Loss as an integral

PDE: $\quad u_{xx} - f = 0 \qquad x \in (0,1)$

Integral loss: $\quad L = \int_0^1 (u_{xx}(x) - f(x))^2 \, dx$

Discretize: $\quad L \approx \sum_{i=1}^{N} \Delta x_i (u_{xx}(x_i) - f(x_i))^2$

Why?
- Error analysis
- Automatic scaling with N
- More accurate quadrature

Integral equations

Ex $\nabla \cdot (u, v, w) = 0$ $\qquad \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0$

$$\Longleftrightarrow \iiint_V \nabla \cdot (u, v, w)\, dx = 0 \quad \text{for any volume } V$$

$$\underset{\text{div thm}}{\Longleftrightarrow} \oiint_S \vec{n} \cdot (u, v, w)\, dS = 0 \quad \text{for any closed surface } S$$

$$L_S = \left(\sum_{i=1}^{N} \vec{n}(x_i) \cdot (u(x_i), v(x_i), w(x_i)) \right)^2 \quad \text{for } x_i \in S$$

$$L = \sum_S L_S \quad \text{for many surfaces } L_S$$

Parameterized geometry

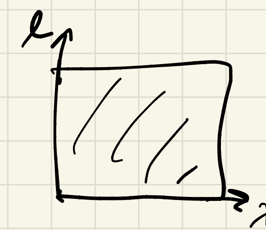
Ex

$$u_{xx} - f = 0 \qquad \text{for} \quad x \in (0, \ell)$$

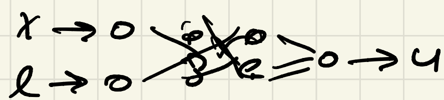
$$u(0) = u(\ell) = 0$$

ℓ is a parameter $\qquad \ell \in [1, 2]$

$\Rightarrow$ want $u(x; \ell)$



PINN



$$L_r = \int_1^2 \int_0^\ell \left(u_{xx}(x;\ell) - f(x)\right)^2 dx\, d\ell$$

$$L_{BC} = \int_1^2 \left((u(0;\ell) - 0)^2 + (u(\ell;\ell) - 0)^2 \right) d\ell$$

Weak solutions

Strong form of PDE: twice-differentiable functions

zero on $\partial\Omega$

Find $u \in H^2(\Omega) \cap H^1_0(\Omega)$ such that

boundary of Ω

$$\Delta u - f = 0 \quad \text{in } \Omega$$

Transform: $$\int_\Omega (\Delta u - f)\, v \, dx = 0 \quad \text{for any } v \in C_0^\infty(\Omega)$$

test functions

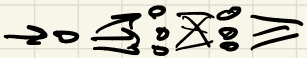
int. by parts: $$\int_{\partial\Omega} \nabla u \cdot \cancelto{0}{\vec{n}\, v}\, dx - \int_\Omega (\nabla u \cdot \nabla v + f v)\, dx = 0$$

once-diff functions

Weak form: find $u \in H_0^1(\Omega)$ such that

$$\int_\Omega (\nabla u \cdot \nabla v + f v)\, dx = 0 \quad \text{for all} \quad v \in H_0^1(\Omega)$$

VPINN – Variational PINN, Kharazmi 2019

NN $u_\theta(x)$ $x \to$  u

choose set of test functions $v_j \in H^1(\Omega)$

variational residual: $R_j(u_\theta) = \int_\Omega (\nabla u_\theta \cdot \nabla v_j + f v_j)\, dx$

boundary residual: $R_{b,j}(u_\theta) = \int_{\partial\Omega} (u_\theta - u_b)\, v_j \, dx$

loss: $L_\theta = \sum_j \left(R_j(u_\theta)\right)^2 + \sum_j \left(R_{b,j}(u_\theta)\right)^2$

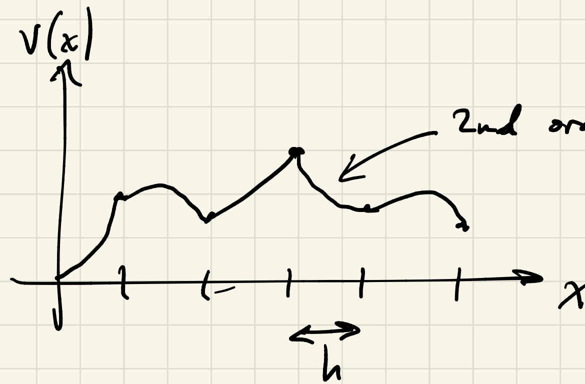
hp - VPINNs (Kharazmi 2020)

h: grid size

p: order of polynomials

u is NN

v is piecewise polynomials
order p
on mesh grid size h



2nd order polys, $p=2$