

```

import torch
import torch.nn as nn
import pandas as pd
import zipfile
import os
import matplotlib.pyplot as plt
from sklearn.metrics import mean_squared_error, r2_score
import joblib
from torch.utils.data import DataLoader, TensorDataset, random_split
import numpy as np
import seaborn as sns
from google.colab import drive

```

```

# Mount Google Drive
drive.mount('/content/drive')

# Set path to dataset files in Google Drive
data_path = '/content/drive/MyDrive/ashrae-energy-prediction/'

# Set random seeds for reproducibility
torch.manual_seed(42)
np.random.seed(42)

```

➞ Drive already mounted at /content/drive; to attempt to forcibly remount, call drive.mount("/content/drive", force\_remount=True).

```

# Load data
building = pd.read_csv(data_path + "building_metadata.csv")
meter = pd.read_csv(data_path + "train.csv")
weather = pd.read_csv(data_path + "weather_train.csv")

```

```

# Merge datasets
data = meter.merge(building, on="building_id")
data = data.merge(weather, on=["site_id", "timestamp"])
data['timestamp'] = pd.to_datetime(data['timestamp'])
data['hour'] = data['timestamp'].dt.hour
data['day'] = data['timestamp'].dt.dayofyear

```

```

# --- Define Model ---
class PINN(nn.Module):
    def __init__(self):
        super(PINN, self).__init__()
        self.layers = nn.Sequential(
            nn.Linear(4, 256),
            nn.ReLU(),
            nn.Dropout(0.2),
            nn.Linear(256, 128),
            nn.ReLU(),
            nn.Dropout(0.2),
            nn.Linear(128, 64),
            nn.ReLU(),
            nn.Linear(64, 1)
        )

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

# --- Physics-Informed Loss Functions ---
def physics_loss(meter_type, pred, delta_T):
    c_p = 4.18 # kJ/kg°C
    m = 0.1 # kg/s
    L = 2260 # kJ/kg, for steam

    if meter_type in [1, 2]: # Chilled Water or Hot Water
        q_phys = m * c_p * delta_T
    elif meter_type == 3: # Steam
        q_phys = m * L * torch.ones_like(delta_T)
    else: # Electricity (simple temp relationship)
        q_phys = 50 + 2 * delta_T

    return torch.mean((pred.squeeze() - q_phys)**2)

```

```

# Assume constant indoor temperature
T_inside = 22.0
for meter_type in range(4):
    print(f"\nTraining model for meter type {meter_type}...")
    subset = data[data['meter'] == meter_type].dropna()

```

```

if subset.empty:
    print("No data for this meter type.")
    continue

subset['delta_T'] = T_inside - subset['air_temperature']
if meter_type == 1:
    subset['delta_T'] = subset['air_temperature'] - T_inside

features = subset[['square_feet', 'hour', 'day', 'delta_T']]
target = subset['meter_reading']
features = (features - features.mean()) / features.std()

X = torch.tensor(features.values, dtype=torch.float32)
y = torch.tensor(target.values.reshape(-1, 1), dtype=torch.float32)

dataset = TensorDataset(X, y)
train_size = int(0.8 * len(dataset))
val_size = len(dataset) - train_size
train_data, val_data = random_split(dataset, [train_size, val_size])

train_loader = DataLoader(train_data, batch_size=256, shuffle=True)
val_loader = DataLoader(val_data, batch_size=256)

model = PINN()
optimizer = torch.optim.AdamW(model.parameters(), lr=0.0003, weight_decay=1e-5)
scheduler = torch.optim.lr_scheduler.StepLR(optimizer, step_size=75, gamma=0.7)
criterion = nn.MSELoss()

loss_data_list, loss_phys_list, val_loss_list = [], [], []

for epoch in range(250):
    model.train()
    epoch_loss_data, epoch_loss_phys = 0.0, 0.0

    for xb, yb in train_loader:
        pred = model(xb)
        delta_T = xb[:, -1]
        loss_data = criterion(pred, yb)
        loss_phys = physics_loss(meter_type, pred, delta_T)
        loss = loss_data + 0.3 * loss_phys

        optimizer.zero_grad()
        loss.backward()
        optimizer.step()

        epoch_loss_data += loss_data.item()
        epoch_loss_phys += loss_phys.item()

    scheduler.step()
    loss_data_list.append(epoch_loss_data)
    loss_phys_list.append(epoch_loss_phys)

    # Validation loss
    model.eval()
    with torch.no_grad():
        val_preds, val_targets = [], []
        for xb, yb in val_loader:
            pred = model(xb)
            val_preds.extend(pred.squeeze().numpy())
            val_targets.extend(yb.squeeze().numpy())
        val_rmse = np.sqrt(mean_squared_error(val_targets, val_preds))
        val_loss_list.append(val_rmse)

    if epoch % 10 == 0:
        print(f"Epoch {epoch}: Train Loss = {loss.item():.4f}, Val RMSE = {val_rmse:.2f}")

print(f"Finished training for meter {meter_type}.")

```



```

Training model for meter type 0...
Epoch 0: Train Loss = 79642.9375, Val RMSE = 232.31
Epoch 10: Train Loss = 41223.6719, Val RMSE = 229.34
Epoch 20: Train Loss = 53636.1406, Val RMSE = 227.39
Epoch 30: Train Loss = 54721.7539, Val RMSE = 224.84
Epoch 40: Train Loss = 28044.7012, Val RMSE = 219.39
Epoch 50: Train Loss = 76166.8828, Val RMSE = 204.47
Epoch 60: Train Loss = 49416.2344, Val RMSE = 203.15
Epoch 70: Train Loss = 38925.4805, Val RMSE = 200.08
Epoch 80: Train Loss = 22581.7109, Val RMSE = 198.14
Epoch 90: Train Loss = 34214.0859, Val RMSE = 194.51
Epoch 100: Train Loss = 45086.3750, Val RMSE = 193.43
Epoch 110: Train Loss = 32113.4258, Val RMSE = 192.27
Epoch 120: Train Loss = 49225.5859, Val RMSE = 187.39
Epoch 130: Train Loss = 35372.5156, Val RMSE = 185.39

```

```
Epoch 140: Train Loss = 40301.0078, Val RMSE = 180.28
Epoch 150: Train Loss = 31318.9746, Val RMSE = 172.31
Epoch 160: Train Loss = 44355.6562, Val RMSE = 174.83
Epoch 170: Train Loss = 72496.8906, Val RMSE = 172.09
Epoch 180: Train Loss = 42203.9180, Val RMSE = 171.03
Epoch 190: Train Loss = 43947.4570, Val RMSE = 172.63
Epoch 200: Train Loss = 26167.9238, Val RMSE = 172.82
Epoch 210: Train Loss = 53689.0391, Val RMSE = 168.07
Epoch 220: Train Loss = 69582.8125, Val RMSE = 171.37
Epoch 230: Train Loss = 44526.4570, Val RMSE = 169.63
Epoch 240: Train Loss = 62259.2422, Val RMSE = 165.71
Finished training for meter 0.
```

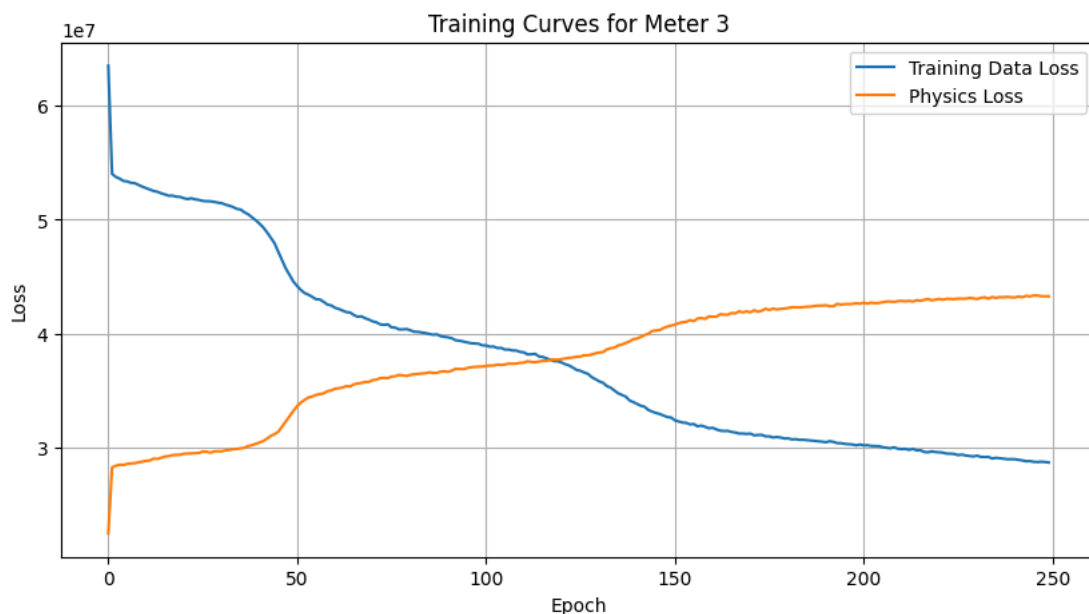
```
Training model for meter type 1...
No data for this meter type.
```

```
Training model for meter type 2...
No data for this meter type.
```

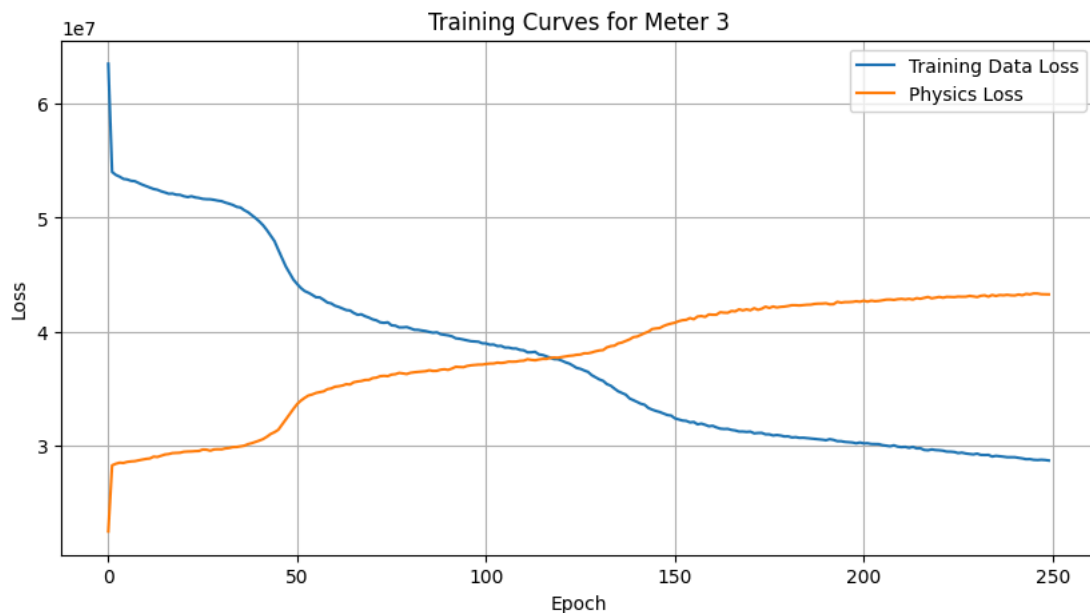
```
Training model for meter type 3...
No data for this meter type.
```

```
subset = subset[subset['meter_reading'] > 0] # Remove pure zeros
subset['meter_reading'] = np.log1p(subset['meter_reading']) # log(1 + x)
```

```
plt.figure(figsize=(10, 5))
plt.plot(loss_data_list, label='Training Data Loss')
plt.plot(loss_phys_list, label='Physics Loss')
plt.title(f'Training Curves for Meter {meter_type}')
plt.xlabel('Epoch')
plt.ylabel('Loss')
plt.legend()
plt.grid(True)
plt.savefig(f"/content/meter_{meter_type}_loss_plot.png")
plt.show()
```



```
# --- Plot Training Curves ---
plt.figure(figsize=(10, 5))
plt.plot(loss_data_list, label='Training Data Loss')
plt.plot(loss_phys_list, label='Physics Loss')
# plt.plot(val_loss_list, label='Validation RMSE') # Removed validation RMSE line
plt.title(f'Training Curves for Meter {meter_type}')
plt.xlabel('Epoch')
plt.ylabel('Loss')
plt.legend()
plt.grid(True)
plt.savefig(f"meter_{meter_type}_loss_plot.png")
plt.show()
```



```
model.eval()
with torch.no_grad():
    preds = model(X).numpy().squeeze()
    true = y.numpy().squeeze()

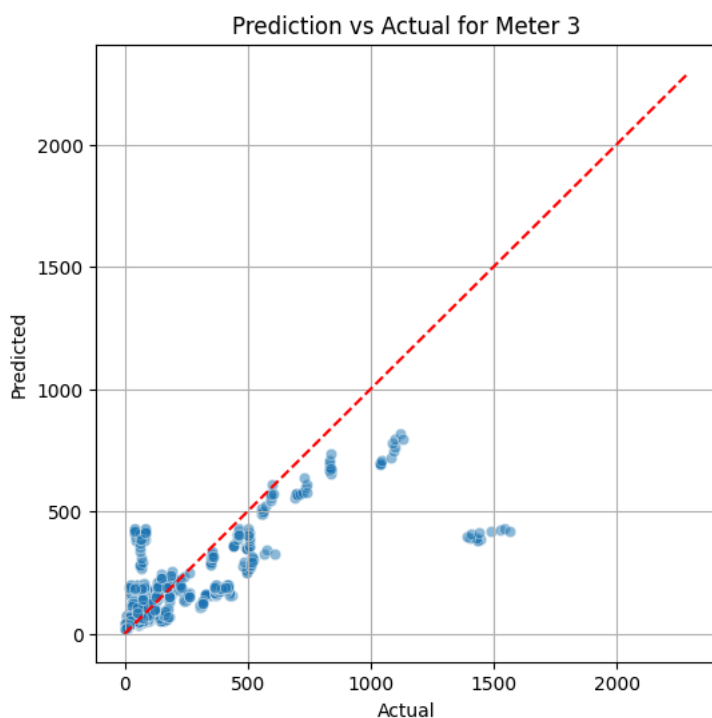
rmse = np.sqrt(mean_squared_error(true, preds))
r2 = r2_score(true, preds)
print(f"Evaluation for meter {meter_type} -> RMSE: {rmse:.2f}, R2: {r2:.2f}")
```



Evaluation for meter 3 -> RMSE: 167.54, R2: 0.66

```
plt.figure(figsize=(6, 6))
sns.scatterplot(x=true[:1000], y=preds[:1000], alpha=0.5)
plt.plot([true.min(), true.max()], [true.min(), true.max()], 'r--')
plt.xlabel("Actual")
plt.ylabel("Predicted")
plt.title(f"Prediction vs Actual for Meter {meter_type}")
plt.grid(True)
plt.savefig(f"/content/meter_{meter_type}_pred_vs_actual.png")
plt.show()

# --- Save Model and Features ---
torch.save(model.state_dict(), f"/content/pinn_model_meter_{meter_type}.pt")
joblib.dump(features.columns.tolist(), f"/content/features_meter_{meter_type}.pkl")
```



f"/content/features\_meter\_3.pkl"

```
# Mean Absolute Percentage Error (MAPE)
mape = np.mean(np.abs((true - preds) / (true + 1e-5))) * 100 # +1e-5 to avoid division by zero

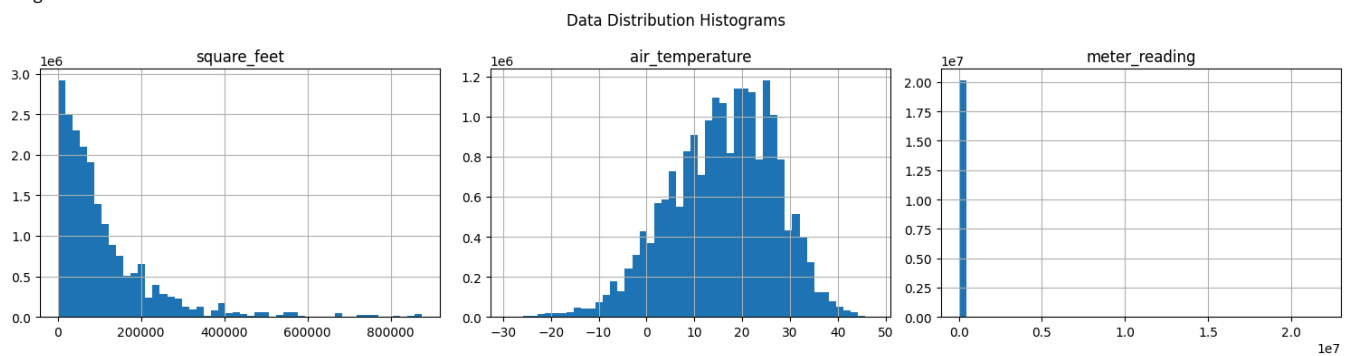
# Custom Accuracy: percentage of predictions within 20% of true values
tolerance = 0.2
within_tolerance = np.abs(true - preds) / (true + 1e-5) < tolerance
custom_accuracy = np.mean(within_tolerance) * 100

print(f"MAPE: {mape:.2f}%")
print(f"Custom Accuracy (within 20% of actual): {custom_accuracy:.2f}%")
```

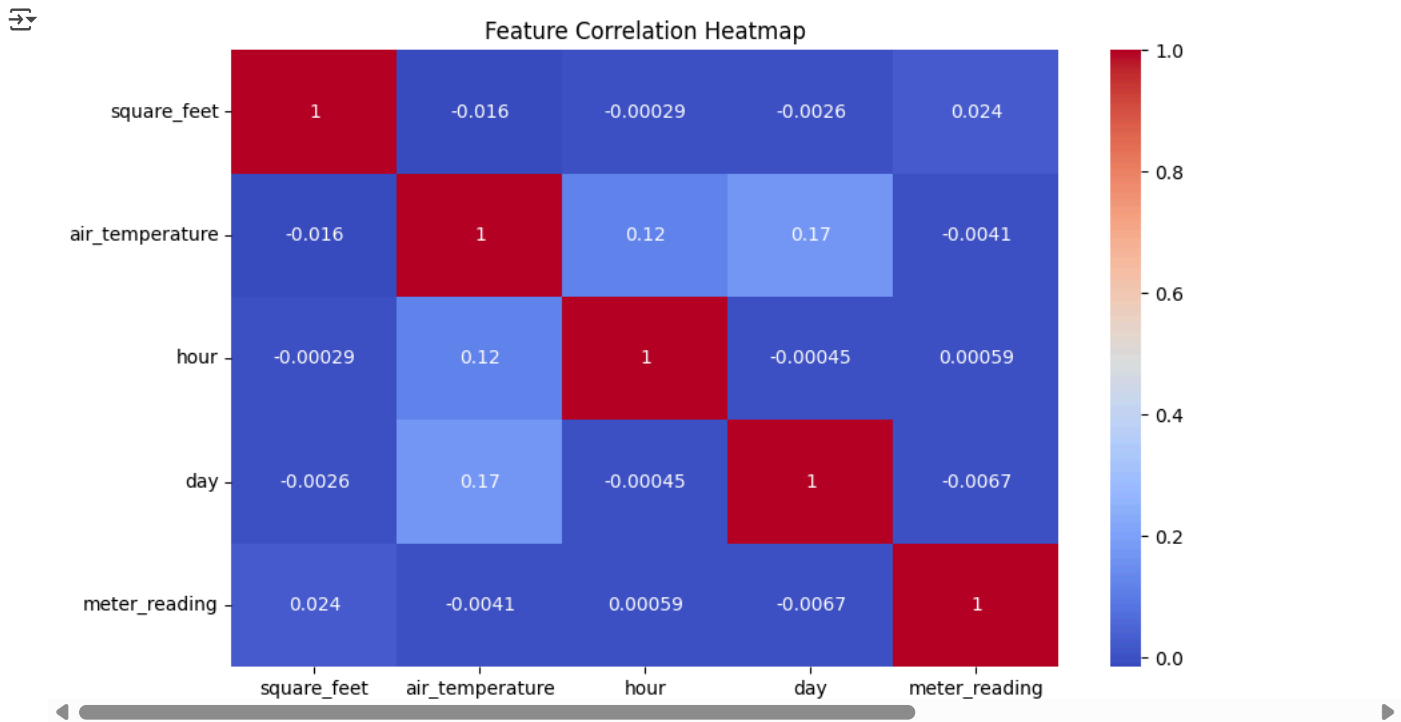
↗ MAPE: 1525785.88%  
Custom Accuracy (within 20% of actual): 17.09%

```
# Plot data distribution histograms
plt.figure(figsize=(12, 8))
data[['square_feet', 'air_temperature', 'meter_reading']].hist(bins=50, layout=(1, 3), figsize=(15, 4))
plt.suptitle('Data Distribution Histograms')
plt.tight_layout()
plt.savefig("/content/data_distribution_histograms.png")
plt.show()
```

↗ <Figure size 1200x800 with 0 Axes>



```
# Feature Correlation Heatmap
plt.figure(figsize=(10, 6))
sns.heatmap(data[['square_feet', 'air_temperature', 'hour', 'day', 'meter_reading']].corr(), annot=True, cmap='coolwarm')
plt.title("Feature Correlation Heatmap")
plt.savefig("/content/feature_correlation_heatmap.png")
plt.show()
```



```
grad_flow_list=[]
total_norm = 0
for p in model.parameters():
    if p.grad is not None:
        param_norm = p.grad.data.norm(2)
        total_norm += param_norm.item() ** 2
grad_flow_list.append(total_norm ** 0.5)
```

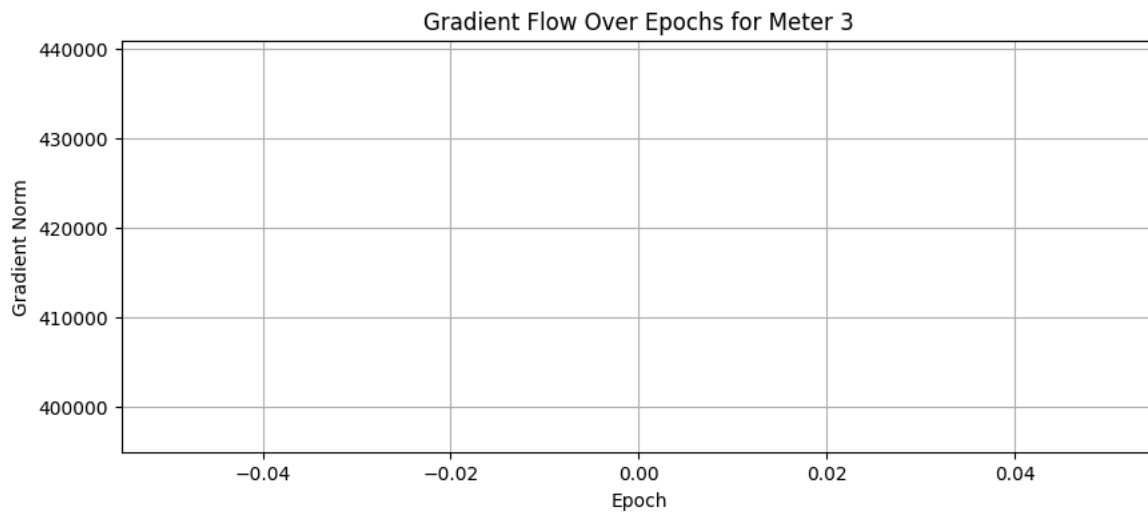
```
plt.figure(figsize=(10, 4))
plt.plot(grad_flow_list, label='Gradient Flow Magnitude')
plt.xlabel("Epoch")
plt.ylabel("Gradient Norm")
plt.title(f"Gradient Flow Over Epochs for Meter {meter_type}")
plt.grid(True)
plt.savefig(f"/content/meter_{meter_type}_gradient_flow.png")
plt.show()

# --- Final Evaluation ---
model.eval()
with torch.no_grad():
    preds = model(X).numpy().squeeze()
    true = y.numpy().squeeze()

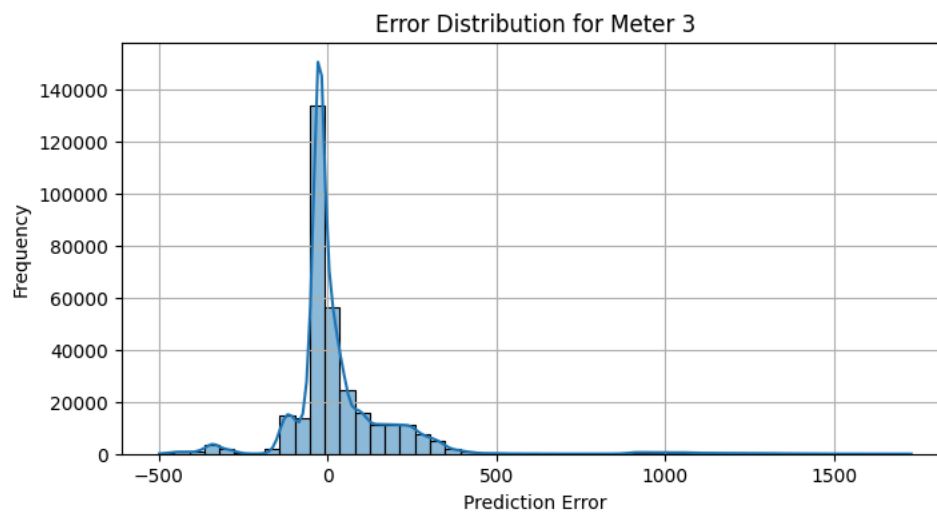
rmse = np.sqrt(mean_squared_error(true, preds))
r2 = r2_score(true, preds)
print(f"Evaluation for meter {meter_type} -> RMSE: {rmse:.2f}, R2: {r2:.2f}")

# --- Error Analysis ---
errors = true - preds
plt.figure(figsize=(8, 4))
sns.histplot(errors, bins=50, kde=True)
plt.title(f"Error Distribution for Meter {meter_type}")
plt.xlabel("Prediction Error")
plt.ylabel("Frequency")
plt.grid(True)
plt.savefig(f"/content/meter_{meter_type}_error_analysis.png")
plt.show()

# --- Save Model and Features ---
torch.save(model.state_dict(), f"/content/pinn_model_meter_{meter_type}.pt")
joblib.dump(features.columns.tolist(), f"/content/features_meter_{meter_type}.pkl")
```



Evaluation for meter 3 -> RMSE: 167.54, R2: 0.66



['/content/features\_meter\_3.pkl']

```
pip install graphviz
```



Requirement already satisfied: graphviz in /usr/local/lib/python3.11/dist-packages (0.20.3)

```
from graphviz import Digraph

dot = Digraph(comment='Physics Loss Breakdown')
dot.attr(rankdir='TB', size='8,10')
dot.attr('node', shape='box', style='filled', color='lightcoral', fontsize='12')

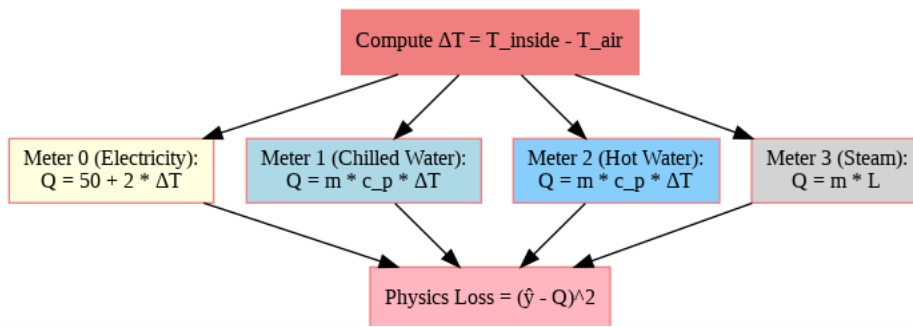
# Base computation
dot.node('A', 'Compute  $\Delta T = T_{\text{inside}} - T_{\text{air}}$ ')

# Meter-specific branches
dot.node('B0', 'Meter 0 (Electricity):  $\dot{Q} = 50 + 2 * \Delta T$ ', fillcolor='lightyellow')
dot.node('B1', 'Meter 1 (Chilled Water):  $\dot{Q} = m * c_p * \Delta T$ ', fillcolor='lightblue')
dot.node('B2', 'Meter 2 (Hot Water):  $\dot{Q} = m * c_p * \Delta T$ ', fillcolor='lightskyblue')
dot.node('B3', 'Meter 3 (Steam):  $\dot{Q} = m * L$ ', fillcolor='lightgray')

dot.node('C', 'Physics Loss =  $(\hat{y} - Q)^2$ ', fillcolor='lightpink')

# Edges
dot.edge('A', 'B0')
dot.edge('A', 'B1')
dot.edge('A', 'B2')
dot.edge('A', 'B3')
dot.edge('B0', 'C')
dot.edge('B1', 'C')
dot.edge('B2', 'C')
dot.edge('B3', 'C')

# Render
dot.render('physics_loss_breakdown', format='png', cleanup=True)
from IPython.display import Image
Image('physics_loss_breakdown.png')
```



```

from graphviz import Digraph

dot = Digraph(comment='Evaluation Process')
dot.attr(rankdir='TB', size='8,10')
dot.attr('node', shape='box', style='filled', color='lightgray', fontsize='12')

# Nodes
dot.node('A', 'Trained PINN Model', fillcolor='lightblue')
dot.node('B', 'Input Test Data\n(features only)', fillcolor='lightyellow')
dot.node('C', 'Generate Predictions ŷ', fillcolor='lightgreen')
dot.node('D', 'Compare with True Values\n(if available)', fillcolor='lightcoral')
dot.node('E', 'Calculate Metrics:\nRMSE, R², MAPE', fillcolor='lightpink')
dot.node('F', 'Plot Results:\nPrediction vs Actual, Error Histograms', fillcolor='lightskyblue')
dot.node('G', 'Export Results:\npredictions.csv, plots', fillcolor='wheat')

# Edges
dot.edges(['AB', 'BC', 'CD', 'DE', 'EF', 'FG'])

# Render
dot.render('/content/evaluation_process_diagram', format='png', cleanup=True)
from IPython.display import Image
Image('/content/evaluation_process_diagram.png')

```

