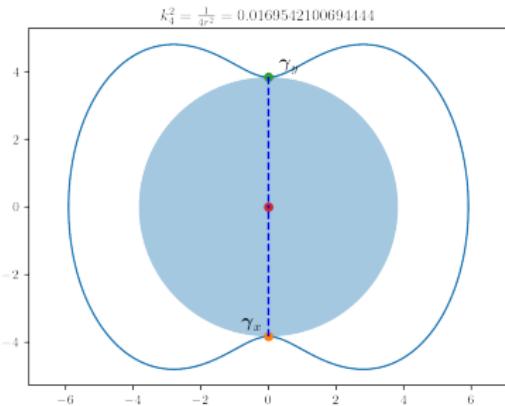
# Intuition

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



# Intuition

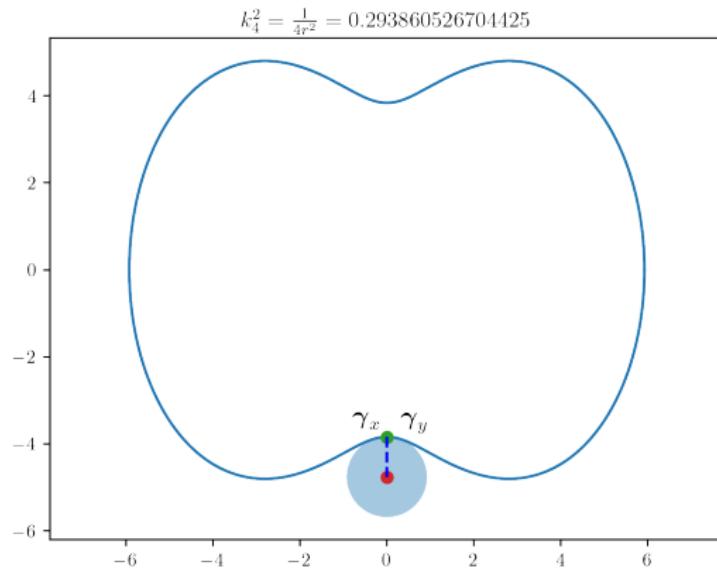
What is the intuition behind the kernel  $k_4^2(\mathbf{p}, \mathbf{q}, \mathbf{T}) := \frac{\|\mathbf{T} \wedge (\mathbf{p} - \mathbf{q})\|^2}{\|\mathbf{p} - \mathbf{q}\|^4}$ ?



## Remark

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

# Intuition



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

## Example (Unit Circle)

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

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

$$= \int_{\theta=0}^{2\pi} \int_{\phi=0}^{2\pi} \frac{\sin^2 \frac{\theta-\phi}{2}}{\sin^4 \frac{\theta-\phi}{2}} d\theta d\phi \quad (4)$$

$$= \pi^2 \quad (5)$$

## Example (Unit Circle)

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

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

$$= \int_{\theta=0}^{2\pi} \int_{\phi=0}^{2\pi} \frac{\sin^2 \frac{\theta-\phi}{2}}{\sin^4 \frac{\theta-\phi}{2}} d\theta d\phi \quad (4)$$

$$= \pi^2 \quad (5)$$

## 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]:

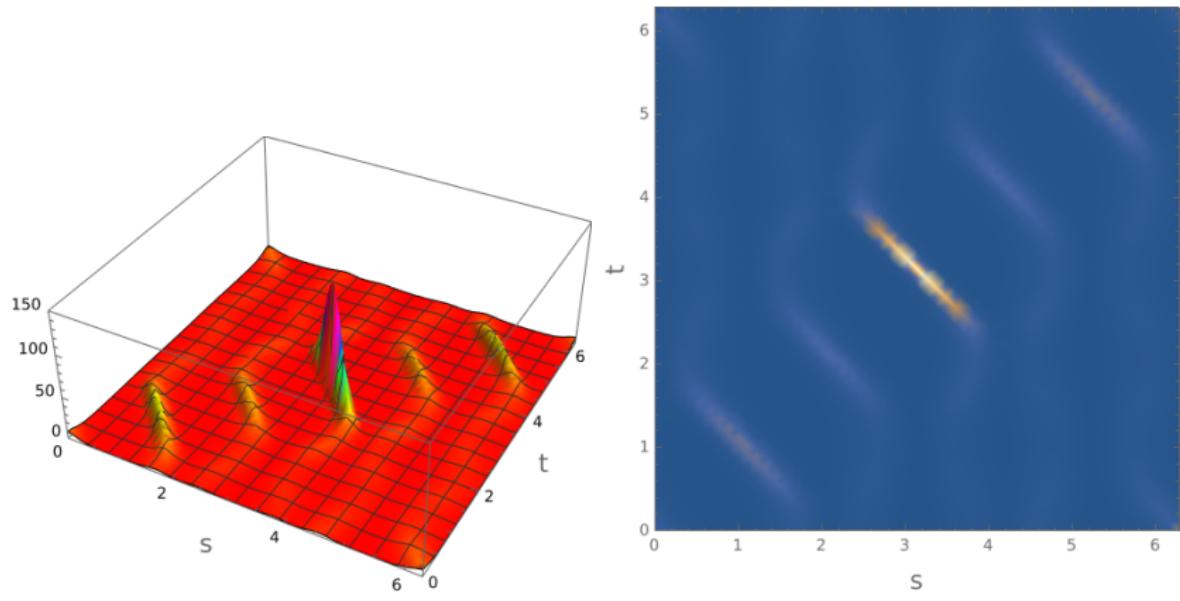
## Definition (Generalised Tangent-Point Energy)

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

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

## Remark

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



**Figure:** Buck-Orloff Tangent-Point Kernel Heat Map

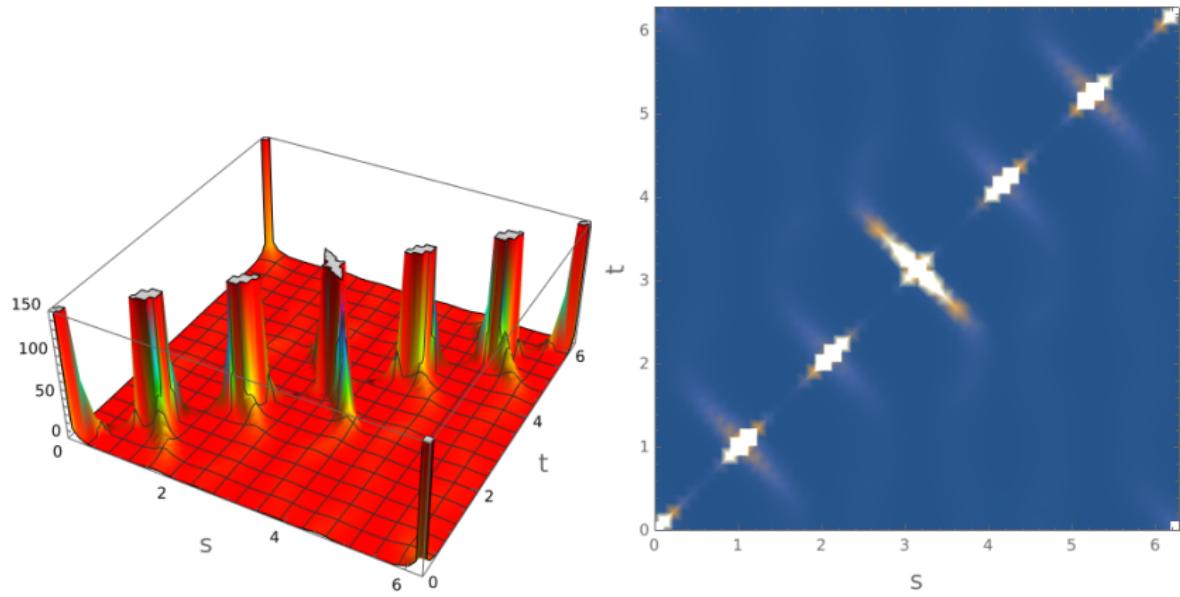


Figure: (2, 4.5) Tangent-Point Kernel Heat Map

# Gradient Flow

# Motivating Gradient Flow

For minimising a functional  $\mathcal{E}(f)$ , we wish to “move”  $f$  in the direction that decreases  $\mathcal{E}$ .

# Motivating Gradient Flow

For minimising a functional  $\mathcal{E}(f)$ , we wish to “move”  $f$  in the direction that decreases  $\mathcal{E}$ .

## Definition (Gradient Flow Equation)

For functional  $\mathcal{E}(f)$ , the **gradient flow equation** is:  $\frac{\partial f}{\partial t} = - \text{grad}_X \mathcal{E}(f)$

# Motivating Gradient Flow

For minimising a functional  $\mathcal{E}(f)$ , we wish to “move”  $f$  in the direction that decreases  $\mathcal{E}$ .

## Definition (Gradient Flow Equation)

For functional  $\mathcal{E}(f)$ , the **gradient flow equation** is:  $\frac{\partial f}{\partial t} = - \text{grad}_X \mathcal{E}(f)$

## Remark

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

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

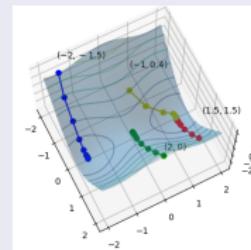


Figure: Steepest Descent [2]

# Gradient in Space of Function?

(Gradient of Function)

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

$$\nabla f(\mathbf{x}) \cdot \mathbf{y} = \frac{\partial}{\partial \epsilon} f(\mathbf{x} + \epsilon \mathbf{y}) \Big|_{\epsilon=0}$$

# Gradient in Space of Function?

(Gradient of Function)

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

$$\nabla f(\mathbf{x}) \cdot \mathbf{y} = \frac{\partial}{\partial \epsilon} f(\mathbf{x} + \epsilon \mathbf{y}) \Big|_{\epsilon=0}$$

(Gradient of Functional)

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

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

where  $X$  is the inner product space of functions (eg.  $L^2, H^1$ )

# Gradient in Space of Function?

(Gradient of Function)

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

$$\nabla f(\mathbf{x}) \cdot \mathbf{y} = \frac{\partial}{\partial \epsilon} f(\mathbf{x} + \epsilon \mathbf{y}) \Big|_{\epsilon=0}$$

(Gradient of Functional)

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

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

where  $X$  is the inner product space of functions (eg.  $L^2$ ,  $H^1$ )

## Remark

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

# Example: Dirichlet Energy in 1D

## Definition (1D Dirichlet Energy)

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

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

# Example: Dirichlet Energy in 1D

## Definition (1D Dirichlet Energy)

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

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

## 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

Because Dirichlet energy is simple enough, we may explicitly write down  $\text{grad}_X E$  for a few inner product function spaces.

# Example: $L^2$ Gradient Flow of Dirichlet Energy

Because Dirichlet energy is simple enough, we may explicitly write down  $\text{grad}_X E$  for a few inner product function spaces.

## Lemma ( $L^2$ Gradient of Dirichlet Energy)

$$\text{grad}_{L^2} E_D(f) = -\Delta f$$

*(for suitable boundary condition if finite interval)*

# Example: $L^2$ Gradient Flow of Dirichlet Energy

Because Dirichlet energy is simple enough, we may explicitly write down  $\text{grad}_X E$  for a few inner product function spaces.

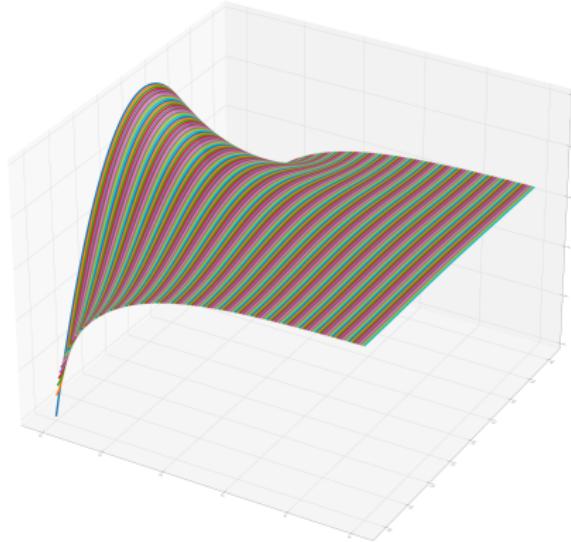
**Lemma ( $L^2$  Gradient of Dirichlet Energy)**

$$\text{grad}_{L^2} E_D(f) = -\Delta f$$

*(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)

- $L^p = \left\{ f \left| \left( \int |f|^p dx \right)^{1/p} < \infty \right. \right\}$ 
  - $\langle \langle f, g \rangle \rangle_{L^2} = \int fg dx$
- $p = 2$  Sobolev Space  $H^k = \left\{ f \left| \sum_{i=0}^k \int |\mathcal{D}^{(i)} f|^2 dx < \infty \right. \right\}$ 
  - $\langle \langle f, g \rangle \rangle_{H^k} = \sum_{i=0}^k \langle \langle \mathcal{D}^{(i)} f, \mathcal{D}^{(i)} g \rangle \rangle_{L^2}$
  - For our case, sufficient to take  $\langle \langle f, g \rangle \rangle_{H^k} = \langle \langle \mathcal{D}^{(k)} f, \mathcal{D}^{(k)} g \rangle \rangle_{L^2}$

# Dirichlet Gradient Flow in Other Function Space

## Definition (Famous Inner Product Function Spaces)

- $L^p = \left\{ f \left| \left( \int |f|^p dx \right)^{1/p} < \infty \right. \right\}$ 
  - $\langle \langle f, g \rangle \rangle_{L^2} = \int fg dx$
- $p = 2$  Sobolev Space  $H^k = \left\{ f \left| \sum_{i=0}^k \int |\mathcal{D}^{(i)} f|^2 dx < \infty \right. \right\}$ 
  - $\langle \langle f, g \rangle \rangle_{H^k} = \sum_{i=0}^k \langle \langle \mathcal{D}^{(i)} f, \mathcal{D}^{(i)} g \rangle \rangle_{L^2}$
  - For our case, sufficient to take  $\langle \langle f, g \rangle \rangle_{H^k} = \langle \langle \mathcal{D}^{(k)} f, \mathcal{D}^{(k)} g \rangle \rangle_{L^2}$
- $L^2 = H^0: \frac{\partial f}{\partial t} = -\Delta f$
- $H^1: \frac{\partial f}{\partial t} = -f$
- $H^{-1}: \frac{\partial f}{\partial t} = -\Delta^2 f$ 
  - $\langle \langle f, g \rangle \rangle_{H^{-1}} = \langle \langle \Delta^{-1} f, \Delta^{-1} g \rangle \rangle_{H^1}$
- $H^2: \frac{\partial f}{\partial t} = \Delta^{-1} f$

# Curve Repulsion

# Gradient Flow on Tangent-Point Energy

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

$$\frac{\partial \gamma}{\partial t} = - \text{grad}_{L^2} \mathcal{E} \quad (7)$$

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

# Gradient Flow on Tangent-Point Energy

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

$$\frac{\partial \gamma}{\partial t} = -\text{grad}_{L^2} \mathcal{E} \quad (7)$$

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

For numerical solution, one discretises the curve.

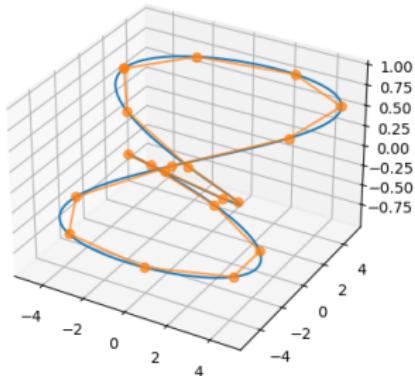


Figure: Discretised Curve

# Gradient Flow on Tangent-Point Energy

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

$$\frac{\partial \gamma}{\partial t} = -\text{grad}_{L^2} \mathcal{E} \quad (7)$$

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

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

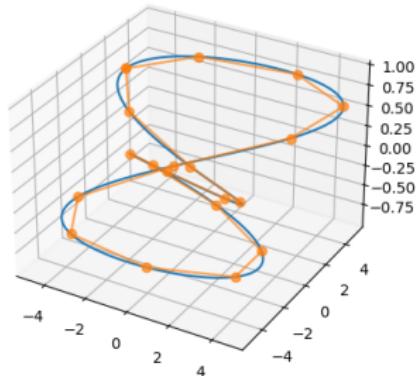
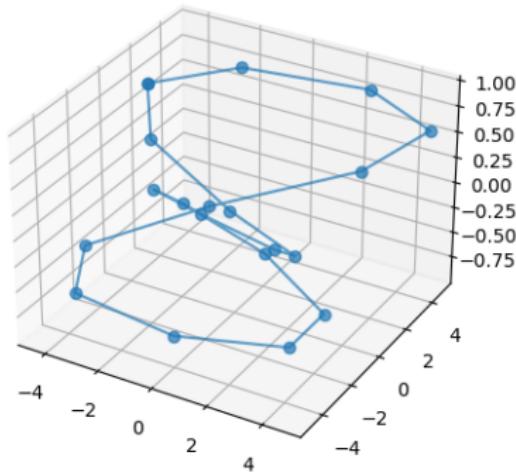


Figure: Discretised Curve

# Subtlety



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

# Energy Discretisation

Note the form of tangent-point energy:

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

# Energy Discretisation

Note the form of tangent-point energy:

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

## Definition (Discretised Energy)

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

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

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

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

# Numerical Scheme

Original  $L^2$  Gradient Flow Equation:

$$\frac{\partial \gamma}{\partial t} = - \text{grad}_{L^2} \mathcal{E} - \underbrace{\mathcal{C}}_{\text{Constraint}} \quad (9)$$

By forward difference, we arrived at an explicit Euler scheme:

$$\frac{\Gamma^{k+1} - \Gamma^k}{\Delta T} = - \underbrace{\frac{\partial E}{\partial \Gamma}}_{\text{Gradient from perturbing each point in each direction}} - \underbrace{\frac{\partial \mathcal{C}}{\partial \Gamma}}_{\text{Derived from Constraint}}$$

where we may further approximate the RHS by central difference scheme, for example:

$$\frac{\partial E}{\partial \Gamma_i} \approx \frac{E|_{\mathbf{x}_i+h} - E|_{\mathbf{x}_i-h}}{2h} \left( = \frac{\partial E}{\partial \Gamma_i} + O(h^2) \right)$$

# Gradient Flow Demo

- Ellipse to Circle (ellipse.mp4)
- Saddle to Circle (saddle.mp4)

# 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](https://doi.org/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](https://doi.org/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](https://doi.org/10.1145/3439429).