Numerical computation for geometric evolution equations using deep learning

Tokuhiro ETO

Graduate School of Mathematical Sciences, The University of Tokyo

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Front tracking method

Heuristic surgery for topological changes:

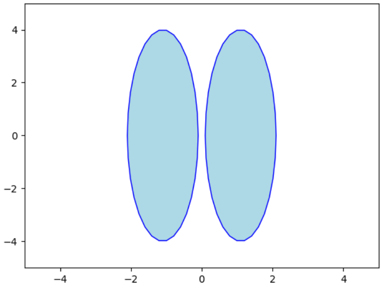


Fig 1: fusion

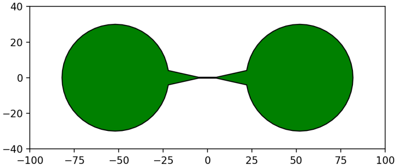


Fig 2: pinch off

Overview of the Level-Set Method

Level-set equation for Mean curvature flow

$$\Phi_t = |\nabla\Phi| \operatorname{div}\left(\frac{\nabla\Phi}{|\nabla\Phi|}\right) \quad \text{in} \quad [0,T]\times\Omega,$$
$$\Phi(0,\cdot) = \Phi_0 \quad \text{in} \quad \Omega.$$

Find a level-set functions

We learn $\Phi : [0,T]\times\Omega \to \mathbb{R}$ via a neural network which satisfies

Φ satisfies the level–set equation.

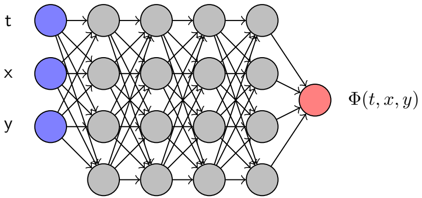
$\Gamma_t = \{x \in \Omega \mid \Phi(t,x) = 0\}$,

inside of $\Gamma_t = \{x \in \Omega \mid \Phi(t,x) < 0\}$,

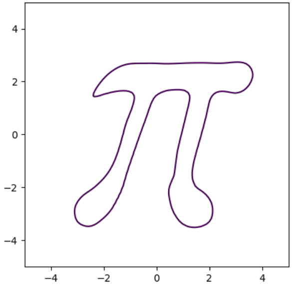
outside of $\Gamma_t = \{x \in \Omega \mid \Phi(t,x) > 0\}$.

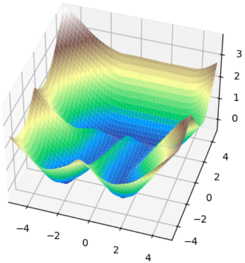
Neural Network Approximation

- **Network Architecture**:
  - 10 fully connected layers
  - tanh activation function
- **Optimization**:
  - Loss function: Residual of the Level-set equation, initial condition
  - Optimizer: ADAM
- **Training**:
  - Data: random sampling

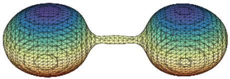


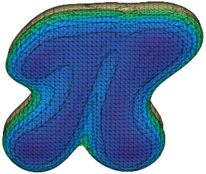
Results for 2D





Results for 3D





Results for contact angle conditions

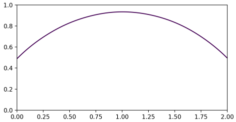


Fig 3: $135^\circ,\ 135^\circ$

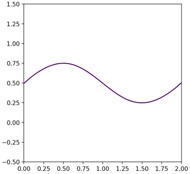


Fig 4: $135^\circ,\ 45^\circ$

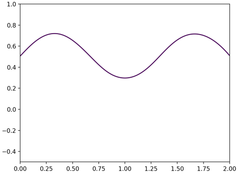


Fig 5: $135^\circ,\ 135^\circ$

Thank you for your attention.

Please visit my website.

For further discussion

Closed curves in 2D

Neural network

For $(t, x) \in [0, T] \times \mathbb{R}^2$, a function $\Phi : [0, T] \times \mathbb{R}^2 \to \mathbb{R}$ is defined by

$$\Phi(t, x) := W_{10}(\alpha(W_9(\cdots \alpha(W_1(t, x)^T + b_1) \cdots) + b_9)) + b_{10}$$

where $W_1 \in \mathbb{R}^{100\times 3}$, $W_i \in \mathbb{R}^{100\times 100}$ $(1 \leq i \leq 9)$, $W_{10} \in \mathbb{R}^{1\times 100}$, $b_i \in \mathbb{R}^{100}$ $(1 \leq i \leq 9)$, $b_{10} \in \mathbb{R}$ and $\alpha := \tanh$.

Method

Update the parameters W_i and b_i to **minimize a loss function** $L(\Phi)$.

Loss function

A non-negative functional $L(\Phi)$ which satisfies $L(\Phi) = 0$ if Φ satisfies the level–set equation.

Closed curves in 2D

Loss function

$$L(\Phi) := M * L_i(\Phi) + L_r(\Phi),$$

$$L_i(\Phi) := MSE(\Phi(0,\cdot), d(\cdot)),$$

$$L_r(\Phi) := MSE\left(\Phi_t, \Delta\Phi - \frac{1}{|\nabla\Phi|^2}\sum_{i,j=1}^{2}\Phi_{x_i}\Phi_{x_j}\Phi_{x_i x_j}\right).$$

Remark

- The signed distance function d is computed by the **fast marching method**.
- Each derivative of Φ is computed with the help of the **automatic differentiation** with respect to the input variables.
- The hyperparameters are set as follows:
  - $M := 100$.
  - Mini–batch size for L_i and $L_r = 1000$.
  - We have used the **ADAM** optimizer with the default learning rate.

Closed surfaces in 3D

Neural network

For $(t,x) \in [0,T] \times \mathbb{R}^3$, a function $\Phi : [0,T] \times \mathbb{R}^3 \to \mathbb{R}$ is defined by

$$\Phi(t,x) := W_5(\alpha(W_4(\cdots\alpha(W_1(t,x)^T + b_1)\cdots) + b_4)) + b_5$$

where $W_1 \in \mathbb{R}^{50\times 4}$, $W_i \in \mathbb{R}^{50\times 50}$ $(1 \le i \le 5)$, $W_5 \in \mathbb{R}^{1\times 50}$,
$b_i \in \mathbb{R}^{50}$ $(1 \le i \le 5)$, $b_5 \in \mathbb{R}$ and $\alpha := \tanh$.

Loss function

We replace L_r as follows:

$$L_r(\Phi) := MSE\left(\Phi_t, \Delta\Phi - \frac{1}{|\nabla\Phi|^2}\sum_{i,j=1}^{3}\Phi_{x_i}\Phi_{x_j}\Phi_{x_ix_j}\right).$$

Remark

We replace the hyperparameters as follows:

- Mini–batch size for $L_i := 5000$ and $L_r := 5000$.

Application to contact angle problems

Mean curvature flow equation with prescribed contact angle

$$\Phi_t = |\nabla \Phi| \operatorname{div}\left(\frac{\nabla \Phi}{|\nabla \Phi|}\right) \quad \text{in} \quad [0,T] \times \Omega,$$

$$\langle \nabla \Phi, \nu_\Omega \rangle + \beta |\nabla \Phi| = 0 \quad \text{on} \quad [0,T] \times \partial\Omega,$$

$$\Phi(0,\cdot) = \Phi_0 \quad \text{in} \quad \Omega,$$

where ν_Ω denotes the outward unit normal vector field on $\partial\Omega$, and $\beta : \partial\Omega \to (-1,1)$ is given as the cosine of the contact angle.

Contact angle problems

Loss function

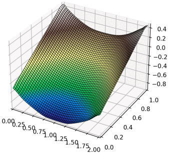
$$L(\Phi) := M * L_i(\Phi) + L_r(\Phi) + B * L_b(\Phi),$$

$$L_i(\Phi) := MSE(\Phi(0,\cdot), d(\cdot)),$$
$$L_r(\Phi) := MSE\left(\Phi_t, \Delta\Phi - \frac{1}{|\nabla\Phi|^2}\left(\Phi_x^2\Phi_{xx} + 2\Phi_x\Phi_y\Phi_{xy} + \Phi_y^2\Phi_{yy}\right)\right),$$
$$L_b(\Phi) := MSE(\langle\nabla\Phi, \nu_\Omega\rangle + \beta|\nabla\Phi|, 0).$$

Remark

- The hyperparameters are set as follows:
  - $M := 100.$
  - $B := 20.$
  - Mini–batch size for L_i and $L_r = 1000.$
  - Mini–batch size for $L_b = 396$ (Mesh points on $\partial\Omega$).

Evolution of line segments (Specify different angles)



Test fixture:

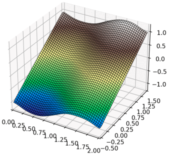
$$\overline{\Omega} = [0,2] \times [0,1].$$

$$\beta(x,y) = \begin{cases} -\frac{1}{\sqrt{2}} = \cos\frac{3}{4}\pi & \text{if } x \in \{0,2\}, \\ 0 = \cos\frac{\pi}{2} & \text{otherwise.} \end{cases}$$

$\Phi(0,\cdot)$ is a level-set function of

$$\left\{ (x,y) \;\middle|\; y = \frac{4}{\pi} \log \left| \cos\left(-\frac{\pi}{4} x + \frac{\pi}{4} \right) \right| + \frac{1}{2} + \frac{2}{\pi} \log 2. \right\}.$$

Evolution of line segments (Convergence to a straight line)



Test fixture:

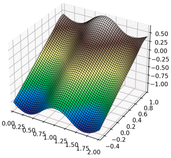
$$\overline{\Omega} = [0, 2] \times [-0.5, 1.5].$$

$$\beta(x, y) = \begin{cases} -\frac{1}{\sqrt{2}} = \cos\frac{3}{4}\pi & \text{if } x = 0, \\ \frac{1}{\sqrt{2}} = \cos\frac{\pi}{4} & \text{if } x = 2, \\ 0 \text{ otherwise.} \end{cases}$$

$\Phi(0, \cdot)$ is a level-set function of

$$\left\{ (x, y) \,\middle|\, y = \frac{1}{4}\sin(\pi x) + \frac{1}{2}. \right\}.$$

Evolution of line segments (Convergence to a soliton)



Test fixture:

$$\overline{\Omega} = [0,2] \times [-0.5, 1].$$

$$\beta(x,y) = \begin{cases} -\frac{1}{\sqrt{2}} = \cos\frac{3}{4}\pi & \text{if } x \in \{0,2\}, \\ \frac{1}{\sqrt{2}} = \cos\frac{\pi}{4} & \text{if } y = 0, \\ 0 \text{ otherwise.} \end{cases}$$

$\Phi(0,\cdot)$ is a level-set function of

$$\left\{ (x,y) \,\middle|\, y = \frac{2}{3\pi}\sin\left(\frac{3}{2}\pi x\right) + \frac{1}{2} \right\}.$$

Issues and Challenges

- Gradient vanishing problem
- Handling bulk-interface models
- What's Convergence criteria ? (e.g. $M = 100$, $B = 20$)