PINN_Damped_HO

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1 Importing Necessary Libraries

[1]:
```
import torch
import torch.nn as nn
import torch.optim as optim

import numpy as np
import matplotlib.pyplot as plt
```

2 Defining Neural Network Model along with Sine activation function

- I am using Sine activation function because it is smooth and more accurately reflects a periodic oscillation

[2]:
```
class SineActivation(nn.Module):
    def forward(self, input):
        return torch.sin(input)

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

    def forward(self, z, xi):
        inputs = torch.cat((z, xi), dim=1)
        return self.net(inputs)
```

3 Declaring Residual and Initial Condition Loss functions

- **physics_loss:** Here I have defined the physics loss by calculating the gradient of x wrt z and subsequently $\frac{dx}{dz}$ wrt z. I have also added a weight term to the residual loss, which is set on the basis of ξ, or damping factor that we take, so that small ξ value will result in higher weight and vice-versa. I did this because for smaller ξ value the solution is more oscillatory and thus the physics loss should be accordingly weighed.
- **initial_condition_loss:** This is just the calculation of loss incurred at initial condition, corresponding to different ξ values taken. I have also added a weighing factor so that the neural network model strictly learns to adjust to the initial condition.

[3]:
```
def physics_loss(model, z, xi):
    z.requires_grad_(True)

    x = model(z, xi)
    dx_dz = torch.autograd.grad(x, z, torch.ones_like(x), create_graph=True)[0]
    d2x_dz2 = torch.autograd.grad(dx_dz, z, torch.ones_like(dx_dz),␣
 ↪create_graph=True)[0]

    residual = d2x_dz2 + 2 * xi * dx_dz + x
    weight = 1 / (1 + xi)
    return torch.mean(weight * residual**2)

def initial_condition_loss(model, lambda_ic, xi_samples):
    z0 = torch.zeros((len(xi_samples), 1), dtype=torch.float32,␣
 ↪requires_grad=True)
    xi0 = xi_samples

    x0_pred = model(z0, xi0)
    v0_pred = torch.autograd.grad(x0_pred, z0, torch.ones_like(x0_pred),␣
 ↪create_graph=True)[0]

    ic_loss = torch.mean((x0_pred - 0.7) ** 2 + (v0_pred - 1.2) ** 2)
    return lambda_ic * ic_loss
```

4 Setting up the model and training it

Here I am setting up the device-agnostic code, so that the model can run on GPU if it's available. Then I am instantiating the model, the optimizer and learning rate scheduler.

[4]:
```
device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
model = PINN().to(device)
optimizer = optim.Adam(model.parameters(), lr=0.01)
scheduler = optim.lr_scheduler.StepLR(optimizer, step_size=5000, gamma=0.7)
```

Setting up the number of epochs, weight factor for loss calculated at intial condition and defining collocation points.

[5]:
```
epochs = 20001
lambda_ic = 10

z_train = torch.linspace(0, 20, 200, dtype=torch.float32).view(-1, 1).to(device)
```

5 Training Loop

In this training loop I am re-weighting the *lambda_ic* factor at every 1000 epochs by a factor of 0.9, as I saw that this helped with the training.

[6]:
```
for epoch in range(epochs):
    optimizer.zero_grad()

    xi_train = (torch.rand(200, 1) * 0.3 + 0.1).to(device)

    loss_pde = physics_loss(model, z_train, xi_train)
    loss_ic = initial_condition_loss(model, lambda_ic, xi_train)
    loss = loss_pde + loss_ic

    loss.backward()
    optimizer.step()
    scheduler.step()

    if epoch % 1000 == 0 and lambda_ic > 1.0:
        lambda_ic *= 0.9

    if epoch % 2000 == 0:
        print(f"Epoch {epoch}, Loss: {loss.item()}", flush=True)
```

```
Epoch 0, Loss: 20.735368728637695
Epoch 2000, Loss: 0.00197867164388299
Epoch 4000, Loss: 0.0015107771614566445
Epoch 6000, Loss: 0.0002502085408195853
Epoch 8000, Loss: 0.00039816793287172914
Epoch 10000, Loss: 0.0005950320046395063
Epoch 12000, Loss: 5.842721293447539e-05
Epoch 14000, Loss: 0.00010185915016336367
Epoch 16000, Loss: 0.0004153420450165868
Epoch 18000, Loss: 2.4799222956062295e-05
Epoch 20000, Loss: 8.915261423680931e-05
```

6 Numerical Method Implementation that serves as a benchmark to validate the performance of the PINN solution.

6.1 `damped_oscillator(z, y, xi)`

Defines the differential equations governing a damped harmonic oscillator.

Parameters: - `z` – Independent variable. - `y` – State vector `[x, v]`. - `xi` – Damping coefficient.

Returns: - A NumPy array `[dx/dz, dv/dz]`, where: - `dx/dz = v` - `dv/dz = -2 * xi * v - x`

6.2 `rk4(f, z, y, h, xi)`

Implements the fourth-order Runge-Kutta (RK4) method for solving ordinary differential equations.

Parameters: - `f` – Function representing the ODE (in our case, `damped_oscillator`). - `z` – Current value of the independent variable. - `y` – Current state `[x, v]`. - `h` – Step size. - `xi` – Damping coefficient.

Returns: - Updated state `[x, v]` after one RK4 step.

6.3 `solve_damped_oscillator_rk4(x0, v0, xi, z_max, h)`

Numerically solves the damped harmonic oscillator using the RK4 method.

Parameters: - `x0` – Initial position. - `v0` – Initial velocity. - `xi` – Damping coefficient. - `z_max` – Maximum value for z. - `h` – Step size.

Returns: - `z_values` – Array of `z` values. - `x_values` – Array of position values `x(z)`.

This method initializes the system with given conditions and iteratively applies RK4 to solve the equations.

[7]:
```
def damped_oscillator(z, y, xi):
    x1, x2 = y
    dx1_dz = x2
    dx2_dz = -2 * xi * x2 - x1
    return np.array([dx1_dz, dx2_dz])

def rk4(f, z, y, h, xi):
    k1 = h * f(z, y, xi)
    k2 = h * f(z + h/2, y + k1/2, xi)
    k3 = h * f(z + h/2, y + k2/2, xi)
    k4 = h * f(z + h, y + k3, xi)
    return y + (k1 + 2*k2 + 2*k3 + k4) / 6

def solve_damped_oscillator_rk4(x0, v0, xi, z_max, h):
    z_values = np.arange(0, z_max + h, h)
    y_values = np.zeros((len(z_values), 2))
    y_values[0] = [x0, v0]

    for i in range(1, len(z_values)):
```

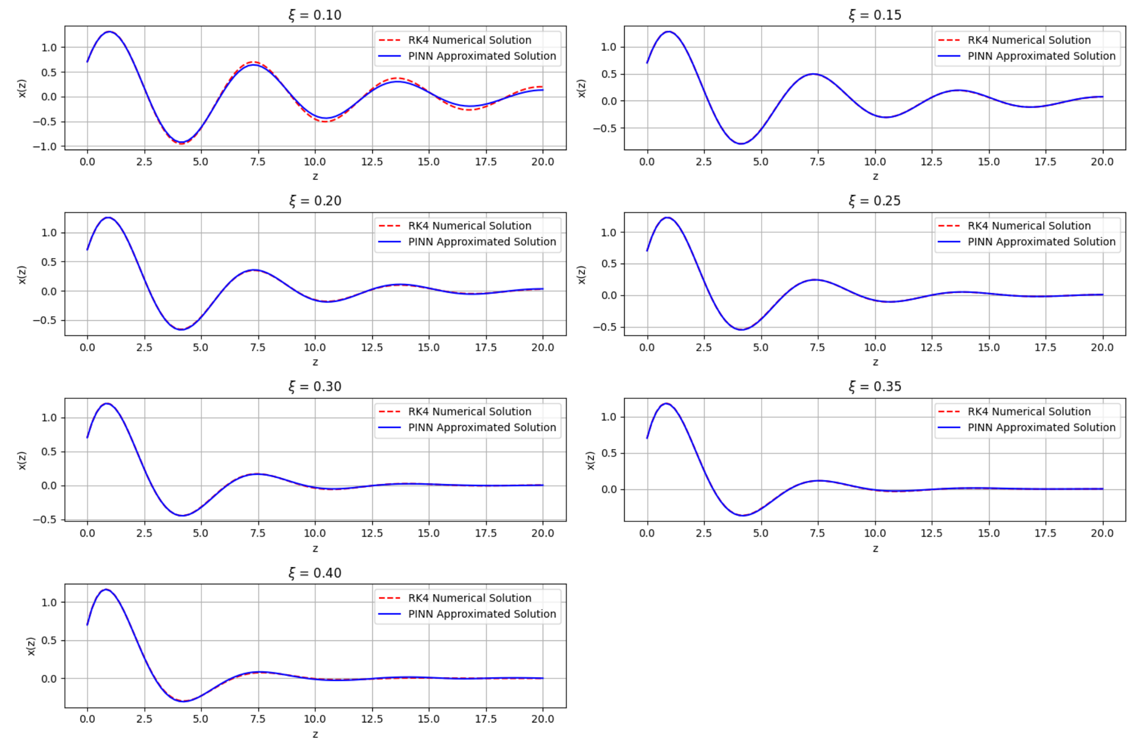
```
        y_values[i] = rk4(damped_oscillator, z_values[i-1], y_values[i-1], h,␣
↪xi)

    return z_values, y_values[:, 0]
```

$x_0 \longrightarrow$ initial position $v_0 \longrightarrow$ initial velocity

[8]:
```
x0, v0 = 0.7, 1.2
z_max, h = 20, 0.05
```

7 Plotting the PINN and RK4 solution for various values of ξ

[10]:
```
xi_test_vals = np.arange(0.1, 0.4, 0.05)

num_plots = len(xi_test_vals)

cols = 2
rows = (num_plots + cols - 1) // cols

fig, axes = plt.subplots(rows, cols, figsize=(15, 10))
axes = axes.flatten()

for i, xi_val in enumerate(xi_test_vals):

    z_values_rk4, x_values_rk4 = solve_damped_oscillator_rk4(x0, v0, xi_val,␣
↪z_max, h)

    z_test = torch.linspace(0, 20, 100).view(-1, 1)
    xi_test = torch.full_like(z_test, xi_val)
    x_pred = model(z_test, xi_test).detach().numpy()

    ax = axes[i]
    ax.plot(z_values_rk4, x_values_rk4, 'r--', label='RK4 Numerical Solution')
    ax.plot(z_test.numpy(), x_pred, 'b-', label='PINN Approximated Solution')
    ax.set_xlabel('z')
    ax.set_ylabel('x(z)')
    ax.set_title(fr'$\xi$ = {xi_val:.2f}')
    ax.legend()
    ax.grid(True)

for j in range(i + 1, len(axes)):
    fig.delaxes(axes[j])

plt.tight_layout()
plt.savefig("Damped_HO.jpg")
plt.show()
```


ξ = 0.10
ξ = 0.15
ξ = 0.20
ξ = 0.25
ξ = 0.30
ξ = 0.35
ξ = 0.40
RK4 Numerical Solution
PINN Approximated Solution
x(z)
z

```
[ ]:
```