AI4PDE

Green Functions and PDEs on manifolds(i)

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Presentation Overview

Section Overview

BINet and Green-BINet

Sources

Literature

- BINet: Learning to Solve Partial Differential Equations with Boundary Integral Networks. Guochang Lin et al. CSIAM Trans. Appl. Math. 2023.
- Green-BINet: Learning Green's functions by boundary integral network. Communications in Mathematics and Statistics. 2023.

Tutorials

- Potential Theory. https://web.stanford.edu/class/math220b/handouts/potential.pdf
- Dependence of the layer heat potentials upon support perturbations. Matteo Dalla Riva.
- Some properties of layer potentials and boundary integral operators for the wave equation.V´ıctor Dom´ınguez.

BI-Net

Motivation

Homogenous PDEs(Possion eq., Helmholtz eq., heat eq. and wave eq. etc.) are determined by its boundary and also can be estimated by **boundary integration**. Benefits are:

- **The dimension of the boundary is lower** and leads to easier computation.
- It **replaces differential operators with integral representation**, which improves the regularity and stability.
- In the unsupervised PINN frame, one needs to determine the ratio between PDE loss and boundary condition loss at advance. And now there is **no such thing called boundary condition loss**.

Remark

Not all PDEs have boundary integral representation.

Preliminary: Potential Theory 1

For simplicity, we only cover the case of Possion equation(TUTORIAL**[1]**). See more in TUTORIAL**[2,3]**.
For instance, to solve the electric potential, we care about the termed **Interior/Exterior Dirichlet/Neumann Problem**.

$$\Delta u = 0, x \in \Omega; u = g, x \in \partial\Omega \tag{1}$$

$$\Delta u = 0, x \in \Omega^C; u = g, x \in \partial\Omega^C \tag{2}$$

$$\Delta u = 0, x \in \Omega; \partial_n u = g, x \in \partial\Omega \tag{3}$$

$$\Delta u = 0, x \in \Omega^C; \partial_n u = g, x \in \partial\Omega^C \tag{4}$$

Remark

Single and double layer potential are applied to Dirichlet and Neumann problems, resp.

Preliminary: Potential Theory 2

Theorem

The fundamental solution of Laplace's equation$\Delta u = 0$ is:

$$\Phi(\mathbf{x}) = -\frac{1}{2\pi}\ln|\mathbf{x}|, n = 2; \Phi(\mathbf{x}) = -\frac{1}{n(n-2)\alpha_n}\frac{1}{|\mathbf{x}|^{n-2}}, n > 2 \tag{5}$$

Def.

The single potential $S[h]$ and double potential $D[h]$ w.r.t. **moment** h:

$$S[h] := -\int_{\partial\Omega} h(y)\Phi(x-y)dS(y) \tag{6}$$

$$D[h] := -\int_{\partial\Omega} h(y)\partial_\nu\Phi(x-y)dS(y) \tag{7}$$

Preliminary: Potential Theory 3

Theorem

$S[h], D[h]$ are both well-defined, harmonic over $\mathbb{R}^n$ and continuous in $\operatorname{int}\Omega, \operatorname{int}\Omega^C$,but on the boundary where ν is the outwards normal vector:

$$\lim_{t\to 0^+} \nabla S[h](x_0+t\nu)\cdot\nu = \frac{1}{2}h(x_0)+S[h]; \lim_{t\to 0^-} \nabla S[h](x_0+t\nu)\cdot\nu = -\frac{1}{2}h(x_0)+S[h] \quad (8)$$

$$\lim_{x\in\Omega\to x_0} D[h] = \frac{1}{2}h(x_0)+D[h](x_0); \lim_{x\in\Omega^C\to x_0} D[h] = -\frac{1}{2}h(x_0)+D[h](x_0) \quad (9)$$

And whence, to solve the interior Dirichlet problem is to look for h s.t.

$$g = D[h] = \frac{1}{2}h(x_0) - \int_{\partial\Omega} h(y)\partial_\nu\Phi(x_0-y)dS(y), x\in\Omega \quad (10)$$

Preliminary: Potential Theory 4

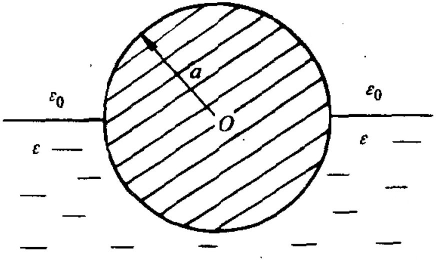

Fig. 1: Physical interpretations of single and double layer potential

See more in https://web.stanford.edu/class/math220b/handouts/potphys.pdf

BI-Net

However, notice that it is impossible to find a closed-form or a simple expansion of h in

$$g(x_0) = D[h] = \frac{1}{2}h(x_0) - \int_{\partial\Omega} h(y)\partial_\nu \Phi(x-y)dS(y), x \in \Omega \tag{11}$$

we instead use a neural network h_θ parametrized θ to evaluate h. This reduces the PINN loss to:

$$\mathscr{L} := \sum_{x_0} \left\| \frac{1}{2}h(x_0) - \int_{\partial\Omega} h(y)\partial_\nu \Phi(x_0-y)dS(y) - g \right\|_{\partial\Omega}^2 \tag{12}$$

Other three problems are simply likewise.

BI-Net Framework

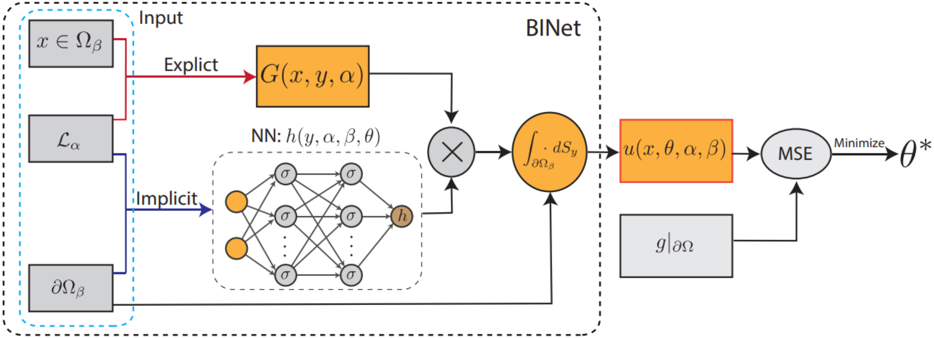

Fig. 2: BI-Net Framework

BI-Net Assess

Drawback

It can only solve homogenous PDEs, which is amended by Green BI-Net.

Generalization

It can be generalized to solve time-involved PDE like heat and wave eq. apart from Possion and Helmholtz eq.

Preliminary:Green Function

Def

For example, the Green function G is defined to solve the PDE where L is a linear differential operator:

$$L[G(x,y)] = \delta(x-y), x, y \in \Omega; G(x,y) = 0, x \in \Omega, y \in \partial\Omega \tag{13}$$

With which one can solve any **non-homogenous** Dirichlet problem:

$$u(x) = \int_{\Omega} G(x,y)f(y)dy + \int_{\partial\Omega} G_{\nu}(x,y)g(y)dS(y) \tag{14}$$

But how to learn such a $G(x,y)$ efficiently?

Green BI-Net

Remove Singularities

Usually, $G(x,y)$ doesn't behave well, i.e., it has lots of singularities. Fortunately, for an unbounded problem s.t. $L[G_0(x,y)] = 0, x, y \in \mathbb{R}^n$, we already know many **fundamental solutions** given by $G_0(x,y) = \Phi(y-x)$.
Define $H(x,y) := G(x,y) - G_0(x,y)$, H has less singularity since the pointwise charge $\delta(y-x)$ is removed.

$$L[H(x,y)] = 0, x, y \in \Omega; H(x,y) = -G_0(x,y), x \in \Omega, y \in \partial\Omega \tag{15}$$

Observe (15) and we find that it is just the **interior Dirichlet Problem** solved by BI-Net!

A More Complicated Task: Interface Problem

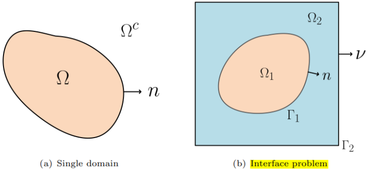

Fig. 3: Interface Problem

The corresponding PDE is:

$$\begin{cases} Lu = f & x \in \Omega \\ [u] = g_1, [\frac{1}{\mu} u_\nu] = g_2, & x \in \Gamma_1 \\ u = g_3 & x \in \Gamma_2 \end{cases} \tag{16}$$

where $[\cdot] := u^+ - u^-$ is the **jump** or **discontinuity** across the boundary.

Green Function in Interface Problems

One can also solve it via:

$$u(x) = (G,f)_\Omega + (\frac{1}{\mu}G_\nu, g_1)_{\Gamma_1} - (G,g_2)_{\Gamma_1} - (\frac{1}{\mu}G_\nu, g_3)_{\Gamma_2} \tag{17}$$

where $(u,v)_\Gamma := \int_\Gamma uvdy$ Usually, the fundamental solution G_0 is not continuous on Γ_1(in different dielectrics, for instance) and thus one can again define $H(x,y)$ as:

$$H(x,y) := G(x,y) - G_0(x,y) \tag{18}$$

and solve:

$$\begin{cases} L[H] = 0 & x \in \Omega \\ [H] = -[G_0], [\frac{1}{\mu}H_\nu] = -[\frac{1}{\mu}\partial_\nu G_0], & x \in \Gamma_1 \\ H = -G_0 & x \in \Gamma_2 \end{cases} \tag{19}$$

Green Function in Interface Problems

From the potential theory, one can show that in consistence with the topology shown in Fig. 3, one have:

$$H(x,y) = \begin{cases} -S[h_1] & ,y \in \Omega_1 \\ -S[h_2] - D[h_3] & ,y \in \Omega_2 \end{cases} \tag{20}$$

where $h_i, i = 1,2,3$ is implemented by networks.
Thus in light of PINN loss, we can add two terms of jump loss L_1, L_2 on Γ_1, i.e., the total loss is:

$$\mathscr{L} := k_1 L_1 + k_2 L_2 + L \tag{21}$$

$$L_1 = \sum_{x_i} |(-S[h_1] + S[h_2] + D[h_3]) + (G_0^+ - G_0^-)|^2 \tag{22}$$

Section Overview

An Intro to PDEs over Manifolds

Literature

- Diffusion maps. Ronald R. Coifman et al. Applied and Computational Harmonic Analysis. 2006.
- SOLVING PDES ON UNKNOWN MANIFOLDS WITH MACHINE LEARNING. Senwei Liang. Applied and Computational Harmonic Analysis. 2024.

Tutorials about Solving PDEs on manifolds

Tutorials: Differential Geometry

- An Introduction to Manifolds. Loring W. Tu.
- Differential Geometry. Loring W. Tu.

Tutorials: Geometric Analysis

- Riemannian geomeotry and geometric analysis. Jurgen Jost.
- Notes for Analysis on Manifolds via the Laplacian. Yaiza Canzani.

Tutorials:Variation

- Introductory Variational Calculus on Manifolds. Ivo Terek.

Numerical Methods

- (ODE)Solving Differential Equations on Manifolds. Ernst Hairer.

Notations about Differential Geometry

Manifold

The tangent space on a n-dimension manifold M at x is $T_x M$ and the tangent bundle $TM : M \times \mathbb{R}^n$ with a natural projection $\pi : TM \to M$.
The cotangent space and the bundle are $T_x^* M$ and $T^* M$.
The smooth vector fields and dual vector fields(1-form) on M are $\mathfrak{X}(M)$,$\Omega(M)$.
The n-forms are $\Omega^n(M)$.

Riemannian Metric

$g : T_x M \times T_x M \to \mathbb{R}$ is the Riemannian metric over M, which is a 2-form. The volume form onwards is $dw := \det g dx$
The unique affine associated connection, i.e., **Levi-Civita connection**, ∇_g. The divergencediv$_g$ and Laplacian operator $\Delta_g := \mathrm{div}_g \circ \nabla_g$ is:

$$\mathrm{div}_g(X) := d\iota_X w, \iota_X w(X_0, X_1, ... X_{n-1}) = w(X, X_1, ... X_{n-1}), w \in \Omega^n(M) \tag{23}$$

What is an ODE on a manifold

Einstein Summation Convention

$$a_i b^i := \sum_i a_i b^i \tag{24}$$

Usually, the solution of an ODE on a manifold is a **curve**(also **flow** in some literature) $\gamma(t)$.

Example

Geodesic. $\gamma(t)$ where $\dot{\gamma} := \frac{d\gamma^i}{dt}\frac{\partial}{\partial x^i}$ is a geodesic iff

$$\nabla_{\dot{\gamma}(t)}\dot{\gamma}(t) = 0 \Leftrightarrow \frac{\mathrm{d}^2}{\mathrm{d}t^2}\gamma^{\mathrm{i}} + \Gamma^i_{jk}\frac{d\gamma^j}{dt}\frac{d\gamma^k}{dt} = 0 \tag{25}$$

where the second Christoffel symbol $\nabla_{\frac{\partial}{\partial x^i}}\frac{\partial}{\partial x^j} =: \Gamma^k_{ij}\frac{\partial}{\partial x^k}$

More Examples

Example

A more generalized version is:

$$\dot{y} = f(y), y(0) = y_0 \tag{26}$$

where $y \in M, f : M \to T_x M$

Usually, the manifold can be viewed as a parameter manifold of a system. The solution of such an ODE/PDE depicts how the system evolves.

Example

(EL-equation in Lagragian Mechanics) $(q, v) \in TM$

$$\frac{\partial L}{\partial q^k} - \frac{d}{dt}\frac{\partial L}{\partial v^k} = 0 \tag{27}$$

More Examples

Example

(**Hamilton Mechanics**) A **Lagragian system** is depicted by a manifold with its tangent space, i.e., **the tangent bundle** TM. A **Hamilton system** instead use a fiber map $F : TM \to T^*M$ given by:

$$F[L(x,v)](w) := \frac{d}{dt}|_{t=0} L(x, v + tw) \tag{28}$$

where L is the Lagragian, $(x,v) \in TM$. Via Riesz Representation Theorem in Hilbert space, we have a one-to-one mapping F, and write as $F : (x,v) \mapsto (x, v_\flat), v \in TM, v_\flat \in T^*M$. The inverse mapping is $F^{-1} : (x,p) \mapsto (x, p^\sharp)$. Given a Hamiltonian $H : M \times T^*M \to \mathbb{R}$ depicted by$(q,p) \in M \times T^*M$, the system follows:

$$\frac{d}{dt} q^k = \frac{\partial H}{\partial p_k}(x(t), p(t)); \frac{d}{dt} p^k = -\frac{\partial H}{\partial q_k}(x(t), p(t)) \tag{29}$$

Naive FDM

If the manifold is embedded in $\mathbb{R}^n$, then one can take the tangent space on M as a subspace in $\mathbb{R}^n$ and use FDM directly.
However, since it always happens that the obtained $y^{n+1} \notin M$ even if $y^n \in M$, a projection step is required.

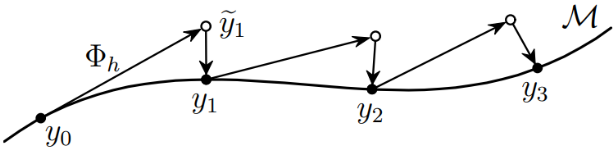

Fig. 4: Naive FDM

PDE on Manifold

Example

A heat eq. can occur on a manifold. Suppose the temperature $u : M \to \mathbb{R}$ on M:

$$u_t - \Delta_g(u) = 0 \tag{30}$$

which is given by:

$$\nabla u := g^{ij} \frac{\partial u}{\partial x^i} \frac{\partial}{\partial x^j} \tag{31}$$

$$\operatorname{div}_g X := \frac{1}{\sqrt{|\det g|}} \frac{\partial}{\partial x^i} (b^i \sqrt{|\det g|}), X = b^i \frac{\partial}{\partial x^i} \tag{32}$$

$$\Delta_g u := \operatorname{div}_g \nabla u = \frac{1}{\sqrt{|\det g|}} \frac{\partial}{\partial x^i} (g^{ij} \frac{\partial u}{\partial x^i} \sqrt{|\det g|}) \tag{33}$$

Elliptic Equations

Δ_g has many good properties and therefore the harmonic analysis rises. Many powerful tools within can be applied to solving PDE with Δ_g, as **[1,2]**.

Example

Elliptic Equation

$$a(x) + \mathrm{div}_g(\kappa(x)\nabla_g u(x)) = 0 \tag{34}$$

Problems to Solve

Suppose we have a point cloud dataset, (x, y) where $x \in M \subset \mathbb{R}^m, y = u(x)$, we are going to solve $u : M \to \mathbb{R}$.

- How to reconstruct the manifold by the point cloud?
- How to solve the PDE given a manifold?
- Another way: can we solve u on an unknown manifold? **[1,2]**

THE END.