1D Poisson Eq.

- Governing eq. : $\frac{d^2y}{dx^2} + \pi^2 \sin(\pi x) = 0$

- Boundary conditions :

  $y(-1) = 0$ and $y(1) = 0$

  → applied to '$loss_{BC}$' :

  $loss_{BC} = (y(-1) - 0)^2 + (y(1) - 0)^2$

- Residual or Loss :

  $$\text{residual or } loss_{PDE} = \frac{d^2 y_{nn}(x)}{dx^2} + \pi^2 \sin(\pi x)$$

  (y_{nn} = y_neural network)

- Total loss : $Loss = Loss_{PDE} + Loss_{BC}$

Key steps for PINNs

1) Define Neural Network

- Input : spatial coordinate x.
- Hidden layer : Non-linear transformations to approximate the solution.
- Output : predicted $y_{nn}(x)$

$\Big\}$ θ parameter

$\hat{y}(x) = N_\theta(x) \rightsquigarrow = y\_pred(x)$

N_θ = NN with θ parmeter

2) Compute Derivatives

- We can use 'tf.GradientTape' to compute $\frac{d^2y}{dx^2}$

3) Define Residual

- Compute the residual of the differential Eq.

$$\underbrace{r(x;\theta) = \text{residual}} = \frac{d^2y(x)}{dx^2} + \pi^2 \sin(\pi x)$$

~ PDE$(x;\theta)$

4) Loss function

- Combine residual loss and boundary loss

'total loss = MSE_residual + MSE_boundary conditions'

e.g., $L_{PDE} = \frac{1}{N}\sum_{i=1}^{N}(r(x_i;\theta))^2$ $\qquad$ $L_{BC} = \frac{1}{N_{bc}}\sum_{j=1}^{N_{bc}}(y_{bc}^{(j)} - \hat{y}(x_{bc}^{(j)}))^2$

- N = # of collocation points
- N_{bc} = # of boundary conditions

5) Training

- Min. loss function using an optimizer
- Optimizer: $\theta \leftarrow \theta - \eta \nabla_\theta L(\theta)$

  How we use $\nabla_\theta L$ by processing it.

parameter θ :

$\theta = [W_1, b_1, W_2, b_2, W_3, b_3, W_{out}, b_{out}]$

- parameters of 3 hidden layers + output layer

- $\nabla_\theta L$ = grads = $\left[\frac{\partial L}{\partial W_1}, \frac{\partial L}{\partial b_1}, \frac{\partial L}{\partial W_2}, \frac{\partial L}{\partial b_2}, \frac{\partial L}{\partial W_3}, \frac{\partial L}{\partial b_3}, \frac{\partial L}{\partial W_{out}}, \frac{\partial L}{\partial b_{out}}\right]$

Additional) Analytical solution.

$$\underbrace{0 = \frac{d^2y(x)}{dx^2} + \pi^2 \sin(\pi x)} \rightsquigarrow y'' = -\pi^2 \sin(\pi x)$$

$x \in [-1, 1]$, $y(-1)=0$, $y(1)=0$

2D linear nonhomogeneous ODE

Homogeneous part : $y''(x) = 0$, $y(x) = Ax + B$

Non-homogeneous part : $y''(x) = -\pi^2 \sin(\pi x)$

$y = \sin(\pi x) \rightsquigarrow y' = \pi\cos(\pi x) \rightsquigarrow y'' = -\pi^2 \sin(\pi x)$

Therefore, $y = \sin(\pi x)$ for non-homogeneous part

⇒ General solution

$$y(x) = \sin(\pi x) + Ax + B$$

BC 1 : $y(-1)=0$, $0 = \overset{\sim 0}{\sin(-\pi)} - A + B \rightsquigarrow A = B$ ①

BC 2 : $y(1)=0$, $0 = \overset{\sim 0}{\sin(\pi)} A + B \rightsquigarrow A + B = 0$ ②

① & ② → $A = 0$, $B = 0$

$\therefore y(x) = \sin(\pi x)$

Loss estimation

- L_2 norm
- L_1, L_∞, etc.
- Weighted norm
- H_1 norm
- Robust loss : Huber, pseudo-Huber loss
- Energy norm : functional from PDE (physics eq.)

Optimizer types

- SGD : Stochastic Gradient Descent
- SGD with momentum : consider step direction
- Nesterov Accelerated Gradient (NAG)
- AdaGrad → RMSProp
- Adam : Momentum + RMSProp
  1st moment (EMA of grad.)
  + 2nd moment (EMA of grad.^{2})
- AdamW
- L-BFGS : rough approx. by Adam
  + Fine-tune by L-BFGS

  PINN에서 같이 사용
- Lion