COMP 309 — Machine Learning Tools and Techniques Assignment 4: Performance Metrics and Optimisation

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2.1 Part 1: Performance Metrics in Regression [35 marks]

For this section I will be performing regression techniques on the diamonds.csv dataset located in $part1/Part\ 1 - regression/diamonds.csv$. I will be using the sci-kit learn tool to perform the regression techniques on this dataset. When running the pipeline, it is preferred to use the Pipeline-Tensor-Flow.py on google colab as some algorithms take about 20 minutes locally.

Loading the dataset:

The first step is to import the required sci-kit learn and basic Python libraries that will help us when we apply our regression techniques. Pandas is developed for fast, efficient & easy practical realworld data manipulation and data analysis. Using pandas, we can load in the diamonds.csv file with simply one line "dataset = pd.read.csv('diamonds.csv').

Initial Data Analysis:

I have attached an image below that helps us analyse some of the initial data. From quickly applying some functions to our dataset, we see there are eleven different attributes to each diamond instance. We can also see there is an *'Unnamed'* attribute, which labels the number of the listed instance. I will remove this as it doesn't help our investigation and more importantly, won't help our regression techniques.

Screenshot of data analytics.py, this gives us a preview of the information in our dataset

```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as seabornInstance
from sklearn.model_selection import train_test_split
from sklearn.linear_model import LinearRegression
from sklearn import metrics
from scipv.io import arff
%matplotlib inline
dataset = pd.read_csv('diamonds.csv')
dataset.shape
(53940, 11)
dataset.columns
dataset.isnull().values.any()
False
dataset.head()
  Unnamed: 0 carat
                   cut color clarity depth table
         1 0.23
                            SI2
                                61.5 55.0 3.95 3.98 2.43
1
         2 0.21 Premium
                      E SI1 59.8 61.0 3.89 3.84 2.31
                                                      326
2
         3 0.23 Good E VS1 56.9 65.0 4.05 4.07 2.31 327
         4 0.29 Premium
                      I VS2 62.4 58.0 4.20 4.23 2.63
         5 0.31
               Good J SI2 63.3 58.0 4.34 4.35 2.75 335
```

Attributes

- Carat: Carat weight of the Diamond.
- Cut: Describe cut quality of the diamond.
- Colour: Colour of the Diamond
- Clarity: Diamond Clarity refers to the absence of the Inclusions and Blemishes
- Depth: The Height of a Diamond, measured from the Culet to the table, divided by its average Girdle Diameter.
- Table: The Width of the Diamond's Table expressed as a Percentage of its Average
- X: Length of the Diamond in mm.
- Y: Width of the Diamond in mm.
- Z: Height of the Diamond in mm.
- Price: The Price of the Diamond.

Description of attributes

- Cut in increasing order Fair, Good, Very Good, Premium, Ideal.
- With D being the best and J the worst.
- (In order from Best to Worst, FL = flawless, I3= level 3 inclusions) FL, IF, VVS1, VVS2, VS1, VS2, SI1, SI2, I1, I2, I3
- Qualitative Features (Categorical): Cut, Colour, Clarity.
- Quantitative Features (Numerical): Carat, Depth, Table, Price, X, Y, Z.
- Price is the Target Variable.

Pre-process Data:

Drop the index from the dataset using "data = data.drop(data.colums[0], axis=1). Cut, Colour and Clarity all have string values, we need to change this these to numerical values this is demonstrated in the screenshot below.

```
# transform cut to int
                                        # drop the index column
def trans_cut(x):
                                        dataset = dataset.drop(dataset.columns[0], axis=1)
    if x == "Fair": return 4
if x == "Good": return 3
                                        dataset.isnull().values.any()
    if x == "Very Good": return 2
if x == "Ideal": return 1
    if x == "Premium": return 0
# transform color into int
def trans_color(x):
    trans_color(x):
if x == "D": return 0
if x == "E": return 1
if x == "F": return 2
if x == "G": return 3
if x == "H": return 4
if x == "I": return 5
if x == "J": return 6
                                                To begin our pre-processing, we need to drop the first
                                                attribute, then run a null value scan to see if there are any
                                                missing values in the dataset. This resulted in 'False,' so we
# transform clarity to int
                                                can continue our investigation and convert each result in a
def trans_clarity(x):
    if x == "I1": return 7
if x == "SI1": return 6
if x == "SI2": return 6
                                                hierarchical numerical structure. (As pictured on the left).
                                                This converts each string result for each attribute in the
    if x == "VS1": return 4
                                                dataset. We are applying this pre-processing technique for
    if x == "VS2": return 3
if x == "VVS1": return 2
                                                our regression algorithms later. From doing this, we should
    if x == "VVS2": return 1
                                                see if there are any correlations between our attributes a lot
    if x == "IF": return 0
                                                easier. This will be described in the later steps.
```

	/	+ [/ - - + -	+ [[1177	0	-11/	4\1
print((datase	t[(data	set[[.x.11	== 0	.all(axi	LS=1)]
print((datase	t[(data	set[[. A. 11	== 0	.all(axi	LS=1)]
print((datase	t[(data	set[[.z.]]	== 0	.all(axi	LS=1)]
	depth	table	х	У	Z	price	
11182	61.6	56.0	0.0	6.62	0.0	4954	
11963	63.3	53.0	0.0	0.00	0.0	5139	
15951		67.0		0.00		6381	
24520	62.2	54.0		0.00		12800	
26243	62.1	59.0			0.0		
27429	62.8	59.0		0.00			
49556	64.1	60.0		0.00		2130	
49557	64.1	60.0	0.0	0.00		2130	
		table	X	у	Z	price	
11963	63.3	53.0	0.0	0.0	0.0	5139	
15951	57.5	67.0		0.0	0.0		
24520	62.2	54.0		0.0	0.0	12800	
26243	62.1	59.0	0.0		0.0	15686	
27429	62.8	59.0	0.0		0.0	18034	
49556	64.1	60.0	0.0	0.0	0.0	2130	
49557	64.1	60.0	0.0	0.0	0.0	2130	
	depth	table	X	,	/ 2	price	
2207	59.1	59.0	6.55				
2314	58.1	59.0	6.66	6.60	0.0	3167	
4791	63.0	59.0	6.50	6.47	7 0.6	3696	
5471	59.2		6.50		7 0.6	3837	
10167	64.0		7.15		4 0.6	4731	
11182	61.6	56.0	0.00	6.62	2 0.6	4954	
11963	63.3	53.0	0.00	0.00	0.0	5139	
13601	59.2	56.0	6.88	6.83	0.6	5564	
15951	57.5	67.0	0.00	0.00	0.6	6381	
24394	59.4	61.0	8.49	8.45	0.6	12631	
24520	62.2	54.0	0.00	0.00	0.0	12800	
26123	61.3	58.0	8.52	8.42	2 0.6	15397	
26243	62.1	59.0	0.00	0.00	0.0	15686	
27112	61.2	59.0	8.42		7 0.6	17265	
27429	62.8	59.0	0.00	0.00	0.0	18034	
27503	62.7	53.0	8.02	7.95	0.6	18207	
27739	63.8	58.0	8.90				
49556	64.1	60.0	0.00		0.6		
49557	64.1	60.0	0.00				
51506	60.4	59.0	6.71	6.6	7 0.6	2383	

Image of zero checking (data cleansing), this can be found in the data_analytics.py file. But is also applied in my pipeline.py.

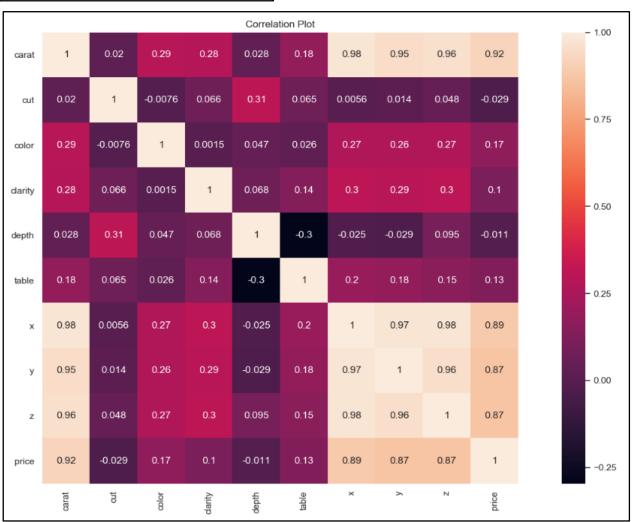
Just because there are no 'null' values present in the dataset, doesn't mean we shouldn't check attributes for inaccurate values. For example, I have individually checked each x, y, z attribute for the number '0.' This is because you physically can't have a diamond with a dimension of 0. For presentation purposes, I have printed every occurrence of this in the dataset. The code I used to drop all 0 occurrences is:

$$data = data [(data[['x', 'y', 'z']] != 0).all(axis=1)]$$

This will give us a far more accurate result when applying our regression algorithms.

Exploratory Data Analysis:

plt.figure(figsize = (15, 10)) sns.heatmap(dataset.corr(), annot = True)



Now let's look at the correlation graph using seaborn heat correlation map:

- We can see x, y, z and carat have extremely high correlations with the price of diamonds.
- Depth has one of the lowest correlations, when comparing to price, we could assume that the depth of a diamond does not affect the price of a diamond, solely because of the close to '0' correlation presented in the heatmap.
- We can also see that table and depth have a strong negative correlation with each other, we may remove this later depending on the performance of our machine learning techniques.

Build classification (or regression) models using the training data

Before we apply our regression algorithm, we must split the data into the required training and test set. As required by the handout, I have applied the random_state = 0 and the test size to be 30% of the dataset. This is done through a simple sci kit function 'train_test_split (x, y, test_size = 0.3, random_state = 309)'

```
# splitting to train and test
X = data.drop(['price'], axis=1)
y = data['price']
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3, random_state=309)
```

We can create an evaluation model by combining common steps, therefor I have created the below function to act on our parsed model type.

```
RSquared_Scores = []
def eval_model(model_type):
   start_time = time.time()
   model = model_type
   model.fit(X_train , y_train)
cross_val_results = cross_val_score(estimator = model, X = X_train, y = y_train, cv = 5,verbose = 1)
   y_predict = model.predict(X_test)
   print('-
   print(model_type)
   print(cross_val_results)
   mse = mean_squared_error(y_test, y_predict)
   rmse = mean_squared_error(y_test, y_predict)**0.5
   r2 = r2_score(y_test, y_predict)
mae = mean_absolute_error(y_test, y_predict)
   print('MSE
                   : %0.2f ' % mse)
   print('RMSE : %0.2f ' % rmse)
                  : %0.2f ' % r2)
: %0.2f ' % mae)
   print('R2 : %0.2f ' % r2)
print('MAE : %0.2f ' % mae)
print("--- %s seconds ---" % (time.time() - start_time))
   print('\n\n')
   RSquared Scores.append(r2)
```

This applies to most models but not all, bringing us to our main () function which will execute all 10 algorithms when run.

```
def main():
    eval_model(LinearRegression())
    eval_model(KNeighborsRegressor())
    eval_model(Ridge(alpha=1.0))
    eval_model(tree.DecisionTreeClassifier())
    ScaledSGDRegression()
    ScaledSVR()
    eval_model(RandomForestRegressor())
    eval_model(RandomForestRegressor())
    eval_model(GradientBoostingRegressor(n_estimators=100, learning_rate=0.1, max_depth=1, random_state=309, loss='ls
    eval_model(LinearSVR(random_state=309, tol=1e-5))
    eval_model(MLPRegressor(max_iter=1000))
```

As you can see both *scaledSVR* and *scaledSGDRegression* require extra work and cannot be passed through the eval_model. Thus, I have created separate functions for these algorithms to be run alongside the rest.

Assess model on the test data.

Model	LinearRegression	Ridge	DecisionTree	SVR	RandomForest
SCORE	0.90	0.90	0.97	0.9416	0.98
MSE	1631602.42	1632206.75	547945.21	949286.03	320793.45
MAE	839.32	839.73	363.80	507.52	285.01
RMSE	1277.34	1277.58	740.23	974.31	566.39
R2	0.90	0.90	0.97	0.94	0.98

Model	GradientBoosting	LinearSVR	MLPRegressor	K-NN	MLP
SCORE	0.91	0.80	0.95	0.95	0.93
MSE	1427945.21	3274041.47	858964.08	752865.31	1128628.63
MAE	699.97	1059.18	541.45	467.84	672.95
RMSE	1194.97	1809.43	926.80	867.68	1062.37
R2	0.91	0.80	0.95	0.95	0.93

Part 2: Performance Metrics in Classification [35 marks]

Step 1. Load Data

There are two methods of approach for loading the data, due to me using google-colab and jupyter notebook. The reason for this is the google TPU runs 4x faster when running the pipelines.

Loading the data via juypter-notebook:

"data train = pd.read csv('adultTrain.csv')" &

Loading the data via google-colab:

Step 2. Initial Data Analysis

- Age: continuous.
- Work-class: Private, Self-emp-not-inc, Self-emp-inc, Federal-gov, Local-gov, State-gov, Without-pay, Never-worked.
- Fnlwgt: continuous.
- Education: Bachelors, Some-college, 11th, HS-grad, Prof-school, Assoc-acdm, Assoc-voc, 9th, 7th-8th, 12th, Masters, 1st-4th, 10th, Doctorate, 5th-6th, Preschool.
- Education-num: continuous.
- Marital-status: Married-civ-spouse, Divorced, Never-married, Separated, Widowed,
- Married-spouse-absent, Married-AF-spouse.
- Occupation: Tech-support, Craft-repair, Other-service, Sales, Exec-managerial, Profspecialty, Handlers-cleaners, Machine-op-inspct, Adm-clerical, Farming-fishing,
- Transport-moving, Priv-house-serv, Protective-serv, Armed-Forces.
- Relationship: Wife, Own-child, Husband, Not-in-family, Other-relative, Unmarried.

[&]quot;data test = pd.read csv('adultTest.csv')"

[&]quot;drive.mount('/content/gdrive')"

[&]quot;train data = pd.read csv('/content/gdrive/My Drive/Colab Notebooks/adultTrain.csv')" &

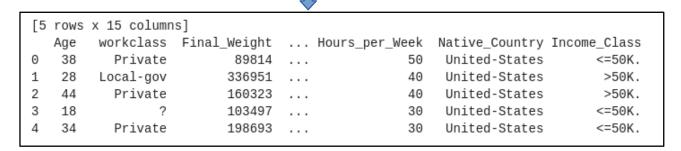
[&]quot;test data = pd.read csv('/content/gdrive/My Drive/Colab Notebooks/adultTest.csv')"

- Race: White, Asian-Pac-Islander, Amer-Indian-Eskimo, Other, Black.
- Sex: Female, Male.
- Capital-gain: continuous.
- Capital-loss: continuous.
- Hours-per-week: continuous.
- Native-country: United-States, Cambodia, England, Puerto-Rico, Canada, Germany,
 Outlying-US(Guam-USVI-etc), India, Japan, Greece, South, China, Cuba, Iran, Honduras,
 Philippines, Italy, Poland, Jamaica, Vietnam, Mexico, Portugal, Ireland, France, DominicanRepublic, Laos, Ecuador, Taiwan, Haiti, Columbia, Hungary, Guatemala, Nicaragua,
 Scotland, Thailand, Yugoslavia, El-Salvador, Trinidad & Tobago, Peru, Hong, HollandNetherlands.
- Income-Class >50K, <=50K. "Extraction was done by Barry Becker from the 1994 Census database. A set of reasonably clean records were extracted using the following conditions: ((AAGE>16) && (AGI>100) && (AFNLWGT>1) && (HRSWK>0))"

Step 3. Pre-process Data

Firstly, we notice both the test and train data files do not have column titles so let's start by assigning a title to each column using dataset.columns command and the column titles discovered in part step 2.

39 State-gov	77516	Bachelors	13	Never-married	Adm-clerical	Not-in-family	White
50 Self-emp-not-inc	83311	Bachelors	13	Married-civ-spouse	Exec-managerial	Husband	White
38 Private	215646	HS-grad	9	Divorced	Handlers-cleaners	Not-in-family	White
53 Private	234721	11th	7	Married-civ-spouse	Handlers-cleaners	Husband	Black



Now also looking more closely at the description of the data in part 2, we see that there is string values we need to convert to numeric values as the decision trees implemented in scikit-learn uses only numerical features and these features are interpreted always as continuous numeric variables. Here are some of the transformations made:

```
# transform work-class to int
def trans_work_class(x):
    if x == " Never-worked":
        return 7
    elif x == " Without-pay":
        return 5
    elif x == " State-gov":
        return 4
    elif x == " Local-gov":
        return 3
    elif x == " Federal-gov":
        return 3
    elif x == " Self-emp-inc":
        return 2
    elif x == " Self-emp-not-inc":
        return 1
    elif x == " Private":
        return 0
    else:
        return "?"
```

Examples of transformation of work-class & education

```
# transform education to int
def trans_education(x):
    if x == " Preschool":
        return 1
    elif x == " 1st-4th":
        return 2
    elif x == " 5th-6th":
        return 3
    elif x == " 7th-8th":
        return 5
    elif x == " 10th":
        return 6
    elif x == " 11th":
        return 7
    elif x == " 12th":
        return 8
    elif x == " 8sograd":
        return 9
    elif x == " 8sograd":
        return 10
    elif x == " 8sograd":
        return 11
    elif x == " 8sograd":
        return 12
    elif x == " 8sograd":
        return 13
    elif x == " Massers":
        return 14
    elif x == " Bachelors":
        return 14
    elif x == " boctorate":
        return 15
    elif x == " boctorate":
        return 16
    else:
        return 17'
```

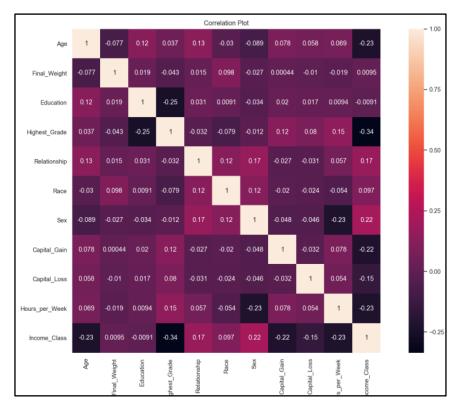
We repeat this process for the other following:

- Marital status
- Education
- Occupation
- Race
- Income class
- Native country

Then calling on the functions we implemented above, we replace all string values within both the train and test set with numeric values respectively as seen below.

```
# replace current columns with new int versions
#train
 train_data['workclass'] = train_data['workclass'].apply(trans_work_class)
 train_data['Education'] = train_data['Education'].apply(trans_education)
train_data['Marital_Status'] = train_data['Marital_Status'].apply(trans_marital_status)
 train_data['Occupation'] = train_data['Occupation'].apply(trans_occupation)
train_data['Relationship'] = train_data['Relationship'].apply(trans_relationship)
train_data['Race'] = train_data['Race'].apply(trans_race)
train_data['Sex'] = train_data['Sex'].apply(trans_sex)
train_data['Native_Country'] = train_data['Native_Country'].apply(trans_native_country)
train_data['Income_Class'] = train_data['Income_Class'].apply(trans_income_class')
 #test
test_data['workclass'] = test_data['workclass'].apply(trans_work_class)
test_data['Education'] = test_data['Education'].apply(trans_education)
test_data['Marital_Status'] = test_data['Marital_Status'].apply(trans_marital_status)
 test_data['Occupation'] = test_data['Occupation'].apply(trans_occupation)
 test_data['Relationship'] = test_data['Relationship'].apply(trans_relationship)
 test_data['Race'] = test_data['Race'].apply(trans_race)
 test_data['Sex'] = test_data['Sex'].apply(trans_sex)
 test_data['Native_Country'] = test_data['Native_Country'].apply(trans_native_country)
test_data['Income_Class'] = test_data['Income_Class'].apply(trans_income_class_test)
50
                  83311
                                            13
                                                                                                                                 13
53
                  234721
                                                                                                                                 40
                                                                                                                                 40
28
                  338409
                                                                                                                                              12
                                             13
37
                  284582
                               10
                                                                                                                                 40
Age workclass
            Final Weight
                         Education
                                  Highest
                                          Grade Marital Status Occupation
                                                                       Relationship
                                                                                   Race
                                                                                         Sex
                                                                                             Capital Gain
                                                                                                         Capital Loss
                                                                                                                      Hours
                                                                                                                               Week Native Country
                                                                                                                                                 Income Class
                   89814
                  336951
                                             12
                                                                                      Θ
                                                                                                                                 40
                                                                                                    7688
                  160323
                                             10
                  103497
                  198693
                               12
                                                                                                                                 30
                                         "Capital_Gain", "Capital_Loss",
                                                            "Capital_Loss", "Hours_per_week"
                      "Race", "5c.
" "Sex",
  "Relationship", "Race
                                                                                "Hours_per_Week", "Native_Country"]].replace('?
                               "Sex", "Capital_Gain",
                                                                                                       "Native_Country"]].replace('?', numpy.NaN)
```

This is the result of applying the transformed data after this technique. Once this is complete we can identify '?' values and replace them with a numpy.NaN value.



Looking at the correlation graph above we can see the both final_weight and education have very low correlation with the class attribute, we can go ahead and remove these two using "data.drop"

Results:

Model	K-NN	GaussianNB	SVM	DecisionTree	RandomForest
ACCURACY	0.85	0.82	0.83	0.82	0.81
PRECISION	0.84	0.81	0.82	0.82	0.84
RECALL	0.91	0.93	0.95	0.87	1.00
F1	0.88	0.87	0.88	0.85	0.91
AUC	0.77	0.71	0.70	0.76	0.59

Model	AdaBoost	GradientBoost	LinearDiscriminant	MLP	Logistic
ACCURACY	0.86	0.87	0.83	0.84	0.84
PRECISION	0.85	0.86	0.82	0.83	0.83
RECALL	0.94	0.95	0.94	0.95	0.94
F1	0.89	0.90	0.87	0.89	0.88
AUC	0.77	0.78	0.71	0.72	0.74

The best performance metric

The accuracy output of a model is not the best metric to evaluate the classifiers performance. The best way to way to evaluate the performance of a classifier is the confusion matrix. This is a combination of accuracy, recall and F1-score. We must use the four outputs to generate our confusion matrix to draw the best conclusions.

The best two algorithms.

The two best classifiers are Adaboost and GradientBoosting, these outperform the other classifiers and are very similar in results. We can see that both algorithms are using 'boosting,' which is a good way to construct a robust model. AdaBoost is adaptive in the sense that weak learners are tweaked in favour of instances misclassified by previous classifiers. **Adaboost** is sensitive to noisy data and

outliers. In some problems in can be less susceptible to the overfitting problem than other learning algorithms.

Gradient boosting is used for both regression and classification problems. This algorithm also allows for the optimization of arbitrary differentiable loss functions. This algorithm constructs a new base learner which needs to be maximally correlated with a negative gradient.

Adaboost

Accuracy: 0.86
Precision: 0.85
Recall: 0.94
F1: 0.89
AUC: 0.77

GradientBoosting

Accuracy: 0.87
Precision: 0.86
Recall: 0.95
F1: 0.90
AUC: 0.78

Part 3: Optimisation Methods [30 marks]

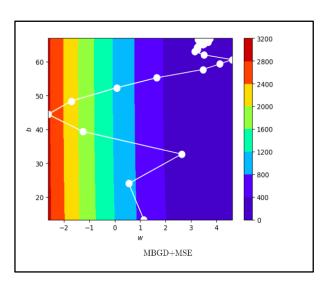
OptimisationMethod.py found at:

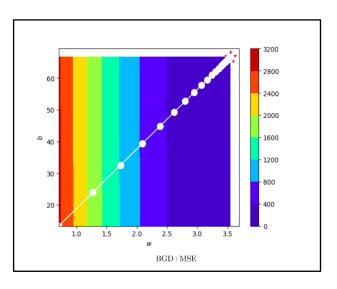
/part3/Part 3 – optimisation/template/Template/LinearRegression/src/

I have had to re-locate the utilities folder as the current release of this program is broken and can't locate the utilities module. It would benefit everyone if this was fixed in the next release of the template code.

1.

a)





• The path of gradient descent of **MBGD** + **MSE** is highly unstable (high path variance). This is because the batch size of MBGD is significantly lower (10) than BGD.

• The path of gradient descent of **BGD** + **MSE** is stable and it is a straight line which go to the local optimal point. This is because there is a larger batch_size, meaning there is less variation.

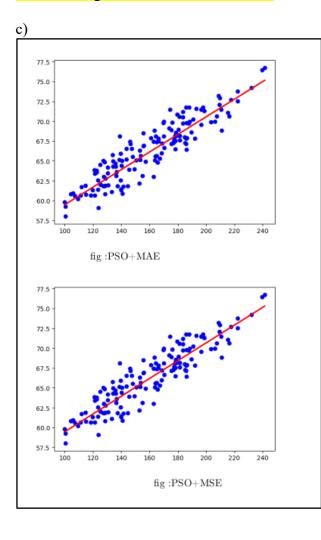
BGD computes the gradient over the entire dataset, averaging over potentially a vast amount of information.

Mini-batch gradient descent is a variation of the gradient descent algorithm that splits the training dataset into small batches that are used to calculate model error and update model coefficients.

b) Results:

	BGD + MSE	MiniBGD + MSE	PSO + MSE	PSO + MAE
MSE	2.41	2.62	2.41	2.43
R-Squared	0.83	0.82	0.84	0.83
MAE	1.28	1.32	1.28	1.28

From the table is shown above, the model optimized by **PSO** + **MSE** has the highest **R-squared value**. It also has the smallest **MSE** and **MAE** value, which means it is the best model among these four models. The **MiniBGD** + **MSE** has the poorest performance. It has the smallest R-squared value and highest MSE and MAE value.



d)

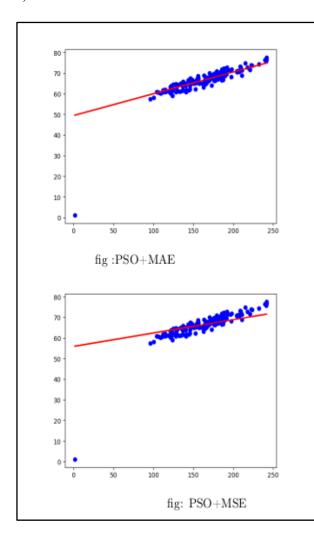
	BGD +	MiniBGD +	PSO +
	MSE	MSE	MSE
Execution Time	0.008	0.015	0.360

From the results table, we can see BGD is the fastest with an execution time of 0.008 seconds. Usually, BGD would be slower than MiniBGD but due to the dataset size being small, the execution time is faster. This could also be due to the MiniBGD batch_size being set inappropriately.

If this is done correctly, with good vectorisation and an appropriate batch_size. MiniBGD will outperform BGD.

PSO is the slowest because it has a low convergence rate in the iterative process.

a)



b)
If we compare the two plots from question one
(c), we can visually see a difference in how they
perform in comparison to question two (a). Firstly,
there is an outlier included in the results of this
algorithm. In comparison we can see that it's more
likely that this algorithm is to be affected by
outliers. This is probably due to the format of the
algorithm (Particle Swarm Optimisation), which
tries to improve a solution regardless of a given
measure of quality.

If we compare the two in this question, it seems that the PSO + MSE line is inaccurate to the groupings, unlike PSO + MAE. Because the MSE is squared before they are average, the MSE gives a relatively high weight to large errors. This means the MSE would be desirable in situations where there aren't outliers. To conclude, the MAE would likely be less prone, because MSE also increases variance associated with the frequency distribution of error magnitude also increases.

We can improve PSO + MAE through gradient boosting (discrete optimisation). In gradient boosting we can work with functions whose derivative is constant. In gradient boosting, you can use functions like MAE and improve them.

References:

 $\underline{https://makingnoise and hearing things.com/2017/12/30/how-to-be-wrong-measuring-error-in-machine-learning-models/}$

https://www.ncbi.nlm.nih.gov/pmc/articles/PMC1464136/