Midterm Exam Part 2 - Solutions

Note that this Notebook contains solutions for the extra questions included in the EEL5934 but not in EEL4930.

In [96]:
```
# Import all necessary libraries and magics

import numpy as np
import matplotlib.pyplot as plt
import pandas as pd
from scipy import stats
%matplotlib inline
plt.style.use('bmh')

from sklearn.model_selection import train_test_split, GridSearchCV, cross_val_score
from sklearn.preprocessing import MinMaxScaler, StandardScaler, PolynomialFeatures, Or
from sklearn.impute import SimpleImputer
from sklearn.pipeline import Pipeline
from sklearn.compose import ColumnTransformer
from sklearn.metrics import classification_report, accuracy_score, confusion_matrix, C
from sklearn.metrics import mean_squared_error, r2_score
from sklearn.linear_model import LinearRegression, Lasso, LogisticRegression, Lasso, R
from sklearn.ensemble import RandomForestClassifier, RandomForestRegressor, BaggingCla
from sklearn.ensemble import AdaBoostClassifier, AdaBoostRegressor
from sklearn.tree import DecisionTreeClassifier, DecisionTreeRegressor
```

Question 1 (20 points)

In this problem, you will be working with the wine dataset that is readily available in `sklearn.datasets`.

This dataset contains 13 numerical attributes. Each sample is labeled as class 0, 1 or 2. Let's load it:

In [2]:
```
from sklearn.datasets import load_wine

wine = load_wine(as_frame=True)

print(wine.DESCR)
```

```
.. _wine_dataset:

Wine recognition dataset
------------------------

**Data Set Characteristics:**

    :Number of Instances: 178 (50 in each of three classes)
    :Number of Attributes: 13 numeric, predictive attributes and the class
    :Attribute Information:
                - Alcohol
                - Malic acid
                - Ash
                - Alcalinity of ash
                - Magnesium
                - Total phenols
                - Flavanoids
                - Nonflavanoid phenols
                - Proanthocyanins
                - Color intensity
                - Hue
                - OD280/OD315 of diluted wines
                - Proline

    - class:
            - class_0
            - class_1
            - class_2

    :Summary Statistics:

    ============================= ==== ===== ======= =====
                                   Min   Max   Mean     SD
    ============================= ==== ===== ======= =====
    Alcohol:                      11.0  14.8    13.0   0.8
    Malic Acid:                   0.74  5.80    2.34  1.12
    Ash:                          1.36  3.23    2.36  0.27
    Alcalinity of Ash:            10.6  30.0    19.5   3.3
    Magnesium:                    70.0 162.0    99.7  14.3
    Total Phenols:                0.98  3.88    2.29  0.63
    Flavanoids:                   0.34  5.08    2.03  1.00
    Nonflavanoid Phenols:         0.13  0.66    0.36  0.12
    Proanthocyanins:              0.41  3.58    1.59  0.57
    Colour Intensity:              1.3  13.0     5.1   2.3
    Hue:                          0.48  1.71    0.96  0.23
    OD280/OD315 of diluted wines: 1.27  4.00    2.61  0.71
    Proline:                       278  1680     746   315
    ============================= ==== ===== ======= =====

    :Missing Attribute Values: None
    :Class Distribution: class_0 (59), class_1 (71), class_2 (48)
    :Creator: R.A. Fisher
    :Donor: Michael Marshall (MARSHALL%PLU@io.arc.nasa.gov)
    :Date: July, 1988

This is a copy of UCI ML Wine recognition datasets.
https://archive.ics.uci.edu/ml/machine-learning-databases/wine/wine.data

The data is the results of a chemical analysis of wines grown in the same
region in Italy by three different cultivators. There are thirteen different
```

```
measurements taken for different constituents found in the three types of
wine.

Original Owners:

Forina, M. et al, PARVUS -
An Extendible Package for Data Exploration, Classification and Correlation.
Institute of Pharmaceutical and Food Analysis and Technologies,
Via Brigata Salerno, 16147 Genoa, Italy.

Citation:

Lichman, M. (2013). UCI Machine Learning Repository
[https://archive.ics.uci.edu/ml]. Irvine, CA: University of California,
School of Information and Computer Science.

.. topic:: References

  (1) S. Aeberhard, D. Coomans and O. de Vel,
  Comparison of Classifiers in High Dimensional Settings,
  Tech. Rep. no. 92-02, (1992), Dept. of Computer Science and Dept. of
  Mathematics and Statistics, James Cook University of North Queensland.
  (Also submitted to Technometrics).

  The data was used with many others for comparing various
  classifiers. The classes are separable, though only RDA
  has achieved 100% correct classification.
  (RDA : 100%, QDA 99.4%, LDA 98.9%, 1NN 96.1% (z-transformed data))
  (All results using the leave-one-out technique)

  (2) S. Aeberhard, D. Coomans and O. de Vel,
  "THE CLASSIFICATION PERFORMANCE OF RDA"
  Tech. Rep. no. 92-01, (1992), Dept. of Computer Science and Dept. of
  Mathematics and Statistics, James Cook University of North Queensland.
  (Also submitted to Journal of Chemometrics).
```

In [3]:
```
X = wine.data

X
```

Out[3]:

	alcohol	malic_acid	ash	alcalinity_of_ash	magnesium	total_phenols	flavanoids	nonflavanoid_
0	14.23	1.71	2.43	15.6	127.0	2.80	3.06	
1	13.20	1.78	2.14	11.2	100.0	2.65	2.76	
2	13.16	2.36	2.67	18.6	101.0	2.80	3.24	
3	14.37	1.95	2.50	16.8	113.0	3.85	3.49	
4	13.24	2.59	2.87	21.0	118.0	2.80	2.69	
...	...	...	...	...	...	...	...	
173	13.71	5.65	2.45	20.5	95.0	1.68	0.61	
174	13.40	3.91	2.48	23.0	102.0	1.80	0.75	
175	13.27	4.28	2.26	20.0	120.0	1.59	0.69	
176	13.17	2.59	2.37	20.0	120.0	1.65	0.68	
177	14.13	4.10	2.74	24.5	96.0	2.05	0.76	

178 rows × 13 columns

In [4]:
```
t = wine.target

t.shape
```

Out[4]:
```
(178,)
```

Answer the following questions:

1. **(2 points) Split the data using a stratified 80/20 random split.**

In [6]:
```
X_train, X_test, t_train, t_test = train_test_split(X, t,
                                                    test_size=0.2,
                                                    stratify=t,
                                                    shuffle=True,
                                                    random_state=0)

X_train.shape, t_train.shape, X_test.shape, t_test.shape
```

Out[6]:
```
((142, 13), (142,), (36, 13), (36,))
```

1. **(4 points) Build a `sklearn` pipeline to (1) scale the data, and (2) train a Random Forest classifier. Carry the experimental design (pick at least 2 hyperparameters) with a 5-fold cross-validation scheme and accuracy as the performance measure. From the values experimented with, which set returned the best accuracy scores?**

In [7]:
```
pipe = Pipeline([('scaling', StandardScaler()),
                 ('random_forest', RandomForestClassifier())])

pipe.get_params()
```

```
Out[7]: {'memory': None,
         'steps': [('scaling', StandardScaler()),
          ('random_forest', RandomForestClassifier())],
         'verbose': False,
         'scaling': StandardScaler(),
         'random_forest': RandomForestClassifier(),
         'scaling__copy': True,
         'scaling__with_mean': True,
         'scaling__with_std': True,
         'random_forest__bootstrap': True,
         'random_forest__ccp_alpha': 0.0,
         'random_forest__class_weight': None,
         'random_forest__criterion': 'gini',
         'random_forest__max_depth': None,
         'random_forest__max_features': 'auto',
         'random_forest__max_leaf_nodes': None,
         'random_forest__max_samples': None,
         'random_forest__min_impurity_decrease': 0.0,
         'random_forest__min_samples_leaf': 1,
         'random_forest__min_samples_split': 2,
         'random_forest__min_weight_fraction_leaf': 0.0,
         'random_forest__n_estimators': 100,
         'random_forest__n_jobs': None,
         'random_forest__oob_score': False,
         'random_forest__random_state': None,
         'random_forest__verbose': 0,
         'random_forest__warm_start': False}
```

```
In [10]: param_grid = {'random_forest__max_depth': list(range(7,15)),
                       'random_forest__n_estimators': np.arange(100,501,100)}

         grid_search = GridSearchCV(pipe, param_grid,
                                    cv=5, scoring='accuracy',
                                   refit=True)

         grid_search.fit(X_train, t_train)

         print(grid_search.best_params_)

         {'random_forest__max_depth': 7, 'random_forest__n_estimators': 100}
```

```
In [11]: # Training final model
         final_pipe_rf = grid_search.best_estimator_

         final_pipe_rf

Out[11]: Pipeline(steps=[('scaling', StandardScaler()),
                         ('random_forest', RandomForestClassifier(max_depth=7))])
```

1. **(4 points) Use your trained pipeline in (2) to make predictions in the training and test sets. Report accuracy, confusion matrices and the 95% confidence interval. Discuss whether the model might be overfitting. Justify your reasoning.**

```
In [12]: # Predicting labels for training/test sets
         y_train = final_pipe_rf.predict(X_train)
         y_test = final_pipe_rf.predict(X_test)
```

```
In [16]: scores_val = cross_val_score(final_pipe_rf, X_train, t_train,
                              scoring='accuracy', cv=5)

confidence = 0.95
stats.t.interval(confidence,
                 len(scores_val)-1,
                 loc = scores_val.mean(),
                 scale=scores_val.std(ddof=1)/np.sqrt(len(scores_val)))
```

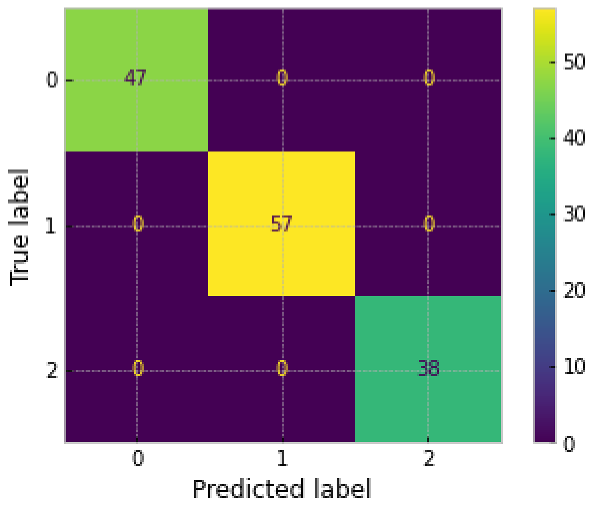
Out[16]:

```
(0.9347375638514634, 0.9953116972322804)
```

In [20]:

```
print('Training Set Accuracy:', accuracy_score(t_train, y_train)*100, '%')
ConfusionMatrixDisplay(confusion_matrix(t_train, y_train)).plot();
```

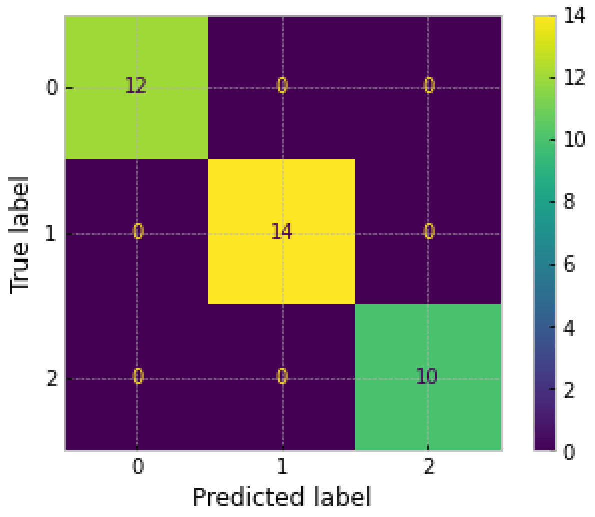
```
Training Set Accuracy: 100.0 %
```



In [21]:

```
print('Test Set Accuracy:', accuracy_score(t_test, y_test)*100, '%')
ConfusionMatrixDisplay(confusion_matrix(t_test, y_test)).plot();
```

```
Test Set Accuracy: 100.0 %
```



1. **(4 points) Build a `sklearn` pipeline to (1) scale the data, and (2) train a Logistic Regression classifier with *a* regularization penalty term. Carry the experimental design (pick at least 2 hyperparameters) with a 5-fold cross-validation scheme and accuracy as the performance measure. From the values experimented with, which set returned the best accuracy scores?**

```
In [24]: pipe = Pipeline([('scaling', StandardScaler()),
                          ('log_reg', LogisticRegression(solver='liblinear'))])

         pipe.get_params()
```

```
Out[24]: {'memory': None,
          'steps': [('scaling', StandardScaler()),
           ('log_reg', LogisticRegression(solver='liblinear'))],
          'verbose': False,
          'scaling': StandardScaler(),
          'log_reg': LogisticRegression(solver='liblinear'),
          'scaling__copy': True,
          'scaling__with_mean': True,
          'scaling__with_std': True,
          'log_reg__C': 1.0,
          'log_reg__class_weight': None,
          'log_reg__dual': False,
          'log_reg__fit_intercept': True,
          'log_reg__intercept_scaling': 1,
          'log_reg__l1_ratio': None,
          'log_reg__max_iter': 100,
          'log_reg__multi_class': 'auto',
          'log_reg__n_jobs': None,
          'log_reg__penalty': 'l2',
          'log_reg__random_state': None,
          'log_reg__solver': 'liblinear',
          'log_reg__tol': 0.0001,
          'log_reg__verbose': 0,
          'log_reg__warm_start': False}
```

```
In [26]: param_grid = {'log_reg__penalty': ['l1','l2'],
                       'log_reg__C': np.linspace(0.0001,5,100)}

         grid_search = GridSearchCV(pipe, param_grid,
                                    cv=5, scoring='accuracy',
                                   refit=True)

         grid_search.fit(X_train, t_train)

         print(grid_search.best_params_)
```

```
{'log_reg__C': 0.15161212121212, 'log_reg__penalty': 'l2'}
```

```
In [27]: # Training final model
         final_pipe_logreg = grid_search.best_estimator_

         final_pipe_logreg
```

```
Out[27]: Pipeline(steps=[('scaling', StandardScaler()),
                         ('log_reg',
                          LogisticRegression(C=0.15161212121212, solver='liblinear'))])
```

1. **(4 points) Use your trained pipeline in (4) to make predictions in the training and test sets. Report accuracy, confusion matrices and the 95% confidence interval. Discuss whether the model might be overfitting. Justify your reasoning.**

```
In [29]: # Predicting labels for training/test sets
```

```
y_train = final_pipe_logreg.predict(X_train)
y_test = final_pipe_logreg.predict(X_test)
```

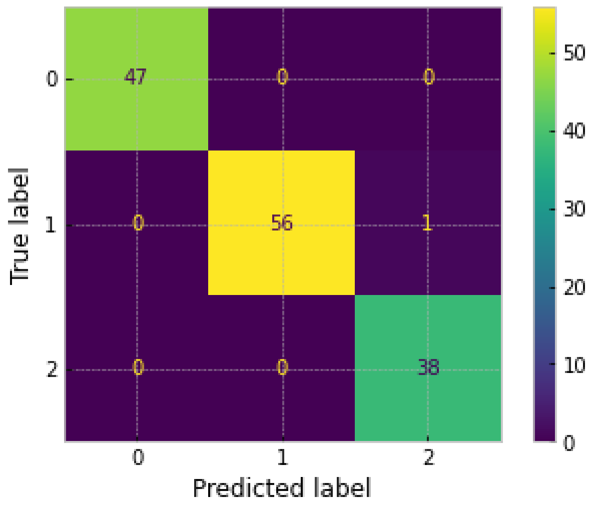
In [30]:
```
scores_val = cross_val_score(final_pipe_logreg, X_train, t_train,
                             scoring='accuracy', cv=5)

confidence = 0.95
stats.t.interval(confidence,
                 len(scores_val)-1,
                 loc = scores_val.mean(),
                 scale=scores_val.std(ddof=1)/np.sqrt(len(scores_val)))
```

Out[30]:
```
(0.9614254506907766, 1.0100031207377949)
```

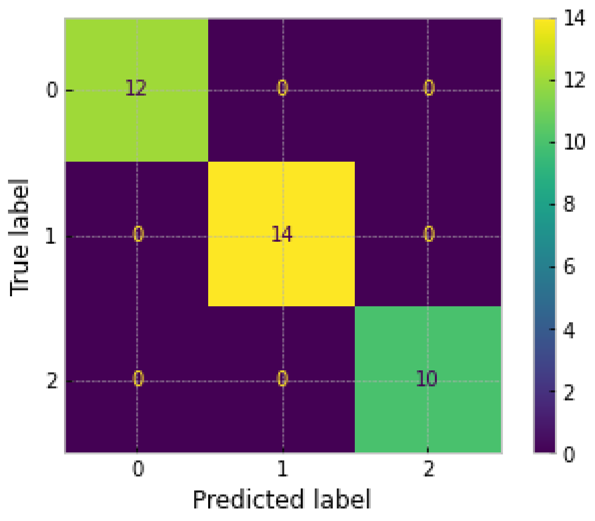
In [31]:
```
print('Training Set Accuracy:', accuracy_score(t_train, y_train)*100, '%')
ConfusionMatrixDisplay(confusion_matrix(t_train, y_train)).plot();
```

```
Training Set Accuracy: 99.29577464788733 %
```



In [32]:
```
print('Test Set Accuracy:', accuracy_score(t_test, y_test)*100, '%')
ConfusionMatrixDisplay(confusion_matrix(t_test, y_test)).plot();
```

```
Test Set Accuracy: 100.0 %
```



1. **(2 points) Based on these results, which model would you select?**

The accuracy in training and test sets are identical in both models, but the 95% for the Logistic Regression model includes larger accuracy scores thus Logistic Regression (with the hyperparameter specified above) performs best for this dataset.

Question 2 (30 points)

In this problem, you will be working with the Air Quality UCI dataset. The dataset contains 9358 instances of hourly averaged responses from an array of metal oxide chemical sensors embedded in an Air Quality Chemical Multisensor Device.

Attribute Information

1. **Date (DD/MM/YYYY)**
2. **Time (HH.MM.SS)**
3. **True hourly averaged concentration CO in mg/m^3 (reference analyzer)**
4. **PT08.S1 (tin oxide) hourly averaged sensor response (nominally CO targeted)**
5. **True hourly averaged overall Non Metanic HydroCarbons concentration in microg/m^3 (reference analyzer)**
6. **True hourly averaged Benzene concentration in microg/m^3 (reference analyzer)**
7. **PT08.S2 (titania) hourly averaged sensor response (nominally NMHC targeted)**
8. **True hourly averaged NOx concentration in ppb (reference analyzer)**
9. **PT08.S3 (tungsten oxide) hourly averaged sensor response (nominally NOx targeted)**
10. **True hourly averaged NO2 concentration in microg/m^3 (reference analyzer)**
11. **PT08.S4 (tungsten oxide) hourly averaged sensor response (nominally NO2 targeted)**
12. **PT08.S5 (indium oxide) hourly averaged sensor response (nominally O3 targeted)**
13. **Temperature in Celsius**
14. **Relative Humidity (%)**
15. **AH Absolute Humidity**

The goal of this problem is to predict the true hourly concentration of CO in mg/m^3.

1. **(5 points) Load the data. Answer the following questions:**
   - **Are there any missing values?**
   - **Visualize how informative each attribute is in predicting the target variable CO(GT).**
   - **Which attributes are most correlated with the target variable?**

In [67]:
```
data = pd.read_csv('AirQualityUCI.csv')
data
```

Out[67]:

	Date	Time	CO(GT)	PT08.S1(CO)	NMHC(GT)	C6H6(GT)	PT08.S2(NMHC)	NOx(GT)
0	3/10/2004	18:00:00	2.6	1360.0	150.0	11.9	1046.0	166.0
1	3/10/2004	19:00:00	2.0	1292.0	112.0	9.4	955.0	103.0
2	3/10/2004	20:00:00	2.2	1402.0	88.0	9.0	939.0	131.0
3	3/10/2004	21:00:00	2.2	1376.0	80.0	9.2	948.0	172.0
4	3/10/2004	22:00:00	1.6	1272.0	51.0	6.5	836.0	131.0
...	...	...	...	...	...	...	...	...
9352	4/4/2005	10:00:00	3.1	1314.0	NaN	13.5	1101.0	472.0
9353	4/4/2005	11:00:00	2.4	1163.0	NaN	11.4	1027.0	353.0
9354	4/4/2005	12:00:00	2.4	1142.0	NaN	12.4	1063.0	293.0
9355	4/4/2005	13:00:00	2.1	1003.0	NaN	9.5	961.0	235.0
9356	4/4/2005	14:00:00	2.2	1071.0	NaN	11.9	1047.0	265.0

9357 rows × 15 columns

In [68]:

```
data.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 9357 entries, 0 to 9356
Data columns (total 15 columns):
 #   Column         Non-Null Count  Dtype  
---  ------         --------------  -----  
 0   Date           9357 non-null   object 
 1   Time           9357 non-null   object 
 2   CO(GT)         7674 non-null   float64
 3   PT08.S1(CO)    8991 non-null   float64
 4   NMHC(GT)       914 non-null    float64
 5   C6H6(GT)       8991 non-null   float64
 6   PT08.S2(NMHC)  8991 non-null   float64
 7   NOx(GT)        7718 non-null   float64
 8   PT08.S3(NOx)   8991 non-null   float64
 9   NO2(GT)        7715 non-null   float64
 10  PT08.S4(NO2)   8991 non-null   float64
 11  PT08.S5(O3)    8991 non-null   float64
 12  T              8991 non-null   float64
 13  RH             8991 non-null   float64
 14  AH             8991 non-null   float64
dtypes: float64(13), object(2)
memory usage: 1.1+ MB
```

There are missing values in all attributes but date and time. Since the target variable CO(GT) only contains 7674, we should drop all samples with missing entries.

In [77]:

```
new_data=data.dropna(subset=['CO(GT)'])

new_data.info()
```

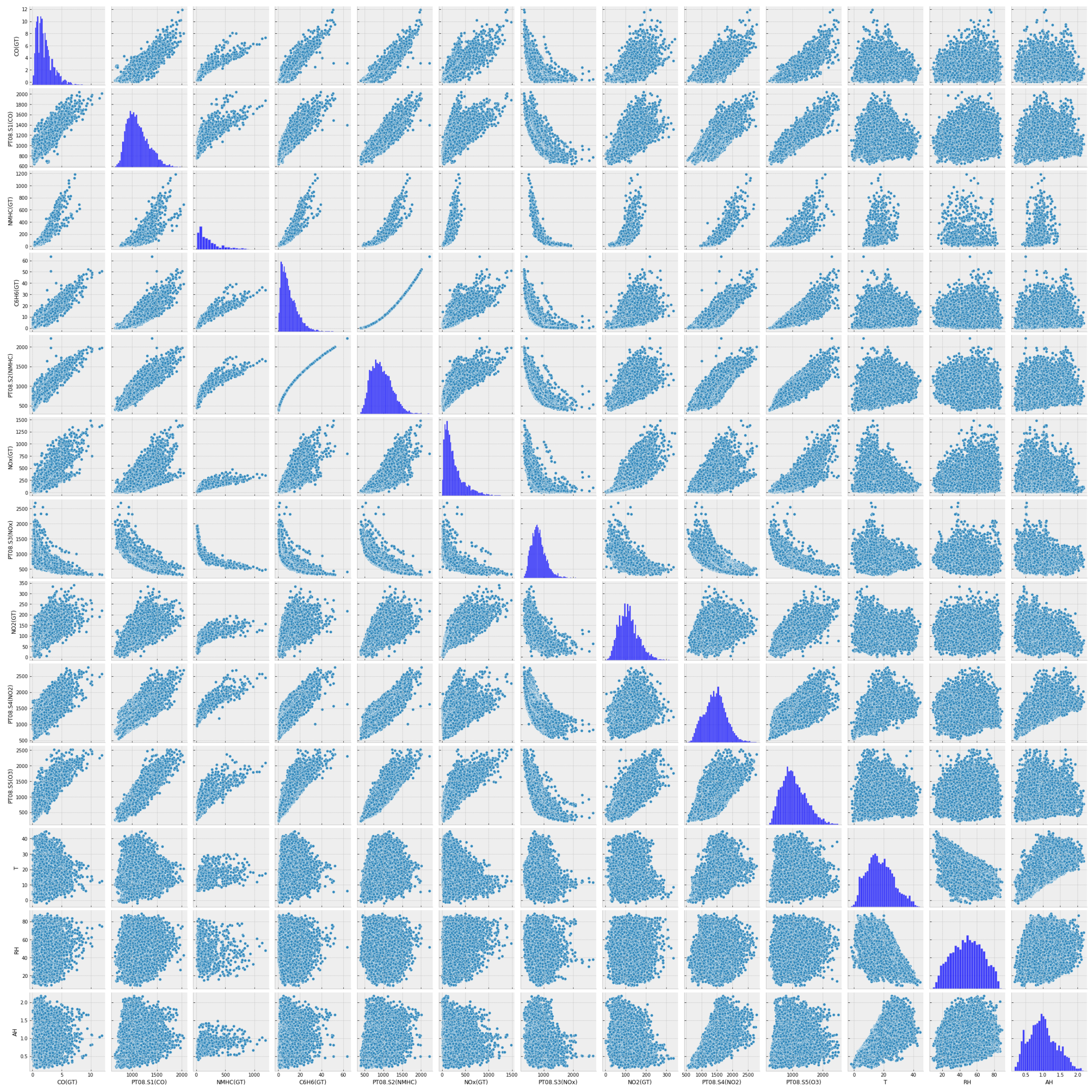
```
<class 'pandas.core.frame.DataFrame'>
Int64Index: 7674 entries, 0 to 9356
Data columns (total 15 columns):
 #   Column         Non-Null Count  Dtype  
---  ------         --------------  -----  
 0   Date           7674 non-null   object 
 1   Time           7674 non-null   object 
 2   CO(GT)         7674 non-null   float64
 3   PT08.S1(CO)    7344 non-null   float64
 4   NMHC(GT)       890 non-null    float64
 5   C6H6(GT)       7344 non-null   float64
 6   PT08.S2(NMHC)  7344 non-null   float64
 7   NOx(GT)        7261 non-null   float64
 8   PT08.S3(NOx)   7344 non-null   float64
 9   NO2(GT)        7258 non-null   float64
 10  PT08.S4(NO2)   7344 non-null   float64
 11  PT08.S5(O3)    7344 non-null   float64
 12  T              7344 non-null   float64
 13  RH             7344 non-null   float64
 14  AH             7344 non-null   float64
dtypes: float64(13), object(2)
memory usage: 959.2+ KB
```

Once we drop the entries in the target variable `CO(GT)`, we see that other entries still have a reasonably large number of missing values. For all other, I will use `SimpleImputer` to impute the missing values with the median. For the attribute `NMHC(GT)`, there are too many missing values. I will drop that atttribute.

In [78]:
```
import seaborn

seaborn.pairplot(new_data)
```

Out[78]:
```
<seaborn.axisgrid.PairGrid at 0x18f86d20df0>
```



In [79]:
```
new_data.corr(method='pearson')['CO(GT)']
```

Out[79]:
```
CO(GT)           1.000000
PT08.S1(CO)      0.879288
NMHC(GT)         0.889734
C6H6(GT)         0.931078
PT08.S2(NMHC)    0.915514
NOx(GT)          0.795028
PT08.S3(NOx)    -0.703446
NO2(GT)          0.683343
PT08.S4(NO2)     0.630703
PT08.S5(O3)      0.854182
T                0.022109
RH               0.048890
AH               0.048556
Name: CO(GT), dtype: float64
```

Attributes C6H6(GT), PT08.S2(NMHC) and NMHC(GT) have the largest Pearson's correlation with the target response (>0.88).

1. **(5 points) Split your data and build a pipeline to encode and scale your attributes. Disregard attributes `Date`, `Time` and any other attribute with less than 1000 non-null entries.**

In [80]:
```
new_data.info()
```

```
<class 'pandas.core.frame.DataFrame'>
Int64Index: 7674 entries, 0 to 9356
Data columns (total 15 columns):
 #   Column         Non-Null Count  Dtype  
---  ------         --------------  -----  
 0   Date           7674 non-null   object 
 1   Time           7674 non-null   object 
 2   CO(GT)         7674 non-null   float64
 3   PT08.S1(CO)    7344 non-null   float64
 4   NMHC(GT)       890 non-null    float64
 5   C6H6(GT)       7344 non-null   float64
 6   PT08.S2(NMHC)  7344 non-null   float64
 7   NOx(GT)        7261 non-null   float64
 8   PT08.S3(NOx)   7344 non-null   float64
 9   NO2(GT)        7258 non-null   float64
 10  PT08.S4(NO2)   7344 non-null   float64
 11  PT08.S5(O3)    7344 non-null   float64
 12  T              7344 non-null   float64
 13  RH             7344 non-null   float64
 14  AH             7344 non-null   float64
dtypes: float64(13), object(2)
memory usage: 959.2+ KB
```

In [101…
```
# Defining feature matrix X and target variable t

t = new_data['CO(GT)']

X = new_data.drop(['CO(GT)'], axis=1)

t.shape, X.shape
```

Out[101]:
```
((7674,), (7674, 14))
```

In [102…
```
X_train, X_test, t_train, t_test = train_test_split(X, t, test_size=0.2, random_state=

X_train.shape, X_test.shape, t_train.shape, t_test.shape
```

Out[102]:
```
((6139, 14), (1535, 14), (6139,), (1535,))
```

In [116…
```
# List of numerical attributes, disregarding "NMHC(GT)"
num_attribs = ['PT08.S1(CO)']+list(data.columns[5:])

# Pipeline for numerical attributes to (1) filling missing values with the median and
num_pipeline = Pipeline([('missing_values',SimpleImputer(strategy='median')),
                         ('std_scaler', StandardScaler())])

# Preprocessing Pipeline
preprocessing_pipeline = ColumnTransformer([('num_attribs', num_pipeline, num_attribs)
                                           remainder='drop')

# Train the pipeline
# preprocessing_pipeline.fit(X_train)
```

1. **(5 points) Train a Linear Regression algorithm with polynomial features of order M and Lasso regularizer.**

Perform hyperparameter tuning to determine which value of M and λ best work for this data. Use r^2 as your performance measure and a 10-fold CV strategy.

Note: You may set `tol=2` in `Lasso` to avoid convergence warnings.

In [127…

```
# Pipeline for Linear Regression with Polynomial Features and Lasso Regularizer
pol_lin_reg = Pipeline([('poly_feat', PolynomialFeatures()),
                        ('lin_reg_lasso', Lasso(tol=2))])

# Full pipeline: Preprocessing + Model
full_pipeline = Pipeline([('preprocessing', preprocessing_pipeline),
                          (['model', pol_lin_reg])])

full_pipeline.get_params()
```

```
Out[127]: {'memory': None,
           'steps': [('preprocessing',
             ColumnTransformer(transformers=[('num_attribs',
                                              Pipeline(steps=[('missing_values',
                                                               SimpleImputer(strategy='media
          n')),
                                                              ('std_scaler',
                                                               StandardScaler())]),
                                              ['PT08.S1(CO)', 'C6H6(GT)', 'PT08.S2(NMHC)',
                                               'NOx(GT)', 'PT08.S3(NOx)', 'NO2(GT)',
                                               'PT08.S4(NO2)', 'PT08.S5(O3)', 'T', 'RH',
                                               'AH'])])),
            ['model',
             Pipeline(steps=[('poly_feat', PolynomialFeatures()),
                             ('lin_reg_lasso', Lasso(tol=2))])]],
           'verbose': False,
           'preprocessing': ColumnTransformer(transformers=[('num_attribs',
                                            Pipeline(steps=[('missing_values',
                                                             SimpleImputer(strategy='median')),
                                                            ('std_scaler',
                                                             StandardScaler())]),
                                            ['PT08.S1(CO)', 'C6H6(GT)', 'PT08.S2(NMHC)',
                                             'NOx(GT)', 'PT08.S3(NOx)', 'NO2(GT)',
                                             'PT08.S4(NO2)', 'PT08.S5(O3)', 'T', 'RH',
                                             'AH'])]),
           'model': Pipeline(steps=[('poly_feat', PolynomialFeatures()),
                           ('lin_reg_lasso', Lasso(tol=2))]),
           'preprocessing__n_jobs': None,
           'preprocessing__remainder': 'drop',
           'preprocessing__sparse_threshold': 0.3,
           'preprocessing__transformer_weights': None,
           'preprocessing__transformers': [('num_attribs',
             Pipeline(steps=[('missing_values', SimpleImputer(strategy='median')),
                             ('std_scaler', StandardScaler())]),
             ['PT08.S1(CO)',
              'C6H6(GT)',
              'PT08.S2(NMHC)',
              'NOx(GT)',
              'PT08.S3(NOx)',
              'NO2(GT)',
              'PT08.S4(NO2)',
              'PT08.S5(O3)',
              'T',
              'RH',
              'AH'])],
           'preprocessing__verbose': False,
           'preprocessing__verbose_feature_names_out': True,
           'preprocessing__num_attribs': Pipeline(steps=[('missing_values', SimpleImputer(strat
          egy='median')),
                           ('std_scaler', StandardScaler())]),
           'preprocessing__num_attribs__memory': None,
           'preprocessing__num_attribs__steps': [('missing_values',
             SimpleImputer(strategy='median')),
            ('std_scaler', StandardScaler())],
           'preprocessing__num_attribs__verbose': False,
           'preprocessing__num_attribs__missing_values': SimpleImputer(strategy='median'),
           'preprocessing__num_attribs__std_scaler': StandardScaler(),
           'preprocessing__num_attribs__missing_values__add_indicator': False,
           'preprocessing__num_attribs__missing_values__copy': True,
           'preprocessing__num_attribs__missing_values__fill_value': None,
 'preprocessing__num_attribs__missing_values__missing_values': nan,
 'preprocessing__num_attribs__missing_values__strategy': 'median',
 'preprocessing__num_attribs__missing_values__verbose': 0,
 'preprocessing__num_attribs__std_scaler__copy': True,
 'preprocessing__num_attribs__std_scaler__with_mean': True,
 'preprocessing__num_attribs__std_scaler__with_std': True,
 'model__memory': None,
 'model__steps': [('poly_feat', PolynomialFeatures()),
  ('lin_reg_lasso', Lasso(tol=2))],
 'model__verbose': False,
 'model__poly_feat': PolynomialFeatures(),
 'model__lin_reg_lasso': Lasso(tol=2),
 'model__poly_feat__degree': 2,
 'model__poly_feat__include_bias': True,
 'model__poly_feat__interaction_only': False,
 'model__poly_feat__order': 'C',
 'model__lin_reg_lasso__alpha': 1.0,
 'model__lin_reg_lasso__copy_X': True,
 'model__lin_reg_lasso__fit_intercept': True,
 'model__lin_reg_lasso__max_iter': 1000,
 'model__lin_reg_lasso__normalize': 'deprecated',
 'model__lin_reg_lasso__positive': False,
 'model__lin_reg_lasso__precompute': False,
 'model__lin_reg_lasso__random_state': None,
 'model__lin_reg_lasso__selection': 'cyclic',
 'model__lin_reg_lasso__tol': 2,
 'model__lin_reg_lasso__warm_start': False}
```

In [128…

```
param_grid = {'model__poly_feat__degree': range(1,5),
             'model__lin_reg_lasso__alpha': [0.0001, 0.001, 0.01, 0.1, 0.2]}

grid_search = GridSearchCV(full_pipeline, param_grid,
                          cv=10, scoring='r2',
                         refit=True)

grid_search.fit(X_train, t_train)

print(grid_search.best_params_)
```

```
{'model__lin_reg_lasso__alpha': 0.0001, 'model__poly_feat__degree': 4}
```

The hyperparameter search should not be exhaustive. Based on these results, in practice, we should go back and increase the range of values <0.0001 since the optimal value lands on the edge of the options provided.

In [129…

```
final_model = grid_search.best_estimator_

final_model
```

```
Out[129]: Pipeline(steps=[('preprocessing',
                 ColumnTransformer(transformers=[('num_attribs',
                                                  Pipeline(steps=[('missing_values',
                                                                   SimpleImputer(stra
tegy='median')),
                                                                  ('std_scaler',
                                                                   StandardScaler
())]),
                                                  ['PT08.S1(CO)', 'C6H6(GT)',
                                                   'PT08.S2(NMHC)', 'NOx(GT)',
                                                   'PT08.S3(NOx)', 'NO2(GT)',
                                                   'PT08.S4(NO2)',
                                                   'PT08.S5(O3)', 'T', 'RH',
                                                   'AH'])])),
                ['model',
                 Pipeline(steps=[('poly_feat', PolynomialFeatures(degree=4)),
                                 ('lin_reg_lasso',
                                  Lasso(alpha=0.0001, tol=2))])]])
```

1. **(4 points) Report the r^2 for training and test sets, and the 95% CI in validation.**

```
In [130…
y_train = final_model.predict(X_train)

y_test = final_model.predict(X_test)
```

```
In [131…
print('Training r^2:', r2_score(t_train, y_train))

scores_val = cross_val_score(final_model, X_train, t_train,
                             scoring='r2', cv=10)
confidence = 0.95
print('95% CI:', stats.t.interval(confidence,
                                  len(scores_val)-1,
                                  loc = scores_val.mean(),
                                  scale=scores_val.std(ddof=1)/np.sqrt(len(scores_val))

print('Test r^2:', r2_score(t_test, y_test))
```

```
Training r^2: 0.8663435932607797
95% CI: (0.852998558572396, 0.8680867800806265)
Test r^2: 0.8486661238853083
```

1. **(5 points) Train a Random Forest regressor. Perform hyperparameter tuning to determine which value for the best number of trees and maximum depth best work for this data. Use r^2 as your performance measure and a 10-fold CV strategy.**

```
In [132…
# Pipeline for Linear Regression with Polynomial Features and Lasso Regularizer
RF_reg = Pipeline([('RF_regressor', RandomForestRegressor())])

# Full pipeline: Preprocessing + Model
full_pipeline = Pipeline([('preprocessing', preprocessing_pipeline),
                          (['model', RF_reg])])

full_pipeline.get_params()
```

```
Out[132]: {'memory': None,
           'steps': [('preprocessing',
             ColumnTransformer(transformers=[('num_attribs',
                                              Pipeline(steps=[('missing_values',
                                                               SimpleImputer(strategy='media
          n')),
                                                              ('std_scaler',
                                                               StandardScaler())]),
                                              ['PT08.S1(CO)', 'C6H6(GT)', 'PT08.S2(NMHC)',
                                               'NOx(GT)', 'PT08.S3(NOx)', 'NO2(GT)',
                                               'PT08.S4(NO2)', 'PT08.S5(O3)', 'T', 'RH',
                                               'AH'])])),
            ['model', Pipeline(steps=[('RF_regressor', RandomForestRegressor())])]],
           'verbose': False,
           'preprocessing': ColumnTransformer(transformers=[('num_attribs',
                                            Pipeline(steps=[('missing_values',
                                                             SimpleImputer(strategy='median')),
                                                            ('std_scaler',
                                                             StandardScaler())]),
                                            ['PT08.S1(CO)', 'C6H6(GT)', 'PT08.S2(NMHC)',
                                             'NOx(GT)', 'PT08.S3(NOx)', 'NO2(GT)',
                                             'PT08.S4(NO2)', 'PT08.S5(O3)', 'T', 'RH',
                                             'AH'])]),
           'model': Pipeline(steps=[('RF_regressor', RandomForestRegressor())]),
           'preprocessing__n_jobs': None,
           'preprocessing__remainder': 'drop',
           'preprocessing__sparse_threshold': 0.3,
           'preprocessing__transformer_weights': None,
           'preprocessing__transformers': [('num_attribs',
             Pipeline(steps=[('missing_values', SimpleImputer(strategy='median')),
                             ('std_scaler', StandardScaler())]),
             ['PT08.S1(CO)',
              'C6H6(GT)',
              'PT08.S2(NMHC)',
              'NOx(GT)',
              'PT08.S3(NOx)',
              'NO2(GT)',
              'PT08.S4(NO2)',
              'PT08.S5(O3)',
              'T',
              'RH',
              'AH'])],
           'preprocessing__verbose': False,
           'preprocessing__verbose_feature_names_out': True,
           'preprocessing__num_attribs': Pipeline(steps=[('missing_values', SimpleImputer(strat
          egy='median')),
                           ('std_scaler', StandardScaler())]),
           'preprocessing__num_attribs__memory': None,
           'preprocessing__num_attribs__steps': [('missing_values',
             SimpleImputer(strategy='median')),
            ('std_scaler', StandardScaler())],
           'preprocessing__num_attribs__verbose': False,
           'preprocessing__num_attribs__missing_values': SimpleImputer(strategy='median'),
           'preprocessing__num_attribs__std_scaler': StandardScaler(),
           'preprocessing__num_attribs__missing_values__add_indicator': False,
           'preprocessing__num_attribs__missing_values__copy': True,
           'preprocessing__num_attribs__missing_values__fill_value': None,
           'preprocessing__num_attribs__missing_values__missing_values': nan,
           'preprocessing__num_attribs__missing_values__strategy': 'median',
           'preprocessing__num_attribs__missing_values__verbose': 0,
           'preprocessing__num_attribs__std_scaler__copy': True,
           'preprocessing__num_attribs__std_scaler__with_mean': True,
           'preprocessing__num_attribs__std_scaler__with_std': True,
           'model__memory': None,
           'model__steps': [('RF_regressor', RandomForestRegressor())],
           'model__verbose': False,
           'model__RF_regressor': RandomForestRegressor(),
           'model__RF_regressor__bootstrap': True,
           'model__RF_regressor__ccp_alpha': 0.0,
           'model__RF_regressor__criterion': 'squared_error',
           'model__RF_regressor__max_depth': None,
           'model__RF_regressor__max_features': 'auto',
           'model__RF_regressor__max_leaf_nodes': None,
           'model__RF_regressor__max_samples': None,
           'model__RF_regressor__min_impurity_decrease': 0.0,
           'model__RF_regressor__min_samples_leaf': 1,
           'model__RF_regressor__min_samples_split': 2,
           'model__RF_regressor__min_weight_fraction_leaf': 0.0,
           'model__RF_regressor__n_estimators': 100,
           'model__RF_regressor__n_jobs': None,
           'model__RF_regressor__oob_score': False,
           'model__RF_regressor__random_state': None,
           'model__RF_regressor__verbose': 0,
           'model__RF_regressor__warm_start': False}
```

In [136…

```
param_grid = {'model__RF_regressor__n_estimators': [50,100],
             'model__RF_regressor__max_depth': [2,4,6]}

grid_search = GridSearchCV(full_pipeline, param_grid,
                           cv=10, scoring='r2',
                          refit=True)

grid_search.fit(X_train, t_train)

print(grid_search.best_params_)
```

```
{'model__RF_regressor__max_depth': 6, 'model__RF_regressor__n_estimators': 50}
```

The hyperparameter search should not be exhaustive. Since the optimal value lands on the edge of the options provided, we should go back and extend the search space beyond those values.

In [137…

```
final_model = grid_search.best_estimator_

final_model
```

Out[137]:
```
Pipeline(steps=[('preprocessing',
                 ColumnTransformer(transformers=[('num_attribs',
                                                  Pipeline(steps=[('missing_values',
                                                                   SimpleImputer(stra
tegy='median')),
                                                                  ('std_scaler',
                                                                   StandardScaler
())]),
                                                  ['PT08.S1(CO)', 'C6H6(GT)',
                                                   'PT08.S2(NMHC)', 'NOx(GT)',
                                                   'PT08.S3(NOx)', 'NO2(GT)',
                                                   'PT08.S4(NO2)',
                                                   'PT08.S5(O3)', 'T', 'RH',
                                                   'AH'])])),
                ['model',
                 Pipeline(steps=[('RF_regressor',
                                  RandomForestRegressor(max_depth=6,
                                                        n_estimators=50))])]])
```

1. **(4 points) Report the r^2 for training and test sets, and the 95% CI in validation.**

In [138…
```
y_train = final_model.predict(X_train)

y_test = final_model.predict(X_test)
```

In [139…
```
print('Training r^2:', r2_score(t_train, y_train))

scores_val = cross_val_score(final_model, X_train, t_train,
                             scoring='r2', cv=10)
confidence = 0.95
print('95% CI:', stats.t.interval(confidence,
                                  len(scores_val)-1,
                                  loc = scores_val.mean(),
                                  scale=scores_val.std(ddof=1)/np.sqrt(len(scores_val))

print('Test r^2:', r2_score(t_test, y_test))
```

```
Training r^2: 0.9238031679943277
95% CI: (0.8927367822180641, 0.9112395230689103)
Test r^2: 0.9043599881276887
```

1. **(2 points) Based on the results you obtain from the previous problems, which model (polynomial linear regression with Lasso penalty or Random Forest regressor) would you select? Explain your reasoning.**

Based on these results, the random forest regressor performs best in training and test sets and produces the best 95% CI in the validation set.
