Assignment 3.

✍️ Written assignment

1. Reading and Explaining Lemmas

   Your task is to read the following paper:

   > **Ryck et al.**, ***On the approximation of functions by tanh neural networks***
   > Link to paper

   Focus on **Lemma 3.1** and **Lemma 3.2**.

Goal: To claim that neural networks with tanh activation function can approximate polynomials very well (both value and their derivative).

Lemma 3.1 (for odd powers)

For odd p, $p \le s$, there exists a one-hidden-layer tanh network of width $\frac{s+1}{2}$ that can simultaneously approximate all $\{y^p\}$ on the interval $[-M, M]$ with error at most ε.

Idea: (1) Expand $\tanh(y)$ in Taylor series

(2) Apply central difference operator δ_h^p to eliminate lower-order terms and remain y^p (odd-power)

(3) When h is small enough, the error can be controlled.

Lemma 3.2 (extending to even powers).

For odd p, there exists a one-hidden-layer tanh network of width $\frac{3(s+1)}{2}$ that can simultaneously approximate all $\{y^k\}_{k\in\mathbb{N}, k\le s}$ on the interval $[-M, M]$ with error at most ε.

Idea: (1) Odd powers are handled by Lemma 3.1

(2) For even power, use algebraic identity:

$$y^{2n} = \frac{1}{2\alpha(2n+1)}\left[(y+\alpha)^{2n+1} - (y-\alpha)^{2n+1} - 2\sum_{k=0}^{n-1}\binom{2n+1}{2k}\alpha^{2(n-k)+1}y^{2k}\right].$$

$\Rightarrow$ even powers can be expressed in terms of odd powers and lower even powers.

(3) By selecting α, the error can be controlled.

Remark. Lemma 3.2 construct a shallow (one-hidden-layer) network to approximate every monomial up to degree s, so we can approximate any polynomial and then approximate smooth functions.

2. Unanswered Questions

   There are unanswered questions from the lecture, and there are likely more questions we haven't covered.

Is there a clear trade-off between network depth versus width in achieving approximation rates?

(Under the constraint of fixed parameter count or computational budget, does there exist a relation that characterizes the optimal depth/width configuration required to minimize the error?)

👨‍💻 Programming assignment

1. Use the **same code** from Assignment 2 - programming assignment 1 to calculate the error in approximating the derivative of the given function.

```
#derivative MSE
net.eval()
x_test = np.linspace(-1, 1, 500).reshape(-1, 1).astype(np.float32)
x_test_tensor = torch.from_numpy(x_test)
x_test_tensor.requires_grad_(True)

y_hat = net(x_test_tensor)
dy_dx_hat = torch.autograd.grad(
    outputs = y_hat,
    inputs = x_test_tensor,
    grad_outputs = torch.ones_like(y_hat),
    retain_graph = False,
    create_graph = False,
)[0]

#f'(x) = -50x/(1+25x^2)^2
with torch.no_grad():
    x_np = x_test
    dy_dx_true_np = -(50.0 * x_np) / (1.0 + 25.0 * x_np**2)**2
    dy_dx_true =
torch.from_numpy(dy_dx_true_np.astype(np.float32))
deriv_mse = torch.mean((dy_dx_hat - dy_dx_true)**2).item()
print(f"Derivative Approximation MSE: {deriv_mse:.6f}")
```

Result: Derivative Approximation MSE: 0.000218.

2. In this assignment, you will use a neural network to approximate both the **Runge function** and its **derivative**. Your task is to train a neural network that approximates:
   a. The function $f(x)$ itself.
   b. The derivative $f'(x)$.
   You should define a **loss function** consisting of two components:
   1). **Function loss:** the error between the predicted $f(x)$ and the true $f(x)$.
   2). **Derivative loss:** the error between the predicted $f'(x)$ and the true $f'(x)$.

   Write a short report (1–2 pages) explaining method, results, and discussion including

   - Plot the true function and the neural network prediction together.
   - Show the training/validation loss curves.
   - Compute and report errors (MSE or max error).

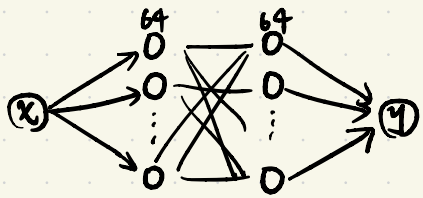
Runge function : $f(x) = \frac{1}{1+25x^2}$, $x \in [-1, 1]$,

$$f'(x) = \frac{-50x}{(1+25x^2)^2}$$

Method : feedforward neural network

dataset : uniformly sampling 200 points from $[-1, 1]$ and the data was split into 80% training and 20% validation sets .

network architecture :



using tanh activations .

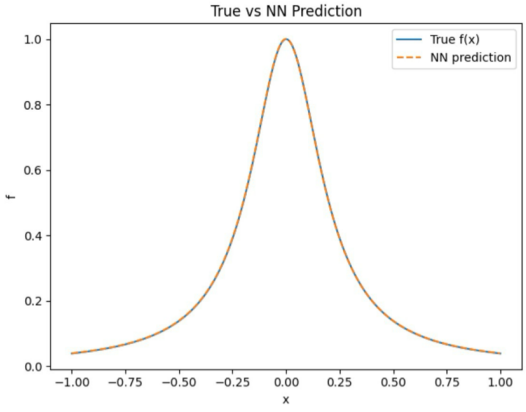
loss function: combined MSE , $\lambda = 1$.

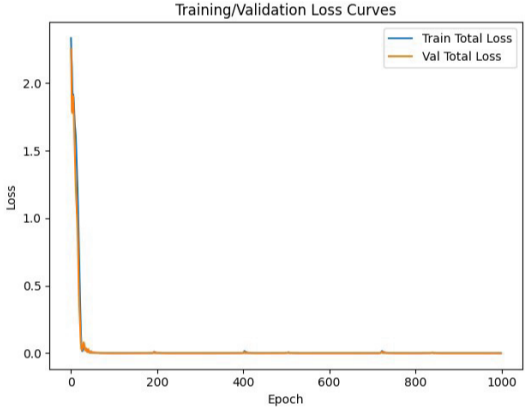
$$L := MSE(f(x), \hat{f}(x)) + \lambda \cdot MSE(f'(x), \hat{f}'(x))$$

optimizer : Adam , learning rate 0.01 , 1000 epochs

Results :

```
Epoch [200/1000] Train Total: 0.000110 (f: 0.000009, f': 0.000102) | Val Total: 0.001828 (f: 0.000045, f': 0.001783)
Epoch [400/1000] Train Total: 0.001762 (f: 0.000117, f': 0.001645) | Val Total: 0.002091 (f: 0.000251, f': 0.001840)
Epoch [600/1000] Train Total: 0.000004 (f: 0.000000, f': 0.000004) | Val Total: 0.000005 (f: 0.000000, f': 0.000005)
Epoch [800/1000] Train Total: 0.000006 (f: 0.000000, f': 0.000006) | Val Total: 0.000008 (f: 0.000000, f': 0.000007)
Epoch [1000/1000] Train Total: 0.000002 (f: 0.000000, f': 0.000002) | Val Total: 0.000003 (f: 0.000000, f': 0.000003)
```






```
Final Test MSE (f):   0.000000
Final Test MSE (f'):  0.000002
```

- Training and validation losses both decrease smoothly
- The network's prediction closely match the true Runge function.

```
import torch
import torch.nn as nn
import torch.optim as optim
import matplotlib.pyplot as plt
import numpy as np
from sklearn.model_selection import train_test_split
torch.manual_seed(0)
np.random.seed(0)

#Runge function and derivative
def runge_function(x):
    return 1.0 / (1.0 + 25.0 * x**2)

def runge_derivative_np(x_np):
    # f'(x) = -50x / (1+25 x^2)^2  (numpy)
    return -(50.0 * x_np) / (1.0 + 25.0 * x_np**2)**2

#dataset
x = np.linspace(-1, 1, 200).reshape(-1, 1).astype(np.float32)
y = runge_function(x).astype(np.float32)
x_train, x_val, y_train, y_val = train_test_split(
    x, y, test_size=0.2, random_state=42
)

x_train_t = torch.from_numpy(x_train)
y_train_t = torch.from_numpy(y_train)
x_val_t = torch.from_numpy(x_val)
y_val_t = torch.from_numpy(y_val)

dy_train_t = torch.from_numpy(runge_derivative_np(x_train).astype(np.float32))
dy_val_t = torch.from_numpy(runge_derivative_np(x_val).astype(np.float32))

#model
class Net(nn.Module):
    def __init__(self):
        super().__init__()
        self.fc1 = nn.Linear(1, 64)
        self.fc2 = nn.Linear(64, 64)
        self.fc3 = nn.Linear(64, 1)
        self.activation = nn.Tanh()
    def forward(self, x):
        x = self.activation(self.fc1(x))
        x = self.activation(self.fc2(x))
        x = self.fc3(x)
        return x

net = Net()

#Loss:= function loss + derivative loss
mse = nn.MSELoss()

train_loss_all, val_loss_all = [], []
train_loss_f, train_loss_df = [], []
val_loss_f, val_loss_df = [], []

lambda_deriv = 1.0
lr = 0.01
optimizer = optim.Adam(net.parameters(), lr=lr)

for epoch in range(epochs):
    net.train()
    optimizer.zero_grad()

    x_train_req = x_train_t.detach().clone().requires_grad_(True)

    y_hat = net(x_train_req)

    dy_hat = torch.autograd.grad(
        outputs = y_hat,
        inputs = x_train_req,
        grad_outputs = torch.ones_like(y_hat),
        create_graph = True,
        retain_graph = True
    )[0]

    loss_f  = (y_hat - y_train_t).pow(2).mean()
    loss_df = (dy_hat - dy_train_t).pow(2).mean()
    loss = loss_f + lambda_deriv * loss_df

    loss.backward()
    optimizer.step()

    net.eval()
    with torch.no_grad():
        y_val_hat = net(x_val_t)
        loss_f_val = (y_val_hat - y_val_t).pow(2).mean().item()

    x_val_req = x_val_t.detach().clone().requires_grad_(True)
    y_val_hat2 = net(x_val_req)
    dy_val_hat = torch.autograd.grad(
        outputs = y_val_hat2,
        inputs = x_val_req,
        grad_outputs = torch.ones_like(y_val_hat2),
        create_graph = False,
        retain_graph = False
    )[0].detach()
    loss_df_val = (dy_val_hat - dy_val_t).pow(2).mean().item()

    train_loss_all.append(loss.item())
    val_loss_all.append(loss_f_val + lambda_deriv * loss_df_val)
    train_loss_f.append(loss_f.item())
    train_loss_df.append(loss_df.item())
    val_loss_f.append(loss_f_val)
    val_loss_df.append(loss_df_val)

    if (epoch + 1) % 200 == 0:
        print(f"Epoch [{epoch+1}/{epochs}] "
              f"Train Total: {train_loss_all[-1]:.6f} "
              f"(f: {train_loss_f[-1]:.6f}, df: {train_loss_df[-1]:.6f}) | "
              f"Val Total: {val_loss_all[-1]:.6f} "
              f"(f: {val_loss_f[-1]:.6f}, df: {val_loss_df[-1]:.6f})")

#true f(x) vs NN prediction
plt.figure(figsize=(12,5))
plt.subplot(1,2,1)
plt.plot(x_test, y_test, label="True f(x)")
plt.plot(x_test, net(torch.from_numpy(x_test)).detach().numpy(),
         "--", label="NN prediction")
plt.xlabel("x"); plt.ylabel("f")
plt.title("True vs NN Prediction")
plt.legend()
plt.tight_layout()
plt.show()

#training/validation total loss curves
plt.figure(figsize=(12,5))
plt.subplot(1,2,2)
plt.plot(train_loss_all, label="Train Total Loss")
plt.plot(val_loss_all, label="Val Total Loss")
plt.xlabel("Epoch"); plt.ylabel("Loss")
plt.title("Training/Validation Loss Curves")
plt.legend()
plt.tight_layout()
plt.show()

#final test MSE
criterion = nn.MSELoss()
with torch.no_grad():
    test_mse_f = criterion(torch.from_numpy(y_test),
net(torch.from_numpy(x_test))).item()
x_test_req2 = torch.from_numpy(x_test).requires_grad_(True)
y_hat_t = net(x_test_req2)
dy_hat_t = torch.autograd.grad(
    outputs = y_hat_t,
    inputs = x_test_req2,
    grad_outputs = torch.ones_like(y_hat_t),
    create_graph = False,
    retain_graph = False
)[0].detach()
test_mse_df = criterion(dy_hat_t, torch.from_numpy(dy_true)).item()

print(f"Final Test MSE (f):   {test_mse_f:.6f}")
print(f"Final Test MSE (f'):  {test_mse_df:.6f}")
```