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2025 USA-NA-AIO Round 2, Problem 1, Part 10

USAAIO 

May 2025

Part 10 (10 points, coding task)

This part asks you to do a mini-batch training of the model.

1. Set the parameter in the PDE $\alpha = 0.1$. (This is not for learning. In PINN, we know the exact form of a PDE. We just need neural networks to help us solve it.)

2. Set the number of epochs as 1000.

3. Define

```
device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
```

4. While iterating over epochs, use `tqdm` to track the progress:

```
for epoch in tqdm(range(num_epochs)):
```

5. In each epoch,

(1) Configure the model to the training mode.

(2) Iterate over all mini-batches of `dataset_train_PDE`.

(3) For each of the above mini-batch of the PDE dataset, while computing the total loss function, you also need to use **all** data in `dataset_train_IC` and `dataset_train_BC`.

(4) Do all these tasks on **GPU**.

6. In each epoch, after training over all mini-batches, if the epoch index is divisible by 100, do the following tasks:

- (1) Configure the model to the evaluation mode.
- (2) Compute the total loss over the entire three datasets: `dataset_train_PDE` ,
`dataset_train_IC` , `dataset_train_BC` .
- (3) Print the epoch index, the residual loss from PDE, the IC loss, the BC loss, and the total loss.
- (4) Do all these tasks on **CPU**.

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

```
alpha = 0.1
num_epochs = 1000
device = torch.device("cuda" if torch.cuda.is_available() else "cpu")

for epoch in tqdm(range(num_epochs)):
    model.train()
    model.to(device)
    for batch_PDE in dataloader_PDE:
        batch_PDE = batch_PDE.to(device)
        optimizer.zero_grad()
        U_PDE = model(batch_PDE)
        U_t_and_x_PDE = autograd.grad(torch.sum(U_PDE), batch_PDE, create_graph=True)
        U_t_PDE = U_t_and_x_PDE[:,0]
        U_x_PDE = U_t_and_x_PDE[:,1]
        U_xx_PDE = autograd.grad(torch.sum(U_x_PDE), batch_PDE, create_graph=True)
        loss_PDE = torch.mean((U_t_PDE - alpha * U_xx_PDE)**2)

    U_IC = model(dataset_train_IC.to(device))
    loss_IC = torch.mean((U_IC - u_IC.to(device))**2)

    U_BC = model(dataset_train_BC.to(device))
    loss_BC = torch.mean(U_BC**2)
```

[Skip to main content](#)

```

        loss = loss_PDE + loss_IC + loss_BC
        loss.backward()
        optimizer.step()

    if epoch % 100 == 0:
        model.eval()
        model.to('cpu')
        batch_PDE = next(iter(dataloader_PDE))
        batch_PDE.requires_grad_(True)
        U_PDE = model(batch_PDE)
        U_t_and_x_PDE = autograd.grad(torch.sum(U_PDE), batch_PDE, create_graph=True)
        U_xx_PDE = autograd.grad(torch.sum(U_t_and_x_PDE[:,1]), batch_PDE, create_graph=True)
        loss_PDE = torch.mean((U_t_and_x_PDE[:,0] - alpha * U_xx_PDE)**2)

        with torch.no_grad():
            U_IC = model(dataset_train_IC)
            loss_IC = torch.mean((U_IC - u_IC)**2)
            U_BC = model(dataset_train_BC)
            loss_BC = torch.mean(model(dataset_train_BC)**2)
            loss = loss_PDE + loss_IC + loss_BC

        print(f"{loss_PDE.item():.4e}, {loss_IC.item():.4e}, {loss_BC.item():.4e}")
        print(f"Epoch {epoch}, Loss: {loss.item():.4e}")

    """ END OF THIS PART """

```

[Skip to main content](#)

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