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In [8]: import torch
import torch.nn as nn
import torch.autograd as autograd
```

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In [9]: import numpy as np
import matplotlib.pyplot as plt
```

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In [10]: device_name = torch.device('cuda' if torch.cuda.is_available() else 'cpu')
```

```
In [11]: def analytic_solution(t, x_0=1.0, v_0=0.0):
return x_0 * np.cos(t) + v_0 * np.sin(t)
```

Architecture for Initial Conditions Fixed Neural Network

```
In [21]: class HarmonicModel(nn.Module):
def __init__(self, x0, v0):
super().__init__()
self.network = nn.Sequential(
nn.Linear(1, 64),
nn.Tanh(),
nn.Linear(64, 64),
nn.Tanh(),
nn.Linear(64, 1)
)
self.x0 = x0
self.v0 = v0

def forward(self, t):
a = self.network(t)
return self.x0 + self.v0 * t + a * t**2
```

```
In [25]: def train_model(model):
num_samples = 200
epochs = 2000
lr = 1e-3
optimizer = torch.optim.Adam(model.parameters(), lr=lr)

values = torch.linspace(0, 2 * np.pi, num_samples, device=device_name).view(-1, 1).requires_grad_()
loss_history = []
for epoch in range(epochs):
optimizer.zero_grad()
x_predicted = model(values)

dx = autograd.grad(x_predicted, values, torch.ones_like(x_predicted), create_graph=True)[0]
d2x = autograd.grad(dx, values, torch.ones_like(dx), create_graph=True)[0]

loss = torch.mean((d2x + x_predicted) ** 2)
loss.backward()
optimizer.step()

if epoch % 500 == 0:
print(f"Epoch {epoch}: Loss = {loss.item():.6f}")

if epoch % 10 == 0:
loss_history.append((epoch, loss.item()))

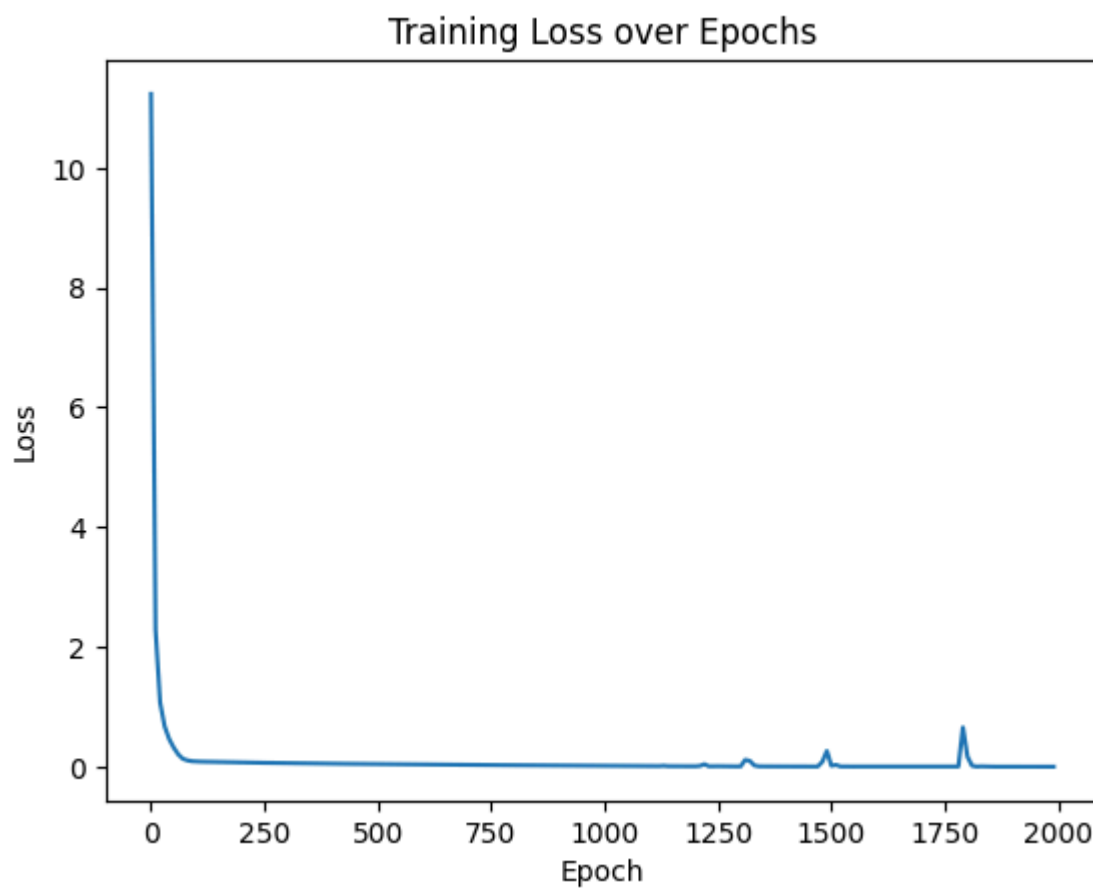
return loss_history
```

```
In [26]: x0 = 1.0
v0 = 1.0
model = HarmonicModel(x0, v0).to(device_name)
```

```
In [27]: loss_history = train_model(model)
plt.plot(*zip(*loss_history), label='Training Loss')
plt.xlabel('Epoch')
plt.ylabel('Loss')
plt.title('Training Loss over Epochs')
```

```
Epoch 0: Loss = 11.233688
Epoch 500: Loss = 0.045333
Epoch 1000: Loss = 0.016686
Epoch 1500: Loss = 0.017797
```

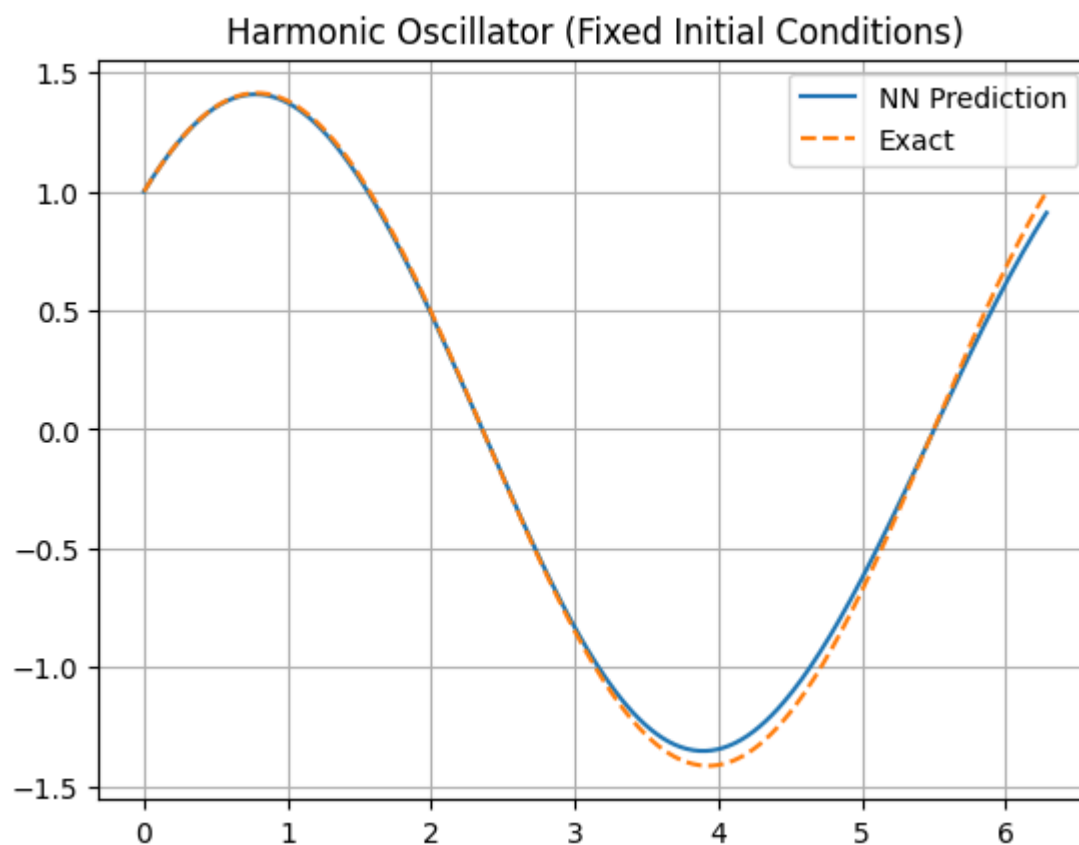
```
Out[27]: Text(0.5, 1.0, 'Training Loss over Epochs')
```



```
In [28]: validation_values = torch.linspace(0, 2 * np.pi, 300, device=device_name).view(-1, 1)
with torch.no_grad():
    x_nn = model(validation_values).cpu().numpy()

x_true = analytic_solution(validation_values.cpu().numpy(), x_0=x0, v_0=v0)

plt.plot(validation_values.cpu(), x_nn, label='NN Prediction')
plt.plot(validation_values.cpu(), x_true, '--', label='Exact')
plt.title("Harmonic Oscillator (Fixed Initial Conditions)")
plt.legend()
plt.grid()
plt.show()
```



Architecture for Boundary Conditions Fixed Neural Network

```
In [48]: class PeriodicResidualNet(nn.Module):
def __init__(self, hidden_dim=32):
    super().__init__()
    self.base = nn.Sequential(
        nn.Linear(2, hidden_dim),
        nn.Tanh(),
        nn.Linear(hidden_dim, hidden_dim),
        nn.Tanh(),
        nn.Linear(hidden_dim, 1)
    )
    self.a0 = nn.Parameter(torch.tensor([0.0]))
    self.a1 = nn.Parameter(torch.tensor([1.0]))
    self.a2 = nn.Parameter(torch.tensor([0.0]))

def forward(self, t):
    base_part = self.a0 + self.a1 * torch.cos(t) + self.a2 * torch.sin(t)
    trig_input = torch.cat([torch.sin(t), torch.cos(t)], dim=1)
```

```
        residual = self.base(trig_input)
        return base_part + residual
```

```
In [49]: def second_derivative(model, t):
        t.requires_grad_(True)
        x = model(t)
        dx = torch.autograd.grad(x, t, torch.ones_like(x), create_graph=True)[0]
        d2x = torch.autograd.grad(dx, t, torch.ones_like(dx), create_graph=True)[0]
        return d2x

# Model and optimizer
model = PeriodicResidualNet().to(device_name)
optimizer = torch.optim.Adam(model.parameters(), lr=5e-4)
```

```
In [50]: epochs = 2000
        N = 256
        t_train = torch.linspace(0, 2 * np.pi, N, device=device).reshape(-1, 1)

        for epoch in range(epochs):
            optimizer.zero_grad()
            d2x = second_derivative(model, t_train)
            x_hat = model(t_train)
            loss = torch.mean((d2x + x_hat)**2) # ODE residual loss

            loss.backward()
            optimizer.step()

            if epoch % 500 == 0:
                print(f"Epoch {epoch} | Loss: {loss.item():.8f}")

# Evaluate
t_eval = torch.linspace(0, 2 * np.pi, 1000, device=device_name).reshape(-1, 1)
x_nn = model(t_eval).detach().cpu().numpy()
x_true = analytic_solution(t_eval.cpu().numpy())

# Plot
plt.figure(figsize=(10, 4))
plt.plot(t_eval.cpu(), x_true, '--', label='Exact Solution')
plt.plot(t_eval.cpu(), x_nn, label='NN Prediction')
plt.xlabel('t')
plt.ylabel('x(t)')
plt.title('Classical Harmonic Oscillator with Periodic Boundary Conditions')
plt.legend()
plt.grid(True)
plt.tight_layout()
plt.show()
```

```
Epoch 0 | Loss: 0.07109271
Epoch 500 | Loss: 0.00000445
Epoch 1000 | Loss: 0.00000115
Epoch 1500 | Loss: 0.00000046
```

