How to work with complex geometries in PINNs ?

Authors:
Frédérique LECOURTIER

Supervisors:
Emmanuel FRANCK
Michel DUPREZ
Vanessa LLERAS

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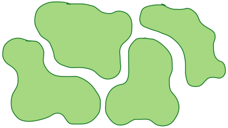
Problem considered



Poisson problem with Dirichlet conditions :
Find $u : \Omega \to \mathbb{R}^d (d = 1, 2, 3)$ such that

$$\begin{cases} -\Delta u(X) = f(X) & \text{in } \Omega, \\ u(X) = g(X) & \text{on } \partial\Omega \end{cases}$$

with Δ the Laplace operator, Ω a smooth bounded open set and Γ its boundary.
For the following examples, we will consider $f(X) = 1$ and $g(X) = 0$.

Standard PINNs : We are looking for θ_u such that

$$\theta_u = \underset{\theta}{\operatorname{argmin}}\, w_r\, J_r(\theta) + w_{bc}\, J_{bc}(\theta)$$

where w_r and w_{bc} are the respective weights associated with

$$J_r = \int_\Omega (\Delta u_\theta + f)^2 \ \text{ and } \ J_{bc} = \int_{\partial\Omega} (u_\theta - g)^2.$$

Remark : In practice, we use a Monte-Carlo method to discretize the cost function by random process.

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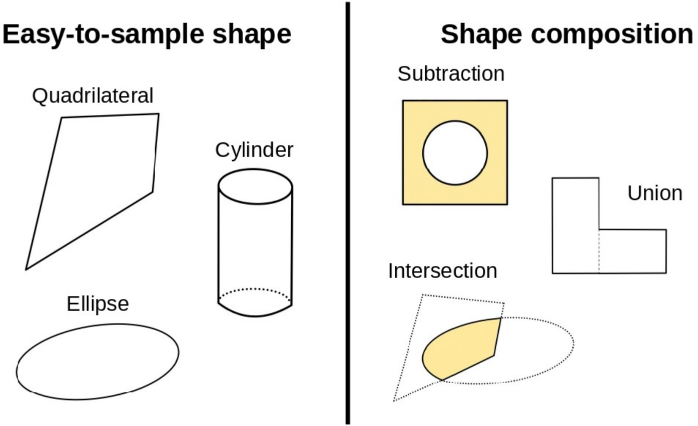
Simple geometry

Claim on PINNs : No mesh, so easy to go on complex geometry !



In practice : Not so easy ! We need to find how to sample in the geometry.

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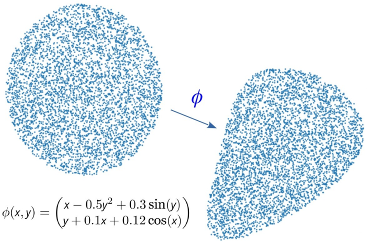
Complex geometry

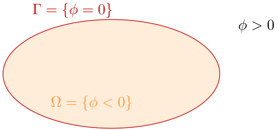
1st approach : Mapping	**2nd approach : LevelSet function**

Idea :

- ➙ Ω_0 a simple domain (as circle)
- ➙ Ω a target domain
- ➙ A mapping from Ω_0 to Ω :

$$\Omega = \phi(\Omega_0)$$





Advantages :

- ➙ Sample is easy in this case.
- ➙ Allow to impose in hard the BC :

$$u_\theta(X) = \phi(X)w_\theta(X) + g(X)$$

Natural LevelSet :

Signed Distance Function (SDF)

Problem : SDF is a $\mathcal{C}^0$ function

$\Rightarrow$ its derivatives explodes

$\Rightarrow$ we need a regular levelset

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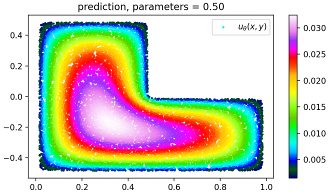
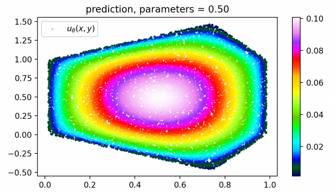
Construct smooth SDF I

1st solution : Approximation theory [5]

$\Delta\phi$ can be singular at the boundary. Sampling at ϵ to it solve the problem.

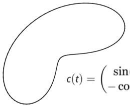
Polygonal domain Appendix 1





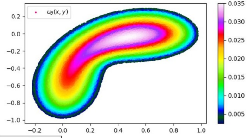
Curved domain Appendix 2

Minus : Use of a parametric curve $c(t)$.

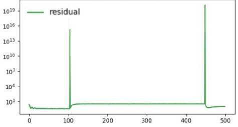


$$c(t) = \begin{pmatrix} \sin(2\pi t) \times (\sin(2\pi t)^3 + \cos(2\pi t)^5) \\ -\cos(2\pi t) \times (\sin(2\pi t)^3 + \cos(2\pi t)^5) \end{pmatrix}$$

Prediction



Loss history



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Construct smooth SDF II

2nd solution : Learn the levelset. [2]

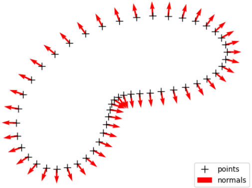
➙ How make that ? with a PINNs.

If we have a boundary domain Γ, the SDF is solution to the Eikonal equation:

$$\begin{cases} ||\nabla\phi(X)|| = 1, \ X \in \mathcal{O} \\ \phi(X) = 0, \ X \in \Gamma \\ \nabla\phi(X) = n, \ X \in \Gamma \end{cases}$$

with $\mathcal{O}$ a box which contains Ω completely and n the exterior normal to Γ.

Advantage : No need for parametric curves.



➙ set of boundary points

➙ exterior normals at Γ

(evaluated at these points)

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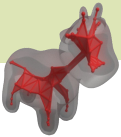
Learn LevelSet I



Objective of the paper :

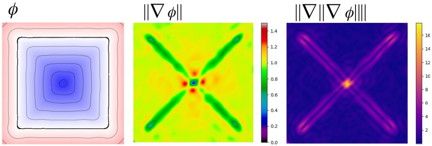
Learn topological Skeleton (by learning SDF) Appendix 3

➙ Skeleton correspond exactly to the gradient singularity

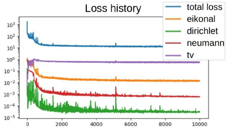
➙ Adding the following term in the loss

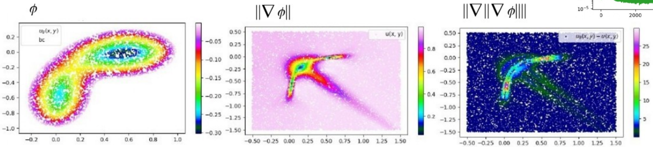
$$\int_{\mathcal{O}} ||\nabla||\nabla\phi||(p)||dp$$

(Total Variation Regularization)



1st test : Eikonal equation with TV Regularization [2]





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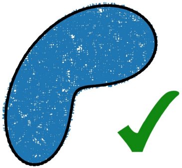
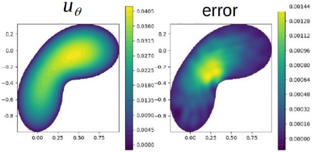
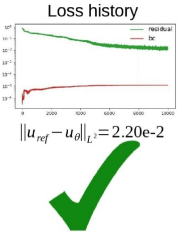
Learn LevelSet I

Sampling :



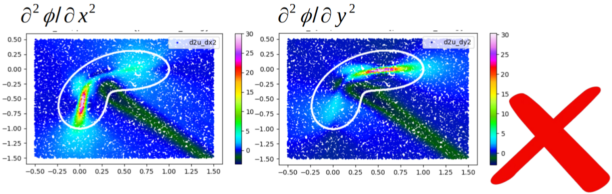
Classical PINNs : Looking for u_θ.





Minus : Costly boundary points generation.

PINNs - Impose BC in hard : Looking for $u_\theta = \phi w_\theta$.



Levelset derivatives explode.

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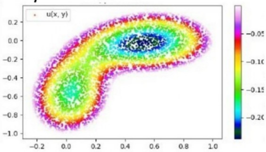
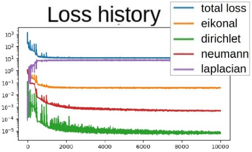
Learn LevelSet II

2nd test : We replace the TV term by a penalization on the laplacian of the levelset

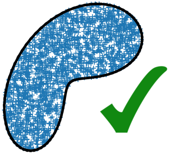
$$J_{reg} = \int_{\mathcal{O}} |\Delta \phi|^2$$

ϕ



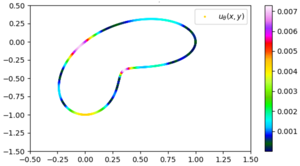


Sampling :



Dirichlet error on the boundary :

Max : 7.29e-3 ; Mean : 1.88e-3



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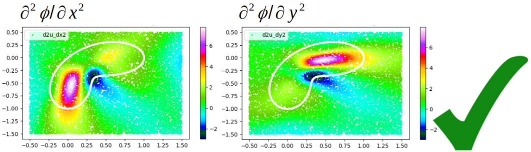
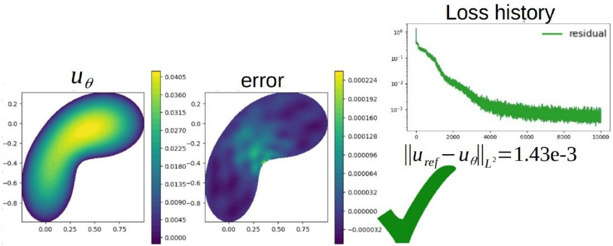
Learn LevelSet II

Derivatives :



$\Rightarrow$ We can impose in hard boundary conditions

PINNs - Impose BC in hard : Looking for $u_\theta = \phi w_\theta$.



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Conclusion

2 main questions :

➙ How to sample in complex domains?

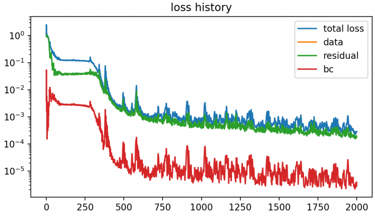
- Using mapping
- Using Levelset (Approximation theory/Learning)

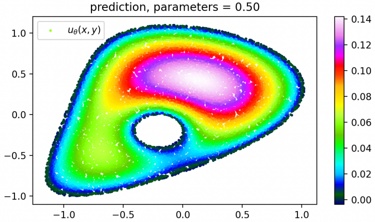
➙ How can we obtain a levelset that usable for imposing boundary conditions in hard ?

By learning the Eikonal equation with penalisation of the levelset Laplacian

To go further : We can combine the option.

(Mapping for the big domain. Level set for the hole.)





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Thank you !

Bibliography

[1] Alexander Belyaev, Pierre-Alain Fayolle, and Alexander Pasko. Signed Lp-distance fields. *Computer-Aided Design*.

[2] Mattéo Clémot and Julie Digne. Neural skeleton: Implicit neural representation away from the surface. *Computers and Graphics*.

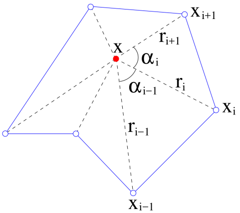
[3] Pierre-Alain Fayolle. Signed Distance Function Computation from an Implicit Surface.

[4] M. Raissi, P. Perdikaris, and G. E. Karniadakis. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *Journal of Computational Physics*.

[5] N. Sukumar and Ankit Srivastava. Exact imposition of boundary conditions with distance functions in physics-informed deep neural networks. *Computer Methods in Applied Mechanics and Engineering*.

[6] Sifan Wang, Shyam Sankaran, Hanwen Wang, and Paris Perdikaris. An Expert's Guide to Training Physics-informed Neural Networks.

Appendix 1 : Polygonal domain [5]



- X_i, $i = 1, \ldots, n$ - coordinates of the polygon
- α_i - angle between X_i and X_{i+1}
- $r_i = ||X_i - X||$ - Euclidean distance between X_i and X
- $R_i = X_i - X$

We define the SDF as

$$\phi(X) = \frac{2}{W(X)}$$

with

$$W(X) = \sum_{i=1}^{n} \left(\frac{1}{r_i} + \frac{1}{r_{i+1}} \right) t_i \quad (r_{n+1} := r_1)$$

and

$$t_i := \tan\left(\frac{\alpha_i}{2}\right) = \frac{det(R_i, R_{i+1})}{r_i r_{i+1} + R_i \cdot R_{i+1}}$$

Remark : The denominator vanishes when $\alpha_i = \pi$, (i.e. when X lies on the boundary of the polygon), but there $\phi_i(X) = 0$.

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Appendix 2 : Curved domain [5]

Considering a nonconvex domain.

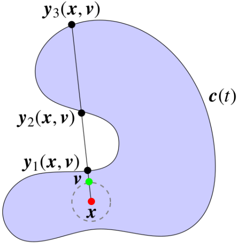
- $c(t)$ - parametrization of the curved boundary $\Gamma : [0,1] \to \mathbb{R}$
- $c'(t)$ - its tangent
- $c'^{\perp}(t)$ - rotating $c'(t)$ through 90° (clockwise)

We define the SDF as

$$\phi(X) = \left(\frac{1}{W_p(X)}\right)^{1/p}$$

with

$$W_p(X) = \int_0^1 \frac{(c(t) - X) \cdot c'^{\perp}(t)}{||c(t) - X||^{2+p}}$$



(Belyaev et al. [1] introduced L_p-distance fields ($p \geq 1$), which approximates the exact distance function.)

Remark : For $X \in \Gamma$ (integral is singular), we set $\phi(X) = 0$.

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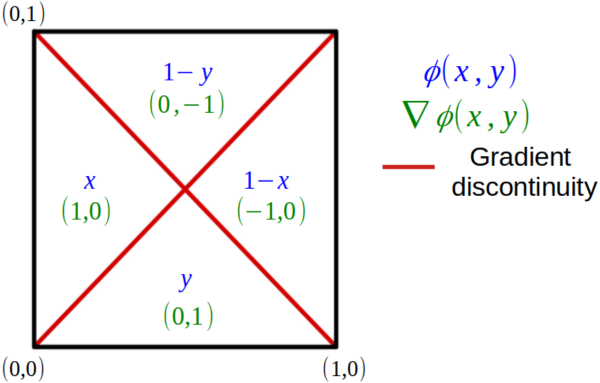
Appendix 3 : Neural Skeleton

Simple example : Skeleton of the unit square.



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