Import libraries

In [1]:
```
import itertools
import torch
import torch.nn as nn
import torch.optim as optim
from torch.utils.data import Dataset, DataLoader
import pandas as pd
from typing import List
import wandb
import joblib
import matplotlib.pyplot as plt
import numpy as np
import json
import os
import csv
```

1. Configuration

1.1 Init

In [2]:
```
WANDB_PROJECT_NAME = "zneus-project-1"
dataset_used = "full_features"
path = f"data/transformed/{dataset_used}" #path of used dataset
IS_WANDB = True
run_id = 1

#using seed for consistent experiments
RANDOM_SEED = 42
np.random.seed(RANDOM_SEED)
torch.manual_seed(RANDOM_SEED)

#if cuda available, use it
device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')
print(f"Device used: {device}")

#model parameters
EPOCH = 50
BATCH_SIZE = 128
LR = 0.001

#transformer for inverse transforms
target_transformer = joblib.load(f"{path}/house_value_scaler.pkl")
```

```
Device used: cuda
```

1.1.1 Wandb init

In [3]:
```
def init_wandb(name=f"{dataset_used}_{run_id}", config_dict=None):
    if IS_WANDB:
```

```
        default_config = {
            "batch_size": BATCH_SIZE,
            "epoch": EPOCH,
            "lr": LR,
            "loss_fn": "MSELoss",
            "dataset_path": path,
            "activation": "LeakyReLU",
            "optimizer": "Adam",
            "weight_decay": 0.0
        }

        #use dict from tuning
        if config_dict is not None:
            default_config.update(config_dict)

        wandb.init(
            project=f"{WANDB_PROJECT_NAME}",
            name=name,
            config=default_config
        )
```

1.2 Model parameters

In [4]:
```
class CSVDataset(Dataset):
    def __init__(self, path: str):
        df = pd.read_csv(path)
        self.X = torch.tensor(df.iloc[:, :-1].values, dtype=torch.float32)
        self.y = torch.tensor(df.iloc[:, -1].values, dtype=torch.float32).view(-1,

    def __len__(self):
        return len(self.X)

    def __getitem__(self, idx):
        return self.X[idx], self.y[idx]

#load datasets from disk
def get_datasets(path: str) -> List[CSVDataset]:
    return [
        CSVDataset(f"{path}/train.csv"),
        CSVDataset(f"{path}/test.csv"),
        CSVDataset(f"{path}/eval.csv")
    ]
```

1.3 Model class - variants

1.3.1 Base

In [5]:
```
class SimpleNN(nn.Module):
    def __init__(self, input_size: int):
        super(SimpleNN, self).__init__()
        self.net = nn.Sequential(
            nn.Linear(input_size, 128),
            nn.LeakyReLU(0.1),
```

```
            nn.Linear(128, 64),
            nn.LeakyReLU(0.1),
            nn.Linear(64, 32),
            nn.LeakyReLU(0.1),
            nn.Linear(32, 1)
        )

    def forward(self, x):
        return self.net(x)
```

1.3.2 Dropout

In [6]:
```
class SimpleNN_dropout(nn.Module):
    def __init__(self, input_size: int):
        super(SimpleNN_dropout, self).__init__()
        self.net = nn.Sequential(
            nn.Linear(input_size, 128),
            nn.LeakyReLU(0.1),
            nn.Dropout(0.1),
            nn.Linear(128, 64),
            nn.LeakyReLU(0.1),
            nn.Dropout(0.3),
            nn.Linear(64, 32),
            nn.LeakyReLU(0.1),
            nn.Linear(32, 1)
        )

    def forward(self, x):
        return self.net(x)
```

1.3.3 Batch Normalization

In [7]:
```
class SimpleNN_batch_norm(nn.Module):
    def __init__(self, input_size: int):
        super(SimpleNN_batch_norm, self).__init__()
        self.net = nn.Sequential(
            nn.Linear(input_size, 128),
            nn.BatchNorm1d(128),
            nn.LeakyReLU(0.3),

            nn.Linear(128, 64),
            nn.BatchNorm1d(64),
            nn.LeakyReLU(0.1),

            nn.Linear(64, 32),
            nn.BatchNorm1d(32),
            nn.LeakyReLU(0.1),

            nn.Linear(32, 1)
        )

    def forward(self, x):
        return self.net(x)
```

1.3.4 Skip connections

In [8]:
```
class SimpleNN_Res(nn.Module): #skip connections
    def __init__(self, input_size: int):
        super(SimpleNN_Res, self).__init__()
        self.fc1 = nn.Linear(input_size, 128)
        self.act1 = nn.LeakyReLU(0.1)

        self.fc2 = nn.Linear(128, 64)
        self.act2 = nn.LeakyReLU(0.1)

        self.fc3 = nn.Linear(64, 32)
        self.act3 = nn.LeakyReLU(0.1)

        self.out = nn.Linear(32, 1)

        #projection for skip connections
        self.skip_proj = nn.Linear(input_size, 64)

    def forward(self, x):
        #first layer
        x1 = self.act1(self.fc1(x))

        #skip connection: input x + projection to 64
        skip = self.skip_proj(x)
        x2 = self.act2(self.fc2(x1) + skip) #residual connection

        #next layer
        x3 = self.act3(self.fc3(x2))

        out = self.out(x3)
        return out
```

1.3.5 Bottleneck layers

In [9]:
```
class SimpleNN_Bottleneck(nn.Module):
    def __init__(self, input_size: int, bottleneck_size: int = 16):
        super(SimpleNN_Bottleneck, self).__init__()

        self.fc1 = nn.Linear(input_size, 128)
        self.act1 = nn.LeakyReLU(0.3)

        #bottleneck layer
        self.fc2 = nn.Linear(128, bottleneck_size)
        self.act2 = nn.LeakyReLU(0.1)

        #output layer
        self.fc3 = nn.Linear(bottleneck_size, 32)
        self.act3 = nn.LeakyReLU(0.1)

        self.out = nn.Linear(32, 1)

    def forward(self, x):
        x1 = self.act1(self.fc1(x))
```

```
        x2 = self.act2(self.fc2(x1))
        x3 = self.act3(self.fc3(x2))
        out = self.out(x3)
        return out
```

1.4 Load data

In [10]:
```
#load datasets and create loss function
train_df, test_df, eval_df = get_datasets(path)
loss_fn = nn.MSELoss()


def create_loaders(batch_size):
    #divide datasets into batches
    train_loader = DataLoader(train_df, batch_size=batch_size, shuffle=True, worker
    test_loader = DataLoader(test_df, batch_size=batch_size, shuffle=True, worker_i
    eval_loader = DataLoader(eval_df, batch_size=batch_size, shuffle=True, worker_i

    return train_loader, test_loader, eval_loader

train_loader, test_loader, eval_loader = create_loaders(BATCH_SIZE) #for base exper
```

1.5 Inverse transform init

In [11]:
```
#inverse transform the input for original values
def get_inverse_transformed(y, y_transformer=None):
    if y_transformer is not None:
        y = y.cpu().numpy().reshape(-1, 1)
        y = y_transformer.inverse_transform(y)
        return torch.tensor(y, dtype=torch.float32, device=device)
    return y
```

1.6 Evaluate model

In [22]:
```
def evaluate(eloader: DataLoader, model, loss_fn, y_transformer=None, is_test=False
    model.eval()
    total_test_loss = 0
    total_test_loss_original = 0
    num_of_batches = len(eloader)

    mse_losses, rmse_losses = [], [] #for test only

    with torch.no_grad():
        if is_test:
            p = "TRAINING" if is_train else "TESTING"
            print(f"\n====={p}====")

        for index, (X, y) in enumerate(eloader):
            X, y = X.to(device), y.to(device)
            y_pred = model(X)

            loss_transformed = loss_fn(y_pred, y).item()
```

```
            mse_losses.append(loss_transformed)
            total_test_loss += loss_transformed

            y_pred = get_inverse_transformed(y_pred, y_transformer)
            y = get_inverse_transformed(y, y_transformer)

            loss_original = loss_fn(y_pred, y).item()
            total_test_loss_original += loss_original
            if is_test:
                rmse = loss_original ** 0.5
                rmse_losses.append(rmse)

                #print(f"{p.lower().capitalize()} eval: Batch {index + 1:03d}: MSE=

    return total_test_loss/num_of_batches, total_test_loss_original/num_of_batches,
```

1.7 Train model

In [21]:

```
def train(train: CSVDataset, train_loader: DataLoader, eval_loader: DataLoader, los
    model = model if model else SimpleNN_Bottleneck(train.X.shape[1]).to(device) #i

    optimizer = optimizer if optimizer else optim.Adam(model.parameters(), lr=LR) #
    train_mse, eval_mse = [], []
    train_rmse, eval_rmse = [], []

    if not tuning: print("\n====TRAINING====")
    for epoch in range(EPOCH):
        model.train()
        total_train_mse = 0
        total_train_rmse = 0

        for X, y in train_loader:
            X, y = X.to(device), y.to(device)
            optimizer.zero_grad()

            #predict y
            y_pred = model(X)

            #calculate loss
            loss = loss_fn(y_pred, y)
            total_train_mse += loss.item()

            #backward pass
            loss.backward()
            optimizer.step()

            #calculate non-normalized loss, for logging
            with torch.no_grad():
                #inverse transform predicted and true y values
                y_orig = get_inverse_transformed(y.detach(), transformer)
                y_pred_orig = get_inverse_transformed(y_pred.detach(), transformer)

                #calculate mse and rmse from results
                mse = loss_fn(y_pred_orig, y_orig).item()
                rmse = mse ** 0.5
```

```
                total_train_rmse += rmse

        #average train mse/rmse per epoch
        avg_train_mse = total_train_mse / len(train_loader)
        avg_train_rmse = total_train_rmse / len(train_loader)

        #test on eval set
        eval_mse_e, eval_mse_original, _, _, _ = evaluate(eval_loader, model, loss_
        eval_rmse_e = eval_mse_original ** 0.5

        #add to arrays
        train_mse.append(avg_train_mse)
        eval_mse.append(eval_mse_e)
        train_rmse.append(avg_train_rmse)
        eval_rmse.append(eval_rmse_e)

        #if not tuning:
            #print(f"Epoch {epoch+1:03d}: train RMSE={avg_train_rmse:.4f}, eval RMS

    return model, train_mse, eval_mse, train_rmse, eval_rmse
```

1.8 Plotting the results locally

In [14]:
```
def plot_res(tr_mse, ev_mse, tr_rmse, ev_rmse, te_mse_losses, te_rmse_losses, test_
    #plot mse losses
    plt.figure(figsize=(8, 5))
    plt.plot(range(1, len(tr_mse) + 1), tr_mse, label="Training MSE", linewidth=2)
    plt.plot(range(1, len(ev_mse) + 1), ev_mse, label="Evaluation MSE", linewidth=2
    plt.title("Training, Evaluation MSE Over Epochs")
    plt.xlabel("Epoch")
    plt.ylabel("MSE")
    plt.legend()
    plt.grid(True, linestyle="--", alpha=0.6)
    plt.tight_layout()
    plt.show()

    #plot rmse - real losses in €
    plt.figure(figsize=(8, 5))
    plt.plot(range(1, len(tr_rmse) + 1), tr_rmse, label="Training RMSE", linewidth=
    plt.plot(range(1, len(ev_rmse) + 1), ev_rmse, label="Evaluation RMSE", linewidt
    plt.title("Training, Evaluation RMSE Over Epochs")
    plt.xlabel("Epoch")
    plt.ylabel("RMSE (€)")
    plt.legend()
    plt.grid(True, linestyle="--", alpha=0.6)
    plt.tight_layout()
    plt.show()

    #test plots - mse
    plt.figure(figsize=(8, 5))
    plt.plot(range(1, test_batches + 1), te_mse_losses, label="Test MSE", linewidth
    plt.title("Test MSE Over Batches")
    plt.xlabel("Epoch")
    plt.ylabel("MSE")
```

```
    plt.legend()
    plt.grid(True, linestyle="--", alpha=0.6)
    plt.tight_layout()
    plt.show()

    #test plots - rmse
    plt.figure(figsize=(8, 5))
    plt.plot(range(1, test_batches + 1), te_rmse_losses, label="Test RMSE", linewid
    plt.title("Test RMSE Over Batches")
    plt.xlabel("Epoch")
    plt.ylabel("RMSE (€)")
    plt.legend()
    plt.grid(True, linestyle="--", alpha=0.6)
    plt.tight_layout()
    plt.show()
```

1.9 Train the model and log the results into WandB and plot locally if allowed in init

In [15]:

```
def run_experiment(model=None, optimizer=None, train_loader=None, test_loader=None,
    #start wandb run
    if tuning:
        init_wandb(tuning_param[0], tuning_param[1])
    else:
        init_wandb()

    #train
    model, tr_mse, ev_mse, tr_rmse, ev_rmse = train(train_df, train_loader, eval_lo

    #evaluate on train dataset, seen data
    train_mse, train_mse_original, _, _, _ = evaluate(train_loader, model, loss_fn,
    train_eval_rmse = train_mse_original ** 0.5

    #evaluate test dataset, unseen data
    test_mse, test_mse_original, te_mse_losses, te_rmse_losses, test_batches = eval
    te_rmse = test_mse_original ** 0.5

    #log results
    if IS_WANDB:
        for epoch, (mse_t, mse_e, rmse_t, rmse_e) in enumerate(zip(tr_mse, ev_mse,
            wandb.log({
                "epoch": epoch,
                "train_MSE": mse_t,
                "eval_MSE": mse_e,
                "train_RMSE": rmse_t,
                "eval_RMSE": rmse_e,
            })

        for batch_idx, (mse, rmse) in enumerate(zip(te_mse_losses, te_rmse_losses),
            wandb.log({
                "batch": batch_idx,
                "test_MSE": mse,
                "test_RMSE": rmse
            })
```

```
        wandb.finish()


    print(f"Train RMSE: {train_eval_rmse:.4f}, Test RMSE: {te_rmse:.4f}")

    if not tuning: #during tuning we dont plot graphs
        plot_res(tr_mse, ev_mse, tr_rmse, ev_rmse, te_mse_losses, te_rmse_losses, t

    return train_eval_rmse, te_rmse
```

Code may output different Test RMSE, that is because we are logging batch RMSE to wandb and then wandb calculates a mean, this is not accurate for comparing models. We calculate RMSE on the whole dataset, that is the correct approach.

In [23]:
```
run_experiment(train_loader=train_loader, test_loader=test_loader, eval_loader=eval
run_id += 1
```

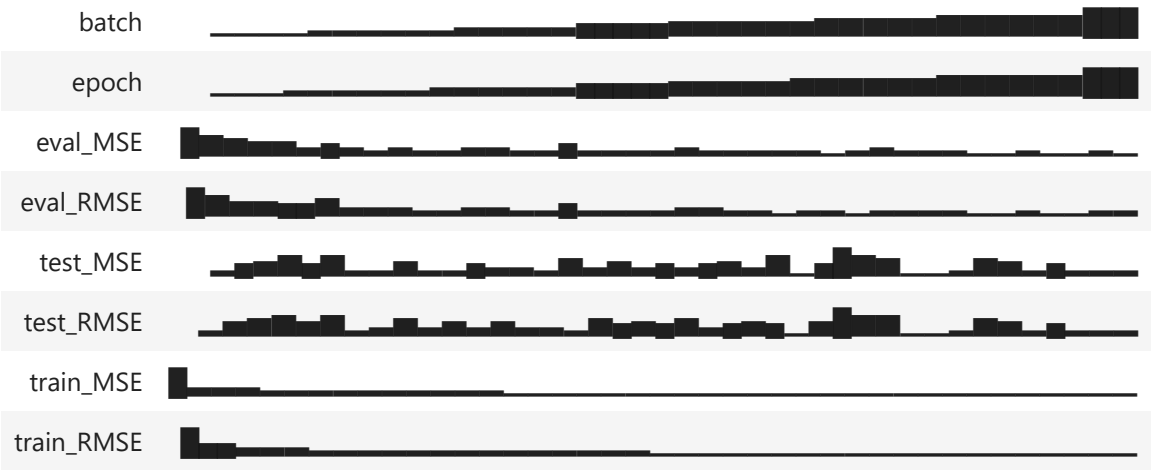
Tracking run with wandb version 0.22.3
Run data is saved locally in `C:\zeus\projekt1\wandb\run-20251109_205457-odofb4l9`
Syncing run **full_features_1** to Weights & Biases (docs)
View project at https://wandb.ai/xhanushchak-slovensk-technick-univerzita-v-bratislave/zneus-project-1
View run at https://wandb.ai/xhanushchak-slovensk-technick-univerzita-v-bratislave/zneus-project-1/runs/odofb4l9

```
====TRAINING====

====TRAINING====

====TESTING====
```

Run history:



Run summary:

batch	49
epoch	50
eval_MSE	0.01189
eval_RMSE	52894.9021
test_MSE	0.00943
test_RMSE	47086.17598
train_MSE	0.01185
train_RMSE	52123.38831

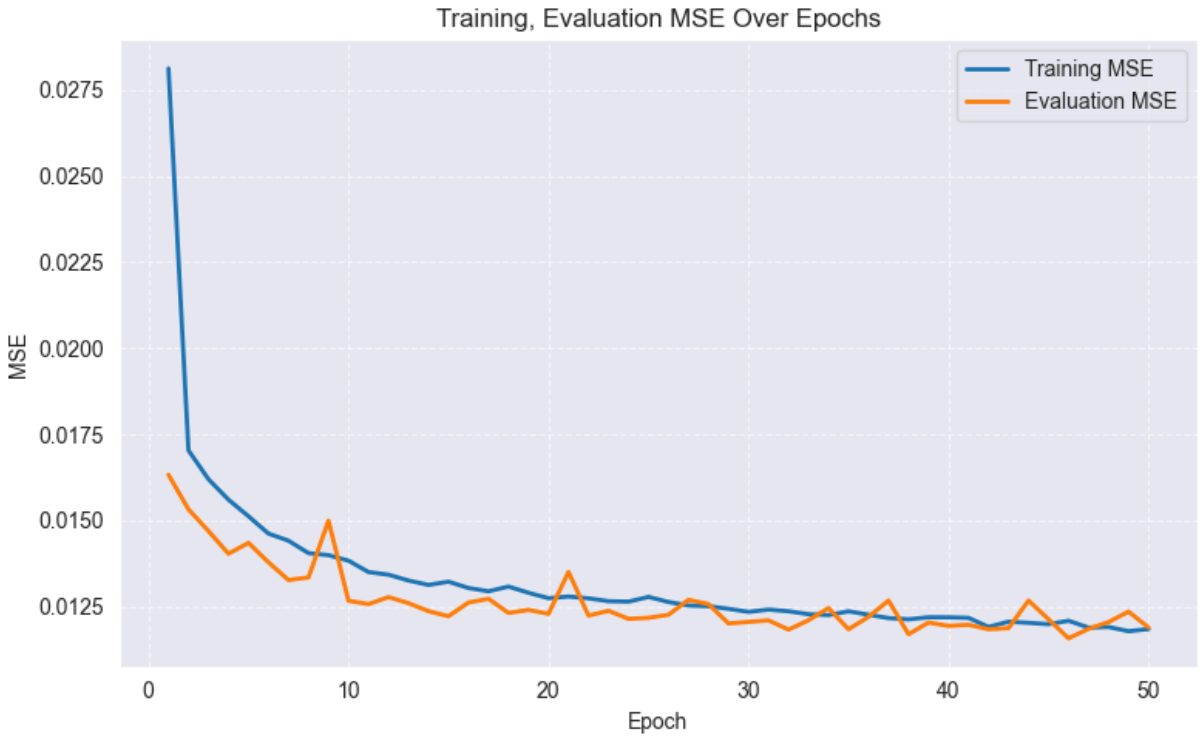
View run **full_features_1** at: https://wandb.ai/xhanushchak-slovensk-technick-univerzita-v-bratislave/zneus-project-1/runs/odofb4l9

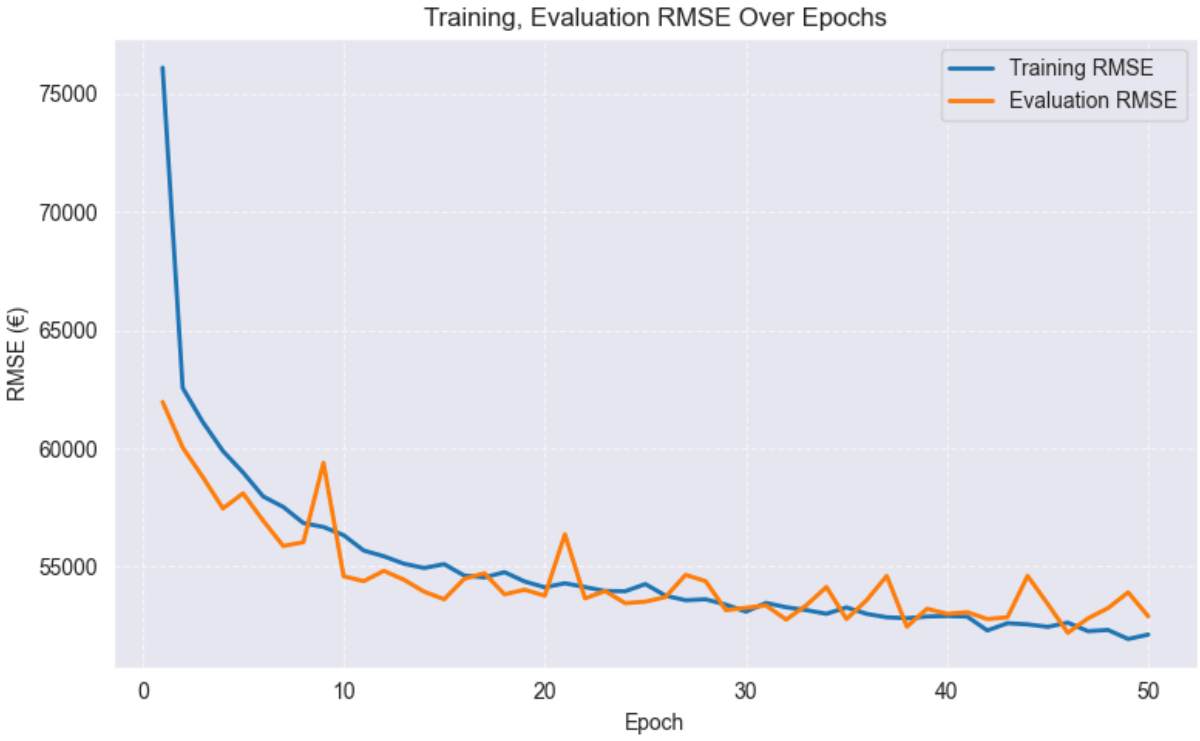
View project at: https://wandb.ai/xhanushchak-slovensk-technick-univerzita-v-bratislave/zneus-project-1

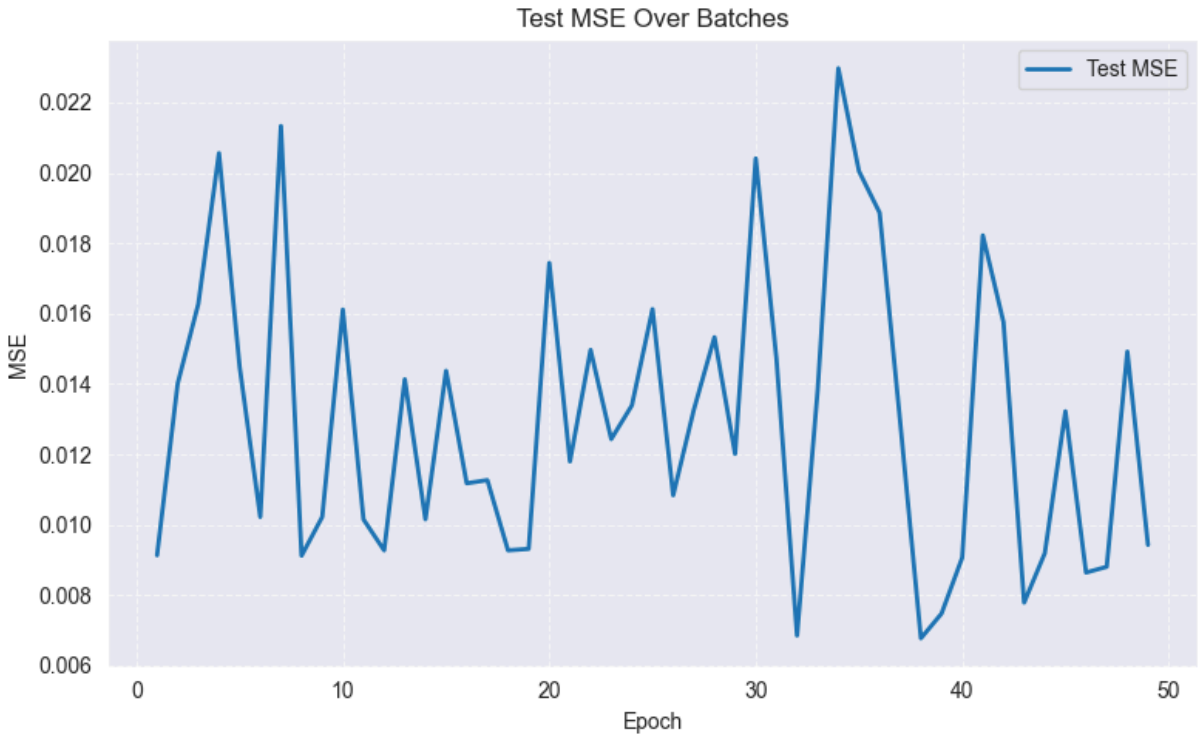
Synced 4 W&B file(s), 0 media file(s), 0 artifact file(s) and 0 other file(s)

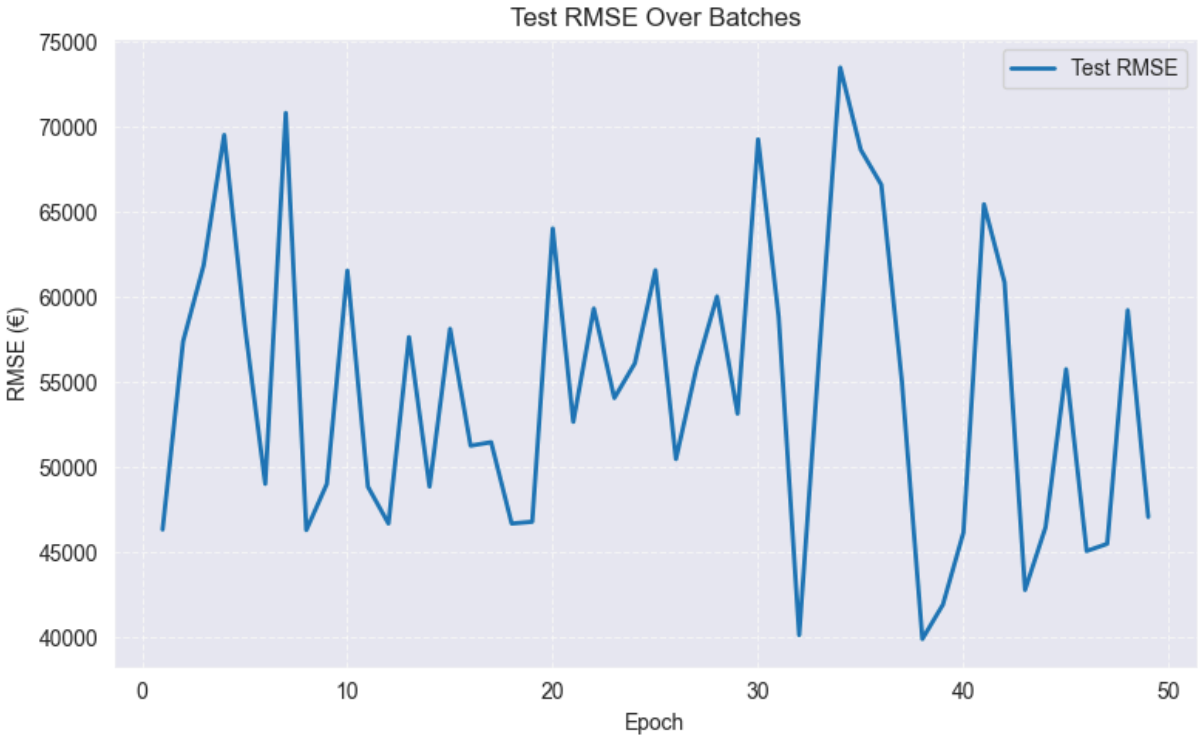
Find logs at: `.\wandb\run-20251109_205457-odofb4l9\logs`

```
Train RMSE: 52090.0550, Test RMSE: 55346.3453
```


Training, Evaluation MSE Over Epochs
Training MSE
Evaluation MSE
MSE
0.0275
0.0250
0.0225
0.0200
0.0175
0.0150
0.0125
0
10
20
30
40
50
Epoch


Training, Evaluation RMSE Over Epochs
Training RMSE
Evaluation RMSE
RMSE (€)
75000
70000
65000
60000
55000
0
10
20
30
40
50
Epoch





1.10 Hyperparameter tuning

In [17]:
```python
def hyperparameter_tuning(train_set: CSVDataset):
    run_id = 0
    best_rmse = float("inf")
    best_config = None
    csv_file = "tuning_results.csv"

    #create file if it does not exist
```

```
if not os.path.exists(csv_file):
    with open(csv_file, mode="w", newline="") as f:
        writer = csv.writer(f)
        writer.writerow([
            "iteration", "activation", "optimizer", "lr",
            "weight_decay", "batch_size", "train_RMSE", "test_RMSE", "new_best"
        ])


#parameter sets
activation_options = [nn.ReLU, lambda: nn.LeakyReLU(0.1)]
optimizer_options = ['Adam', 'SGD']
learning_rates = {
    'Adam': [1e-4, 3e-4, 1e-3],
    'SGD': [1e-2, 3e-3, 1e-3]
}
batch_sizes = [64, 128]
weight_decays = [0, 1e-4]

param_grid = list(itertools.product(
    activation_options,
    optimizer_options,
    batch_sizes,
    weight_decays
))

total_runs = sum(len(learning_rates[o]) for _, o, _, _ in param_grid)
print(f"Starting hyperparameter tuning: {total_runs} total runs\n")

#for effectivity, lets init all needed data loaders needed for experiments
loaders = []
for b in batch_sizes:
    train_loader, test_loader, eval_loader = create_loaders(b)
    loaders.append([train_loader, test_loader, eval_loader]) #index of b in bat

for act_fn, opt_name, batch, wd in param_grid:
    loader_idx = batch_sizes.index(batch)
    for lr in learning_rates[opt_name]:
        activation = act_fn()
        model = SimpleNN_Res(train_set.X.shape[1]).to(device)
        model.act1 = activation
        model.act2 = activation
        model.act3 = activation

        #optimizer
        if opt_name == 'Adam':
            optimizer = optim.Adam(model.parameters(), lr=lr, weight_decay=wd)
        elif opt_name == 'SGD':
            optimizer = optim.SGD(model.parameters(), lr=lr, momentum=0.9, weig

        exp_name = f"{dataset_used}_parameter_tuning_{run_id}"
        config_dict = {
            "activation": act_fn.__name__ if hasattr(act_fn, "__name__") else "
            "batch_size": batch,
            "epoch": EPOCH,
            "lr": lr,
```

```
                "loss_fn": "MSELoss",
                "dataset_path": path,
                "optimizer": opt_name,
                "weight_decay": wd
            }

            print(f"[{run_id+1}/{total_runs}] Starting: "
                  f"{config_dict['optimizer']} | act={config_dict['activation']} |
                  f"lr={lr} | wd={wd} | batch={batch}")


            train_rmse, test_rmse = run_experiment(model=model, optimizer=optimizer

            new_best = False #if it the new best model yet
            if test_rmse < best_rmse:
                best_rmse = test_rmse
                best_config = config_dict
                new_best = True
                print(f"New best RMSE: {best_rmse:.4f} with config {best_config}")


            #write results to csv
            with open(csv_file, mode="a", newline="") as f:
                writer = csv.writer(f)
                writer.writerow([run_id+1, config_dict["activation"], opt_name, lr,

            run_id += 1

    if best_config is not None:
        with open("best_config.json", "w") as f:
            json.dump({"best_rmse": best_rmse, "config": best_config}, f, indent=4)
        print(f"\nBest configuration saved to best_config.json:")
        print(json.dumps(best_config, indent=4))
    else:
        print("No valid configuration found!")
```

In [18]:
```
#hyperparameter_tuning(train_df) #start hyperparameter tuning
```

In [20]:
```
#best iterations
tuning_res = pd.read_csv("models_tuning/tuning_improvements.csv")
tuning_res
```

Out[20]:

	iteration	activation	optimizer	lr	weight_decay	batch_size	train_RMSE	t
0	1	ReLU	Adam	0.0001	0.0	64	53373.203790	568
1	2	ReLU	Adam	0.0003	0.0	64	51067.636097	556
2	3	ReLU	Adam	0.0010	0.0	64	48283.271055	552
3	9	ReLU	Adam	0.0010	0.0	128	49679.079022	549
4	27	LeakyReLU(0.1)	Adam	0.0010	0.0	64	47995.374228	539

1.11 Best Model Results

In [24]:
```python
with open("models_tuning/best_config.json", "r") as f: #load best config
    best = json.load(f)

best_rmse = best["best_rmse"]
config = best["config"]
print(f"Best RMSE: {best_rmse}")
print("Config:", config)

#create model
model = SimpleNN_Res(train_df.X.shape[1]).to(device)

#create activation function
activation = nn.LeakyReLU(0.1)

#apply activation
model.act1 = activation
model.act2 = activation
model.act3 = activation

#create optimizer
lr = config["lr"]
weight_decay = config["weight_decay"]

if config["optimizer"] == "Adam":
    optimizer = optim.Adam(model.parameters(), lr=lr, weight_decay=weight_decay)


#create loader
batch_size = config["batch_size"]
train_loader, test_loader, eval_loader = create_loaders(batch_size)

#run experiment
train_rmse, test_rmse = run_experiment(
    model=model,
    optimizer=optimizer,
    train_loader=train_loader,
    test_loader=test_loader,
    eval_loader=eval_loader,
    tuning=False #print results also
)
```

```
Best RMSE: 53968.44942545371
Config: {'activation': 'LeakyReLU(0.1)', 'batch_size': 64, 'epoch': 50, 'lr': 0.001,
'loss_fn': 'MSELoss', 'dataset_path': 'data/transformed/full_features', 'optimizer':
'Adam', 'weight_decay': 0}
```

Tracking run with wandb version 0.22.3

Run data is saved locally in `C:\zeus\projekt1\wandb\run-20251109_205618-gvlsqjyq`

Syncing run **full_features_1** to Weights & Biases (docs)

View project at https://wandb.ai/xhanushchak-slovensk-technick-univerzita-v-bratislave/zneus-project-1

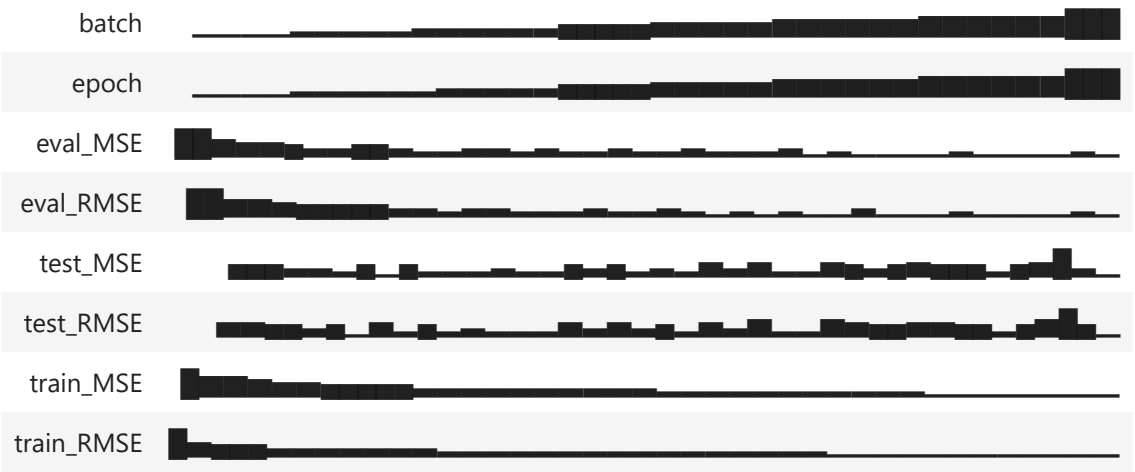
View run at https://wandb.ai/xhanushchak-slovensk-technick-univerzita-v-bratislave/zneus-project-1/runs/gvlsqjyq

```
====TRAINING====

====TRAINING====

====TESTING====
```

Run history:



Run summary:

batch	49
epoch	50
eval_MSE	0.01135
eval_RMSE	51665.07952
test_MSE	0.00616
test_RMSE	38054.22321
train_MSE	0.01059
train_RMSE	49376.0815

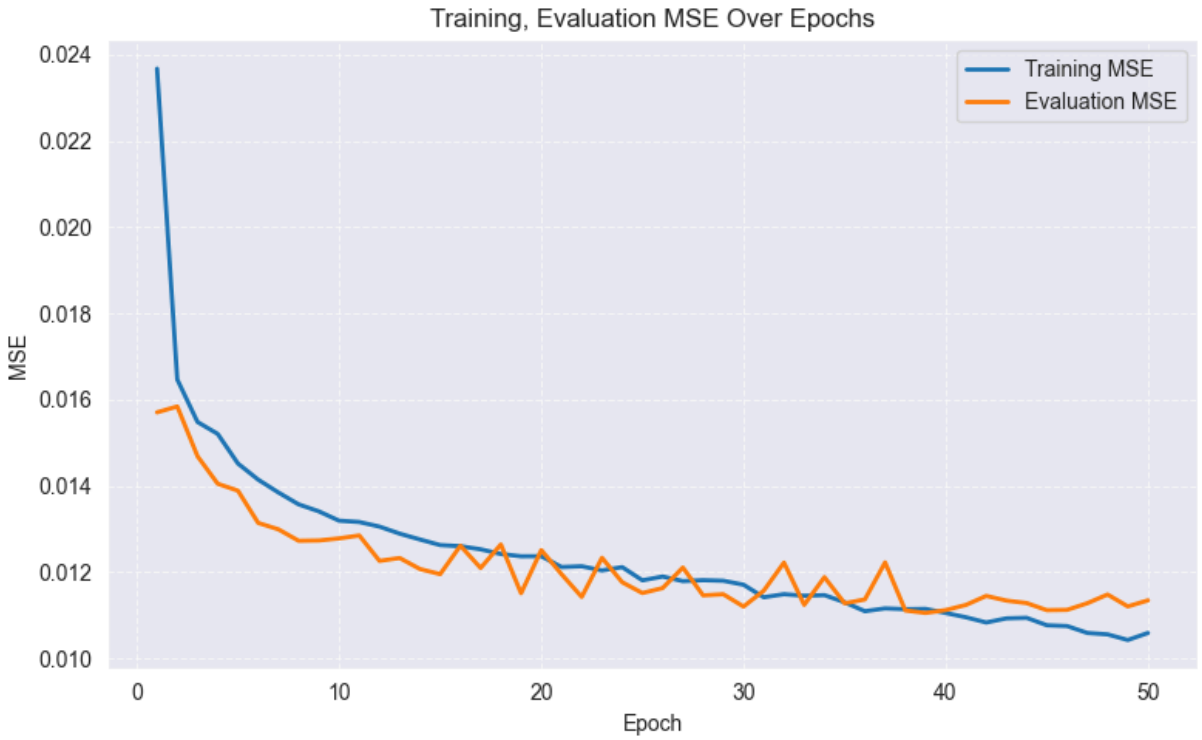
View run **full_features_1** at: https://wandb.ai/xhanushchak-slovensk-technick-univerzita-v-bratislave/zneus-project-1/runs/gvlsqjyq

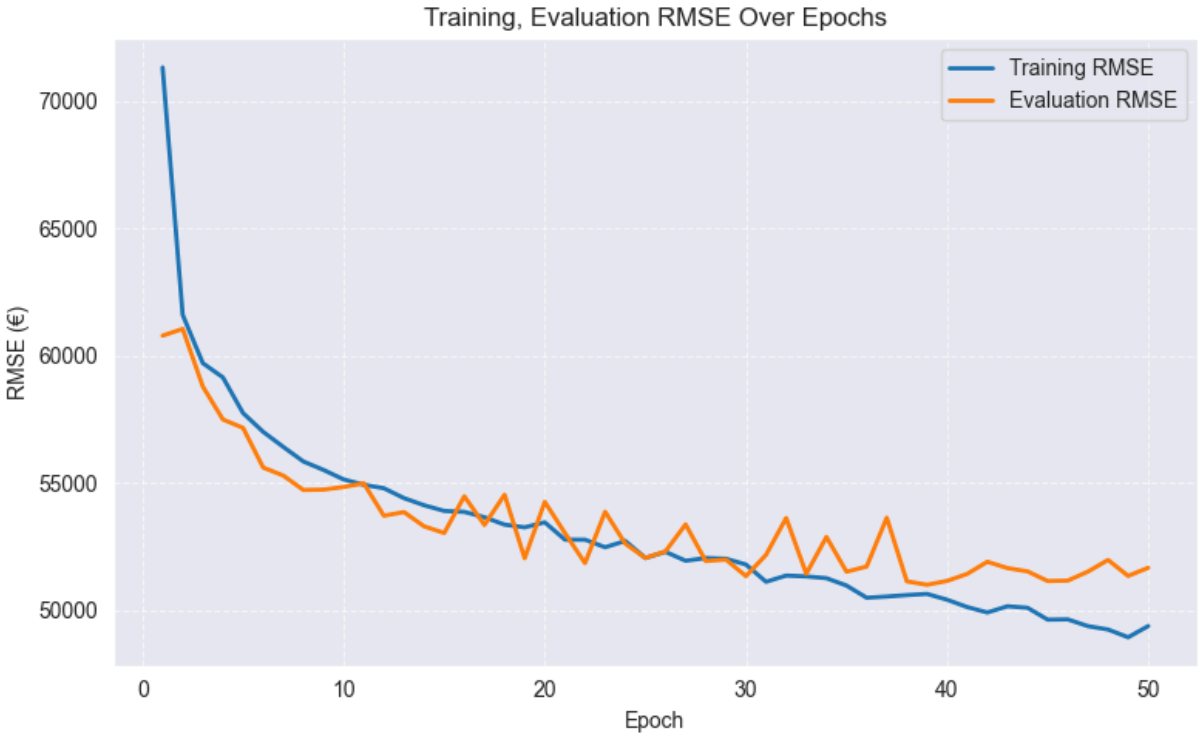
View project at: https://wandb.ai/xhanushchak-slovensk-technick-univerzita-v-bratislave/zneus-project-1

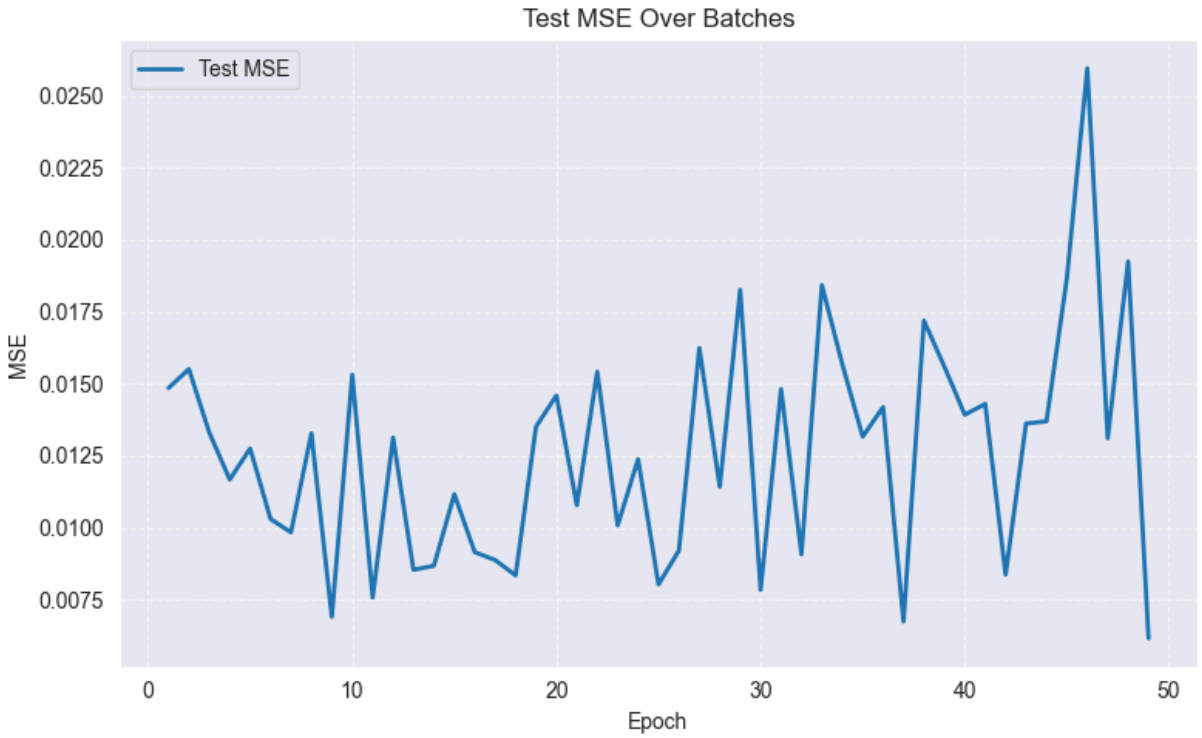
Synced 4 W&B file(s), 0 media file(s), 0 artifact file(s) and 0 other file(s)

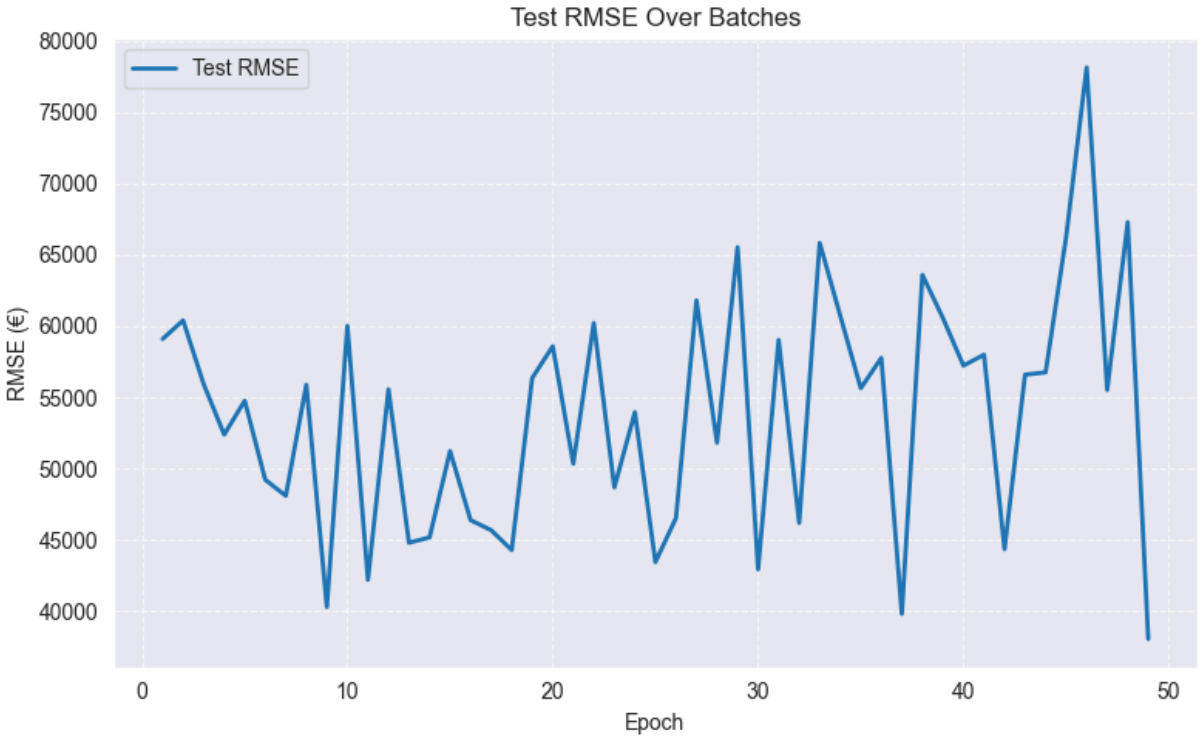
Find logs at: `.\wandb\run-20251109_205618-gvlsqjyq\logs`

```
Train RMSE: 48883.2118, Test RMSE: 54498.1586
```






Test MSE Over Batches
Test MSE
MSE
0.0250
0.0225
0.0200
0.0175
0.0150
0.0125
0.0100
0.0075
0
10
20
30
40
50
Epoch


Test RMSE Over Batches
Test RMSE
RMSE (€)
80000
75000
70000
65000
60000
55000
50000
45000
40000
0
10
20
30
40
50
Epoch