2025 USA-NA-AIO Round 2, Problem 1, Part 2

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The high level idea of PINN is as follows:

1. **(Neural network)** We design a neural network (functional mapping) $U\left(\cdot,\cdot \mid \theta\right) : [0,1]^2 \rightarrow \mathbb{R}$, such that

   ○ θ: learnable parameters in U.

   ○ Inputs are time t and position x.

   ○ Output is the predicted temperature.

2. **(Training data)** To train U (equivalently, to learn θ), we use the following three groups of temporal-spacial data (t, x):

   ○ **(Training data for PDE)** (t, x) are randomly sampled from $[0,1]^2$.

      Denote by $\mathcal{D}_{PDE}$ the set of these data points.

   ○ **(Training data for IC)** $(0, x)$ with x that are evenly distributed on $[0, 1]$.

      Denote by $\mathcal{D}_{IC}$ the set of these data points.

   ○ **(Training data for BC)** $(t, 0)$ and $(t, 1)$ with t that are evenly distributed on $[0, 1]$.

      Denote by $\mathcal{D}_{BC}$ the set of these data points.

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3. **(Loss function in training)**

$$L_{total} = L_{PDE} + L_{IC} + L_{BC},$$

where

- Residual loss in PDE:

$$L_{PDE} = \frac{1}{|\mathcal{D}_{PDE}|} \sum_{(t,x)\in\mathcal{D}_{PDE}} \left(\frac{\partial U(t,x|\theta)}{\partial t} - \alpha \frac{\partial^2 U(t,x|\theta)}{\partial x^2} \right)^2.$$

- IC loss:

$$L_{IC} = \frac{1}{|\mathcal{D}_{IC}|} \sum_{(t,x)\in\mathcal{D}_{IC}} \left(U(t,x|\theta) - u(t,x) \right)^2.$$

- BC loss:

$$L_{BC} = \frac{1}{|\mathcal{D}_{BC}|} \sum_{(t,x)\in\mathcal{D}_{BC}} \left(U(t,x|\theta) - u(t,x) \right)^2.$$

Part 2 (10 points, coding task)

In this part, you are asked to build a deep neural network that is used to output PDE solutions.

1. The class name is `HeatPINN`.

   It subclasses `nn.Module`.

2. The model consists of the following layers that are sequentially conntected:

(1) Fully connected layer with `out_features = 64` (you need to determine `in_features` taken from the input).

(2) Activation layer with tanh function.

(3) Fully connected layer with `in_features = 64` and `out_features = 64`.

(4) Activation layer with tanh function.

(5) Fully connected layer with `in_features = 64` (you need to determine `out_features` as the output of the entire model).

3. Construct a model who is an object of this class and is called as `model`.

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```python
### WRITE YOUR SOLUTION HERE ###

class HeatPINN(nn.Module):
    def __init__(self):
        super().__init__()
        self.net = nn.Sequential(
            nn.Linear(2, 64),
            nn.Tanh(),
            nn.Linear(64, 64),
            nn.Tanh(),
            nn.Linear(64, 1)
        )

    def forward(self, x):
        return self.net(x)

model = HeatPINN()

""" END OF THIS PART """
```

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