

Configuration Manual

MSc Research Project MSc in Data Analytics

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MSc Project Submission Sheet

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Performance Using Machine Learning models

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Configuration Manual

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1 Introduction

This document provides detailed information about the kind of configuration required to perform the code. This document discusses both the software and hardware requirements to set up the environment.

2 Environment

This section provides information about the software and hardware configuration required to the execute the code.

2.1 Hardware Configuration

Hardware specification used to execute the project is displayed using Figure 1.

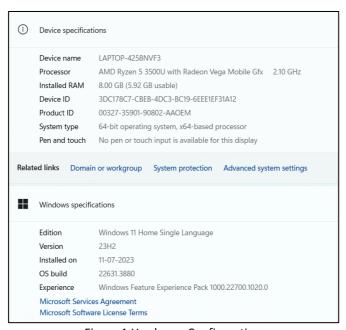


Figure 1 Hardware Configuration

2.2 Software Requirements

Python programming language is used to perform the research project. This python code was written using the jupyter notebook environment, which is interactive IDE to perform analysis and modelling. This is performed on python version 3

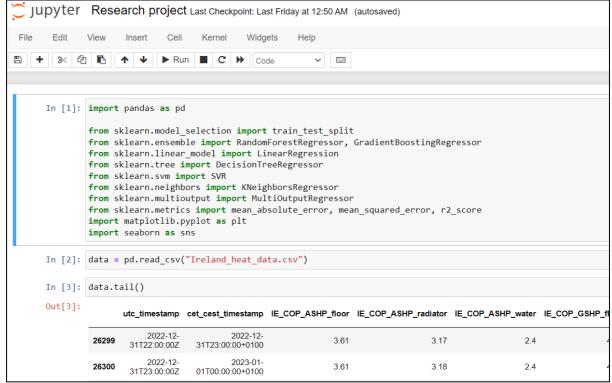


Figure 2 Jupyter Notebook Overview

3 Packages Required

Importing the necessary packages is the first step of the research, these packed can be installed using the pip command. Initially some packages such pandas, numpy and matplotlib are required to load the dataset and understand the data performing some operations which may require numpy. Other libraries can be loaded at the later stage of the project.

```
In [1]: import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns

from sklearn.model_selection import train_test_split
from sklearn.ensemble import RandomForestRegressor, GradientBoostingRegressor
from sklearn.linear_model import LinearRegression
from sklearn.tree import DecisionTreeRegressor
from sklearn.svm import SVR
from sklearn.neighbors import KNeighborsRegressor
from sklearn.multioutput import MultiOutputRegressor
from sklearn.metrics import mean_absolute_error, mean_squared_error, r2_score
from sklearn.model_selection import learning_curve
```

Figure 3 Importing Libraries

4 Dataset Description

Two datasets are being used in this research project, one dataset contains information about heat pumps¹ and other contains information about weather². Both the datasets are merged using excel based on a common column time stamp.

dat	data.head()								
	utc_timestamp	cet_cest_timestamp	IE_COP_ASHP_floor	IE_COP_ASHP_radiator	IE_COP_ASHP_water	IE_COP_GSHP_floor			
0	2020-01-01 00:00:00	2020-01- 01T01:00:00+0100	3.72	3.30	2.44	5.02			
1	2020-01-01 01:00:00	2020-01- 01T02:00:00+0100	3.70	3.28	2.43	5.00			
2	2020-01-01 02:00:00	2020-01- 01T03:00:00+0100	3.68	3.25	2.42	4.97			
3	2020-01-01 03:00:00	2020-01- 01T04:00:00+0100	3.62	3.18	2.40	4.87			
4	2020-01-01 04:00:00	2020-01- 01T05:00:00+0100	3.54	3.09	2.36	4.76			
5 r	5 rows × 25 columns								

Figure 4 Dataset Imported

5 Data Preparation

The data is being prepared by deleting all the null values and also performed feature selection afterwards the data is being divided into train and test set to train model.

```
In [25]:

data = data.dropna()
Y = [
    'IE_COP_ASHP_floor', 'IE_COP_ASHP_radiator', 'IE_COP_ASHP_water',
    'IE_COP_ASHP_floor', 'IE_COP_ASHP_radiator', 'IE_COP_GSHP_water',
    'IE_COP_MSHP_floor', 'IE_COP_WSHP_radiator', 'IE_COP_WSHP_water'
]

X = data.drop(columns=Y + ['utc_timestamp', 'cet_cest_timestamp'])

corr_matrix = X.corr().abs()

upper = corr_matrix.where(np.triu(np.ones(corr_matrix.shape), k=1).astype(np.bool_))

# correlation greater than 0.8
to_drop = [column for column in upper.columns if any(upper[column] > 0.8)]

X_selected = X.drop(columns=to_drop)

print("Selected Features after correlation filtering: ", X_selected.columns)

Selected Features after correlation filtering: Index(['IE_heat_profile_space_COM', 'IE_heat_profile_water_COM',
    'IE_heat_profile_water_MFH', 't2m', 'prectotland (mm/h)',
    'precsnoland (mm/h)', 'snomas (kg/m)', 'rhoa (kg/m)', 'swgdn (W/m)',
    'cldtot'],
    dtype='object')
```

Figure 5 Feature Selection

¹ https://data.open-power-system-data.org/when2heat/latest/

² https://www.renewables.ninja/#/country

```
X_train, X_test, y_train, y_test = train_test_split(X_selected, data[Y], test_size=0.2, random_state=42)
```

Figure 6 Train and test split

6 Model Preparation

There are six machine learning model and two deep learning models used in this research. The six machine learning model are Random Forest, Gradient Boost, Decision Tree, KNN, Support Vector Regression and Vector Regressor and the two deep learning model are LSTM and MLP.

6.1 Random Forest

A Random Forest model was employed using 100 estimators, with a maximum depth of 10, and minimum samples split and leaf values set to 5 and 2, respectively. K-Fold cross-validation (with 4 splits) was performed to evaluate the performance, using negative mean squared error (MSE).

```
from sklearn.model selection import KFold, cross val score
import numpy as np
import time
# K-Fold Cross Validation setup
kfold = KFold(n_splits=4, shuffle=True, random_state=42)
# List to store computation times for each model
computation_times = []
model_rf = RandomForestRegressor(
    n_estimators=100,
    max_depth=10,
    min_samples_split=5,
    min_samples_leaf=2,
    random state=42,
    n jobs=-1 # Parallel processing
start_time = time.time()
cv_scores_rf = cross_val_score(model_rf, X_train, y_train, cv=kfold, scoring='neg_mean_squared_error', n_jobs=-1)
end_time = time.time()
computation_times.append(('Random Forest', end_time - start_time))
print(f'Random Forest Cross-Validation MSE Scores: {-cv scores rf}')
print(f'Mean MSE: {-np.mean(cv scores rf)}')
print(f'Computational Time: {end_time - start_time:.2f} seconds\n')
model_rf.fit(X_train, y_train)
predictions = model_rf.predict(X_test)
```

Figure 7 Random Forest

6.2 Gradient Boosting

A Gradient Boosting Regressor was used and wrapped in a MultiOutputRegressor to handle multi-output regression. The model was configured with 110 estimators, a learning rate of 0.05, and a maximum depth of 5, with additional hyperparameters for controlling split and leaf size. K-Fold cross-validation (4 splits) was applied to evaluate the model, using negative MSE, and the computation time was recorded. After evaluation, the model was fitted and used to predict on the test set.

```
GB_model = MultiOutputRegressor(GradientBoostingRegressor(
    n_estimators=110,
    learning_rate=0.05,
   max_depth=5,
   min_samples_split=10,
   min_samples_leaf=4,
    random_state=42
start_time = time.time()
cv_scores_gb = cross_val_score(GB_model, X_train, y_train, cv=kfold, scoring='neg_mean_squared_error', n_jobs=-1)
end time = time.time()
computation_times.append(('Gradient Boosting', end_time - start_time))
print(f'Gradient Boosting Cross-Validation MSE Scores: {-cv_scores_gb}')
print(f'Mean MSE: {-np.mean(cv_scores_gb)}')
print(f'Computational Time: {end_time - start_time:.2f} seconds\n')
GB_model.fit(X_train_scaled, y_train)
GB predict = GB model.predict(X test)
```

Figure 8 Gradient Boosting

6.3 Decision Tree

A Decision Tree Regressor was configured with a maximum depth of 8, a minimum sample split of 10, and a minimum sample leaf size of 5. K-Fold cross-validation with 4 splits was performed to evaluate the model using negative mean squared error (MSE) as the performance metric. After recording the computational time, the model was trained on the training set and used to make predictions on the test set.

```
DT_model = DecisionTreeRegressor(
    max_depth=8,
    min_samples_split=10,
    min_samples_leaf=5,
    random_state=24
)

start_time = time.time()
    cv_scores_dt = cross_val_score(DT_model, X_train, y_train, cv=kfold, scoring='neg_mean_squared_error', n_jobs=-1)

DT_model.fit(X_train, y_train)

DT_predict = DT_model.predict(X_test)
end_time = time.time()
computation_times.append(('Decision Tree', end_time - start_time))

print(f'Decision Tree Cross-Validation MSE Scores: {-cv_scores_dt}')
    print(f'Mean MSE: {-np.mean(cv_scores_dt)}')
    print(f'Computational Time: {end_time - start_time:.2f} seconds\n')
```

Figure 9 Decision Tree

6.4 K – Nearest Neighbour (KNN)

The K-Nearest Neighbors (KNN) Regressor was implemented with 7 neighbors and a distance-based weighting scheme. Cross-validation was performed using K-Fold to assess model

performance using negative mean squared error. The computation time was recorded, and the model was trained on the training set before making predictions on the test set.

```
KNN_model = KNeighborsRegressor(
    n_neighbors=7,
    weights='distance',
    algorithm='auto',
    leaf_size=30,
    p=2
)

start_time = time.time()
    cv_scores_knn = cross_val_score(KNN_model, X_train, y_train, cv=kfold, scoring='neg_mean_squared_error', n_jobs=-1)
KNN_model.fit(X_train|, y_train)
KNN_predict = KNN_model.predict(X_test)
end_time = time.time()
computation_times.append(('KNN', end_time - start_time))
print(f'KNN Cross-Validation MSE Scores: {-cv_scores_knn}')
print(f'Mean MSE: {-np.mean(cv_scores_knn)}')
print(f'Computational Time: {end_time - start_time:.2f} seconds\n')
```

Figure 10 KNN

6.5 Support Vector Regression (SVR)

A Support Vector Regressor (SVR) was employed using a radial basis function (RBF) kernel, with a regularization parameter C=1.0, an epsilon value of 0.1, and the gamma parameter set to 'scale'. The model was wrapped in a MultiOutputRegressor to handle multi-output regression tasks. K-Fold cross-validation (4 splits) was conducted to evaluate performance.

Figure 11 SVR

6.6 Voting Regressor

A Voting Regressor was built by combining two base models Gradient Boosting Regressor and a Support Vector Regressor (SVR). This ensemble approach aggregates the predictions from both models to improve overall performance. The model was wrapped in a MultiOutputRegressor to handle multi-output regression tasks. The Voting Regressor was trained and evaluated using the test set using the evaluation metrics.

```
from sklearn.ensemble import VotingRegressor
start time vr = time.time()
gb = GradientBoostingRegressor()
svr = SVR()
voting regressor = VotingRegressor(estimators=[('gb', gb), ('svr', svr)])
multi voting regressor = MultiOutputRegressor(voting regressor)
multi voting regressor.fit(X train, y train)
y pred voting = multi voting regressor.predict(X test)
end time vr = time.time()
print(f"Computation Time of LSTM Model: {end time vr - start time vr:.2f} seconds")
mae = mean_absolute_error(y_test, y_pred_voting)
mse = mean_squared_error(y_test, y_pred_voting)
r2 = r2_score(y_test, y_pred_voting)
print(f"Voting Regressor - Mean Absolute Error: {mae}")
print(f"Voting Regressor - Mean Squared Error: {mse}")
print(f"Voting Regressor - R-squared: {r2}")
```

Figure 12 Voting Regressor

6.7 Long Short-Term Memory (LSTM)

An LSTM neural network was implemented for the time-series prediction task, consisting of two LSTM layers with 100 and 50 units, respectively. A Dense layer with 32 units and ReLU activation was added, followed by an output layer to predict the target variables. The model was trained for 50 epochs with a batch size of 32, using the Adam optimizer and mean squared error as the loss function. After training, predictions were made on the reshaped test data, and key evaluation metrics such as MAE, MSE, and R² were calculated.

```
# Reshape data
X train = np.array(X train)
X \text{ test} = np.array(X \text{ test})
X_train_lstm = np.reshape(X_train, (X_train.shape[0], 1, X_train.shape[1]))
X_test_lstm = np.reshape(X_test, (X_test.shape[0], 1, X_test.shape[1]))
lstm_model = Sequential()
lstm\_model.add(LSTM(units=100, return\_sequences= \textit{True}, input\_shape=(X\_train\_lstm.shape[1], X\_train\_lstm.shape[2]))) \\
lstm_model.add(LSTM(units=50, return_sequences=False)) # Second LSTM Layer
lstm_model.add(Dense(units=32, activation='relu')) # Dense Layer after LSTM Layers
lstm_model.add(Dense(units=y_train.shape[1])) # Output Layer
lstm model.compile(optimizer='adam', loss='mean squared error')
lstm_model.fit(X_train_lstm, y_train, epochs=50, batch_size=32)
y_pred_lstm = lstm_model.predict(X_test_lstm)
mae = mean_absolute_error(y_test, y_pred_lstm)
mse = mean_squared_error(y_test, y_pred_lstm)
r2 = r2_score(y_test, y_pred_lstm)
print(f"LSTM - Mean Absolute Error: {mae}")
print(f"LSTM - Mean Squared Error: {mse}")
print(f"LSTM - R-squared: {r2}")
```

Figure 13 LSTM

6.8 Multi-Layer Perceptron (MLP)

A Multi-Layer Perceptron (MLP) model was constructed using a series of dense layers with ReLU activation. The model architecture included layers with 256, 128, 64, and 32 units, followed by an output layer corresponding to the target dimensions. The model was trained for 50 epochs with a batch size of 32, using the Adam optimizer and mean squared error as the loss function. After training, predictions were made on the test set.

```
from keras.models import Sequential
from keras.layers import Dense
start time mlp = time.time()
mlp model = Sequential()
mlp model.add(Dense(units=256, activation='relu', input dim=X train.shape[1]))
mlp model.add(Dense(units=128, activation='relu'))
mlp model.add(Dense(units=64, activation='relu'))
mlp model.add(Dense(units=32, activation='relu'))
mlp_model.add(Dense(units=y_train.shape[1]))
mlp_model.compile(optimizer='adam', loss='mean_squared_error')
mlp_model.fit(X_train, y_train, epochs=50, batch_size=32)
y_pred_mlp = mlp_model.predict(X_test)
end time mlp = time.time()
print(f"Computation Time of LSTM Model: {end time mlp - start time mlp:.2f} seconds")
mae = mean_absolute_error(y_test, y_pred_mlp)
mse = mean_squared_error(y_test, y_pred_mlp)
r2 = r2_score(y_test, y_pred_mlp)
print(f"MLP - Mean Absolute Error: {mae}")
print(f"MLP - Mean Squared Error: {mse}")
print(f"MLP - R-squared: {r2}")
```

Figure 14 MLP