S09 T02: Aprenentatge Supervisat - Regressions - part 1

In [2]:
```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
import seaborn as sns
pd.set_option('display.max_columns', None)
import warnings
warnings.filterwarnings('ignore')
```

In [3]:
```
# open dataset from the previous exercise
# this file has data cleaned (we handled missing values and droped non useful columns, explained in oprevious e
# this file does not have yet dummy columns, I will generate them later before doing the regressions
data = pd.read_csv('data.csv')
data.head()
```

Out[3]:

	ArrDelay	ActualElapsedTime	CRSElapsedTime	AirTime	DepDelay	Distance	Speed	TaxiIn	TaxiOut	CarrierDelay	WeatherDelay	NASDelay
0	-14.0	128.0	150.0	116.0	8.0	810	418.97	4.0	8.0	0.0	0.0	0.0
1	2.0	128.0	145.0	113.0	19.0	810	430.09	5.0	10.0	0.0	0.0	0.0
2	14.0	96.0	90.0	76.0	8.0	515	406.58	3.0	17.0	0.0	0.0	0.0
3	34.0	90.0	90.0	77.0	34.0	515	401.30	3.0	10.0	2.0	0.0	0.0
4	11.0	101.0	115.0	87.0	25.0	688	474.48	4.0	10.0	0.0	0.0	0.0

This dataset is already cleaned from previous exercise. Because of memory issues and due to the large dataset, I'm having trouble performing the models, so I will select a sample of the dataset consisting of the 10% of the observations. I will stratify by UniqueCarrier to have a good representation of all Carriers.

In [4]:
```
data_sample = data.groupby('UniqueCarrier', group_keys= False).apply(lambda x : x.sample(frac=0.1, random_state
```

In [5]:
```
data_sample.shape
```

Out[5]:
```
(192825, 24)
```

We are going to do a describe both for our data and for the sample to check if the sample represents the data correctly:

In [6]:
```
data.describe().round(2)
```

Out[6]:

	ArrDelay	ActualElapsedTime	CRSElapsedTime	AirTime	DepDelay	Distance	Speed	TaxiIn	TaxiOut	CarrierDelay
count	1928255.00	1928255.00	1928255.00	1928255.00	1928255.00	1928255.00	1928255.00	1928255.00	1928255.00	1928255.00
mean	42.20	133.31	134.20	108.28	43.09	764.97	396.75	6.81	18.22	12.41
std	56.78	72.06	71.23	68.64	53.26	573.89	75.87	5.26	14.31	36.20
min	-70.00	14.00	-21.00	3.00	6.00	11.00	21.29	0.00	0.00	0.00
25%	9.00	80.00	82.00	58.00	12.00	338.00	351.86	4.00	10.00	0.00
50%	24.00	116.00	116.00	90.00	24.00	606.00	403.82	6.00	14.00	0.00
75%	56.00	165.00	165.00	137.00	53.00	997.00	448.14	8.00	21.00	10.00
max	2461.00	1114.00	660.00	1091.00	2467.00	4962.00	993.60	240.00	422.00	2436.00

In [7]:
```
data_sample.describe().round(2)
```

Out[7]:

	ArrDelay	ActualElapsedTime	CRSElapsedTime	AirTime	DepDelay	Distance	Speed	TaxiIn	TaxiOut	CarrierDelay
count	192825.00	192825.00	192825.00	192825.00	192825.00	192825.00	192825.00	192825.00	192825.00	192825.00
mean	42.22	133.35	134.26	108.33	43.13	765.28	396.75	6.79	18.23	12.29
std	56.92	72.03	71.20	68.60	53.56	573.94	75.75	5.24	14.23	35.81
min	-59.00	15.00	15.00	7.00	6.00	31.00	51.67	0.00	0.00	0.00
25%	9.00	80.00	82.00	58.00	12.00	338.00	352.08	4.00	10.00	0.00
50%	24.00	116.00	116.00	90.00	24.00	606.00	403.90	6.00	14.00	0.00
75%	56.00	165.00	165.00	137.00	53.00	998.00	447.90	8.00	21.00	10.00
max	1655.00	687.00	660.00	652.00	1597.00	4962.00	960.00	197.00	356.00	1312.00

We can observe the summary statistics are very similar, some min and max values change because we are taking only 10% of the data so these values may be a litlle different (we have in this dataset some heavy outliers).

We will check if we have stratified correctly according to 'UniqueCarrier' column:

In [8]:
```
# we use normalize = True because this way it´s easier to compare
data.UniqueCarrier.value_counts(normalize= True)
```

Out[8]:
```
WN    0.195096
AA    0.099006
MQ    0.073238
UA    0.073073
OO    0.068329
DL    0.058978
XE    0.053490
CO    0.051721
US    0.050827
EV    0.042396
NW    0.040888
FL    0.036804
YV    0.034621
B6    0.028480
OH    0.027185
9E    0.026742
AS    0.020231
F9    0.014636
HA    0.003875
AQ    0.000385
Name: UniqueCarrier, dtype: float64
```

In [9]:
```
data_sample.UniqueCarrier.value_counts(normalize= True)
```

Out[9]:
```
WN    0.195094
AA    0.099007
MQ    0.073237
UA    0.073071
OO    0.068331
DL    0.058976
XE    0.053489
CO    0.051720
US    0.050828
EV    0.042396
NW    0.040887
FL    0.036805
YV    0.034622
B6    0.028482
OH    0.027185
9E    0.026744
AS    0.020231
F9    0.014635
HA    0.003874
AQ    0.000384
Name: UniqueCarrier, dtype: float64
```

The proportions of Unique Carrier column are the same in our sample dataframe as in the original data.

I generate again the dummy columns explained in the previous exercise, including the Delay Interval column I generated for delay intervals. I prefer to generate the dummies directly in the Notebook and not opening a file with dummy columns because doing it this way makes the dataframe less heavy in size (this is because of the data types).

In [10]:
```
# now i will generate the dummy columns that are already explained in the previous exercise
# create a column to categorize ArrDelay, explained in previous exercise
def delay_interval(x):
    if x < 15:
        return "Less than 15"
    elif x < 30:
        return "Between 15 and 30"
    elif x < 60:
        return "Between 30 and 60"
    else:
        return "More than 60"


data_sample['DelayInterval'] = data_sample['ArrDelay'].apply(delay_interval)
data_sample.head()
```

Out[10]:

	ArrDelay	ActualElapsedTime	CRSElapsedTime	AirTime	DepDelay	Distance	Speed	TaxiIn	TaxiOut	CarrierDelay	WeatherDelay
143019	21.0	95.0	88.0	63.0	14.0	364	346.67	11.0	21.0	14.0	0.0
1886001	24.0	139.0	126.0	105.0	11.0	813	464.57	18.0	16.0	0.0	0.0
1881989	2.0	86.0	102.0	65.0	18.0	490	452.31	9.0	12.0	0.0	0.0
1030789	37.0	114.0	90.0	87.0	13.0	442	304.83	4.0	23.0	13.0	0.0
687997	10.0	90.0	88.0	61.0	8.0	382	375.74	7.0	22.0	0.0	0.0

In [11]:
```
# creating the dummy columns
# we´ll use the param drop first = True so we don t have duplicated information
# we are doing it the same way as previous exercise
data_sample= pd.get_dummies(data = data_sample, columns = ['UniqueCarrier','Origin', 'Dest'],
                            drop_first= True)
# map dummies for DelayInterval
data_sample['DelayInterval'] = data_sample['DelayInterval'].map({"Less than 15": 0, "Between 15 and 30": 1,
                        "Between 30 and 60" : 2, "More than 60": 3})
data_sample.info()
```

```
&lt;class 'pandas.core.frame.DataFrame'&gt;
Int64Index: 192825 entries, 143019 to 1544585
Columns: 637 entries, ArrDelay to Dest_YUM
dtypes: float64(15), int64(7), uint8(615)
memory usage: 146.9 MB
```

In [12]:
```
data_sample.head()
```

Out[12]:

	ArrDelay	ActualElapsedTime	CRSElapsedTime	AirTime	DepDelay	Distance	Speed	TaxiIn	TaxiOut	CarrierDelay	WeatherDelay
143019	21.0	95.0	88.0	63.0	14.0	364	346.67	11.0	21.0	14.0	0.0
1886001	24.0	139.0	126.0	105.0	11.0	813	464.57	18.0	16.0	0.0	0.0
1881989	2.0	86.0	102.0	65.0	18.0	490	452.31	9.0	12.0	0.0	0.0
1030789	37.0	114.0	90.0	87.0	13.0	442	304.83	4.0	23.0	13.0	0.0
687997	10.0	90.0	88.0	61.0	8.0	382	375.74	7.0	22.0	0.0	0.0

- Exercici 1

Crea almenys tres models de regressió diferents per intentar predir el millor possible l'endarreriment dels vols (ArrDelay) de DelayedFlights.csv.

Model 1 : Simple Linear Regression

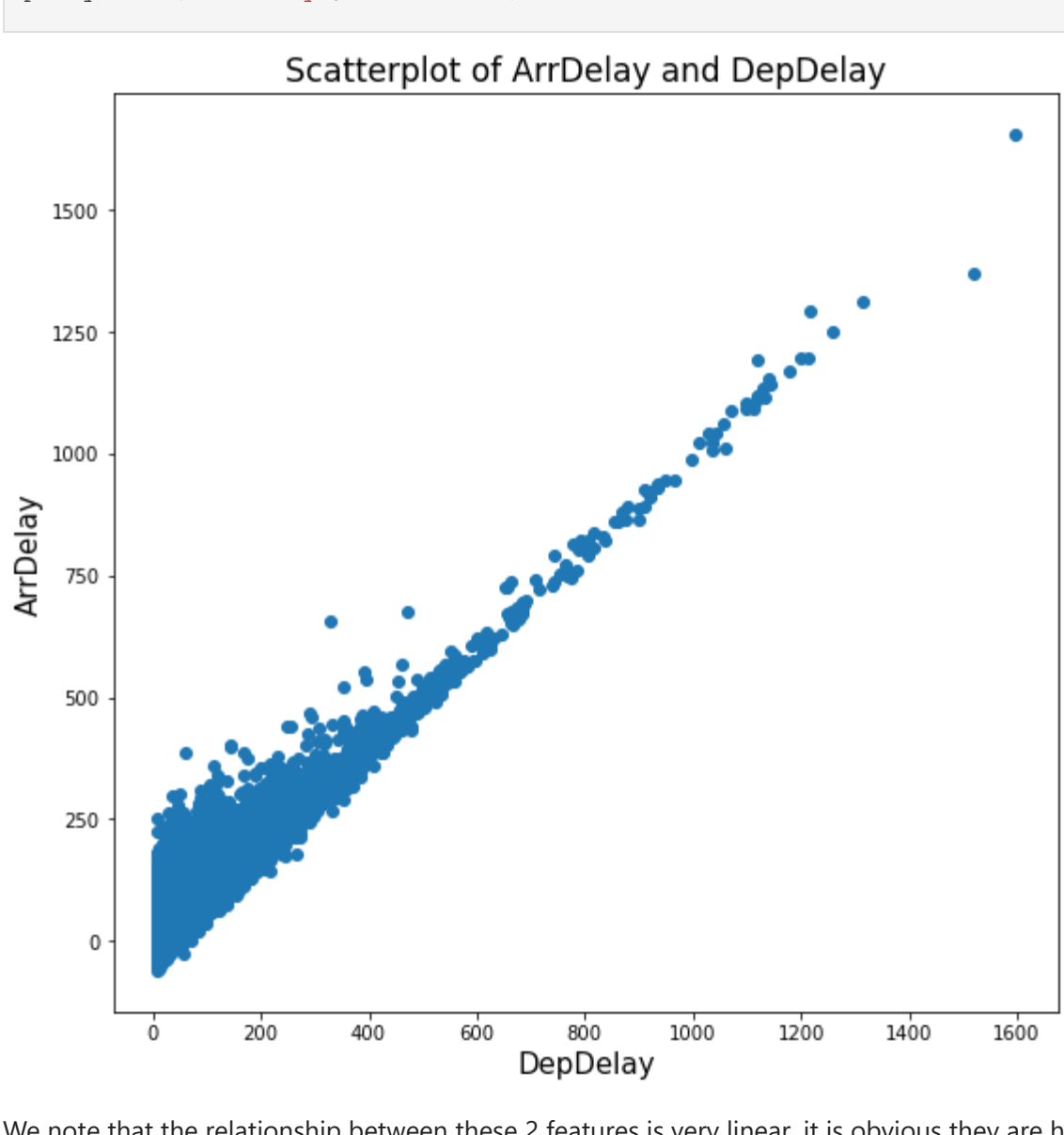
First we´ll try a simple linear regression model. We´ll choose the feature that has a higher correlation with ArrDelay which is DepDelay, this way we can have a better understanding between the relation of these 2 features:

In [13]:
```
from sklearn.model_selection import train_test_split
```

In [14]:
```
# choose dependent variable
y_simple = data_sample['ArrDelay']
# choose independent variable
x_simple = data_sample['DepDelay']
```

First let´s explore the relation between 'ArrDelay' and 'DepDelay:

In [15]:
```
# scatterplot of dependent vs independent variable
plt.figure(figsize = (9,9))
plt.scatter(x_simple, y_simple)
plt.title('Scatterplot of ArrDelay and DepDelay', fontsize = 17)
plt.xlabel('DepDelay',fontsize=15)
plt.ylabel('ArrDelay',fontsize=15);
```



We note that the relationship between these 2 features is very linear, it is obvious they are highly correlated.

In [16]:
```
# since the input has only 1 dimension, (1 feature), we reshape first
x_simple = x_simple.values.reshape(-1, 1)
x_simple.shape
```

Out[16]:
```
(192825, 1)
```

In [17]:
```
from sklearn.linear_model import LinearRegression
from sklearn.model_selection import train_test_split
# we´ll use a test size of 30%
simple_x_train, simple_x_test, simple_y_train, simple_y_test = train_test_split(x_simple,
                              y_simple, test_size= 0.3, random_state= 10)
```

In [18]:
```
# doing the regression
simple_reg = LinearRegression()
simple_reg.fit(simple_x_train, simple_y_train)
```

Out[18]:
```
LinearRegression()
```

In [19]:
```
# import modules for the metrics
from sklearn.metrics import r2_score
from sklearn.metrics import mean_squared_error
import sklearn.metrics as metrics
```

We define functions to print the results:

In [20]:
```
def print_results_test(true, predicted):

    r2_square = metrics.r2_score(true, predicted)
    mse = metrics.mean_squared_error(true, predicted)

    print('R2 for test set : ', r2_square)
    print('MSE (mean squared error) for test set: ', mse)
    print('-----------------------------------------')
```

In [21]:
```
def print_results_train(true, predicted):

    r2_square = metrics.r2_score(true, predicted)
    mse = metrics.mean_squared_error(true, predicted)

    print('R2 for train set : ', r2_square)
    print('MSE (mean squared error) for train set: ', mse)
```

In [22]:
```
# predictions for test set
simple_pred_test = simple_reg.predict(simple_x_test)

# predictions for train test
simple_pred_train = simple_reg.predict(simple_x_train)
```

In [23]:
```
print_results_test(simple_y_test, simple_pred_test)
print_results_train(simple_y_train, simple_pred_train)
```

```
R2 for test set :  0.9095964548101837
MSE (mean squared error) for test set:  290.4797885539615
-----------------------------------------
R2 for train set :  0.9098436088946702
MSE (mean squared error) for train set:  293.1189766509487
```

Despite we are using only 1 variable (DepDelay), the regression has a R2 for test set of 0.9098, which seems pretty high.

- R2 shows the percentage in the dependent variable (in our case 'ArrDelay') that is explained by the independent variables collectively (in this first example we are only using 'DepDelay'). So we oberve that DepDelay alone is able to explain 91% of the variability of ArrDelay!!
- MSE (Mean Squared Error) is a measure that tells us how close the regression is of the observed points. It measures the distance to the true observations. The lowe MSE, the better. In our Regression model we see MSE is a little higher in test set than in train set.

In [24]:
```
# define a function to get the results to a dataframe:
def get_results(true, predicted):
    r2_square = metrics.r2_score(true, predicted)
    mse = metrics.mean_squared_error(true, predicted)

    return r2_square, mse
```

In [25]:
```
# we will store the results on a Dataframe:

results_df = pd.DataFrame(data = [['Simple Linear Regression', get_results(simple_y_test, simple_pred_test)[0],
                         get_results(simple_y_test, simple_pred_test)[1], get_results(simple_y_train, simple_pre
                         get_results(simple_y_train, simple_pred_train)[1]]], columns = ['Model', 'R2_test', 'MS
                         'R2_train', 'MSE_train'])

results_df
```

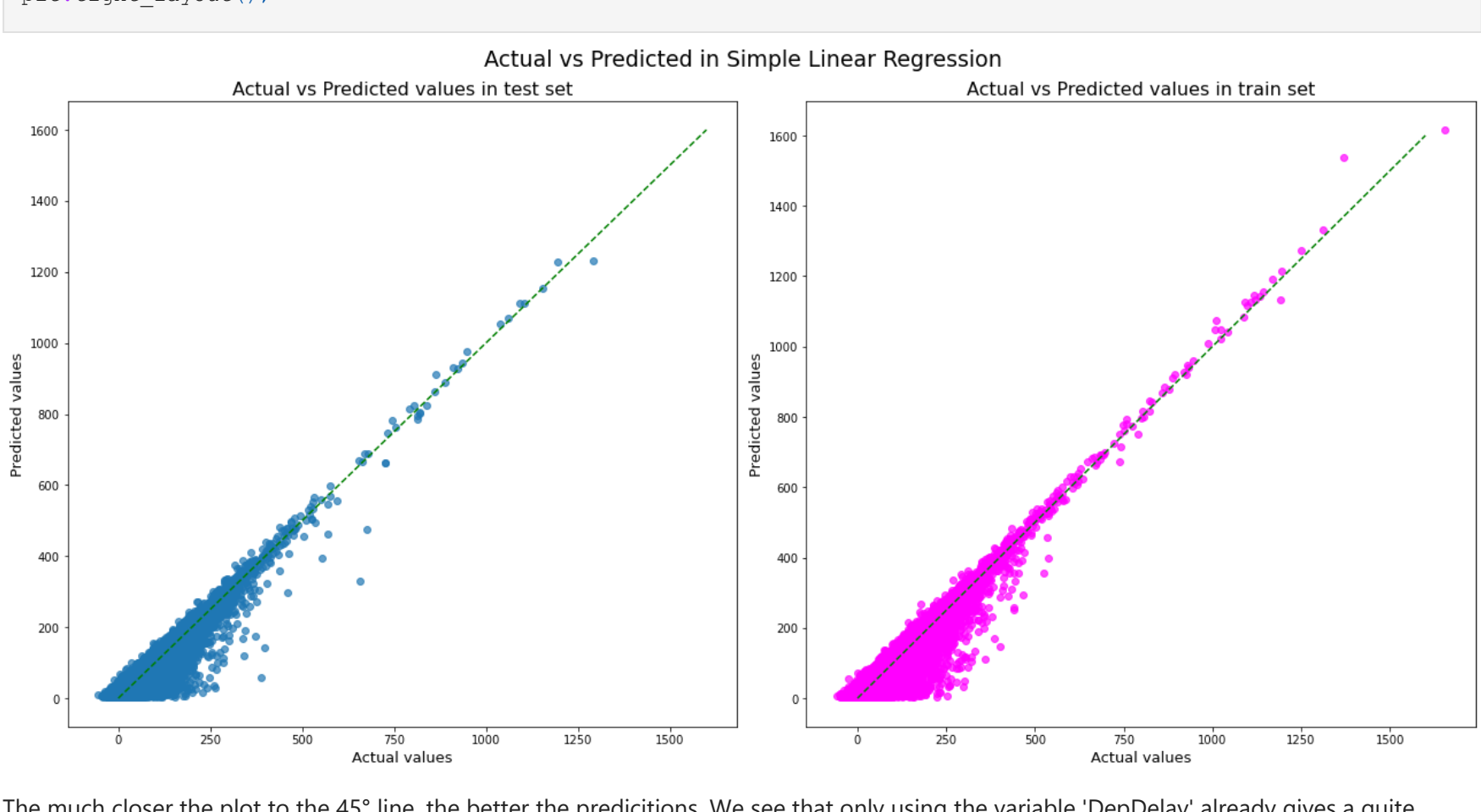
Out[25]:

	Model	R2_test	MSE_test	R2_train	MSE_train
0	Simple Linear Regression	0.909596	290.479789	0.909844	293.118977

We can plot the results in a graph of Actual against Predicted values, we will draw a 45° line, the closer the scatterplot to that line mean the better the predictions are.

In [26]:
```
# we´ll do a df for test predictions and another one for train predictions
simple_pred_test = pd.DataFrame({'y_test': simple_y_test, 'test_predictions' : simple_pred_test})

simple_pred_train = pd.DataFrame({'y_train' : simple_y_train, 'train_predictions' : simple_pred_train})
```

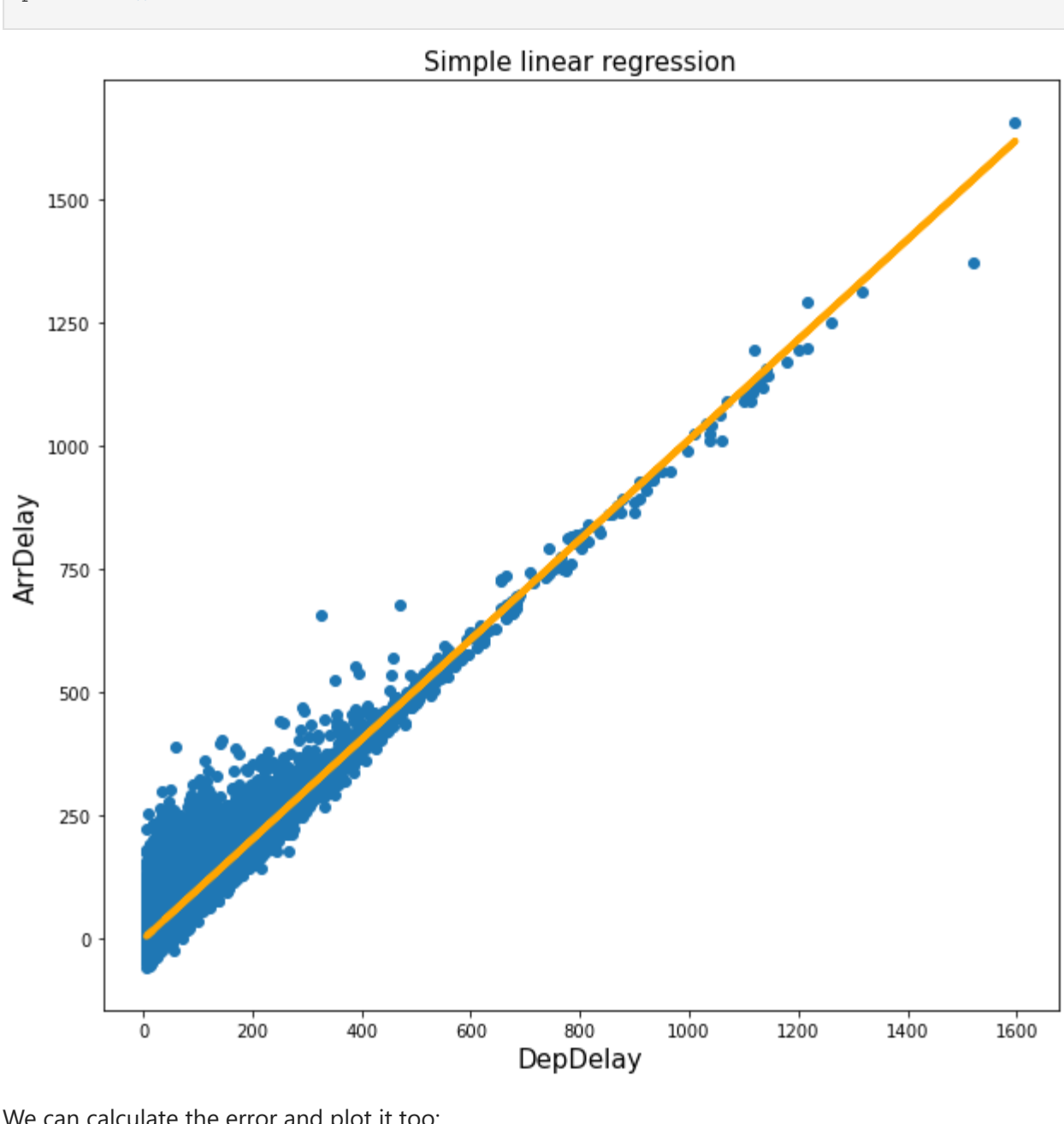
In [27]:
```
#now we plot them
plt.figure(figsize = (18,9))
plt.suptitle('Actual vs Predicted in Simple Linear Regression', fontsize = 19)

plt.subplot(121)
plt.scatter(x= simple_pred_test['y_test'], y= simple_pred_test['test_predictions'] , alpha = 0.7)
plt.plot([0, 1600], [0, 1600], color = 'green', linewidth = 1.5, linestyle = 'dashed')
plt.xlabel('Actual values', fontsize= 13)
plt.ylabel('Predicted values', fontsize = 13)
plt.title('Actual vs Predicted values in test set', fontsize = 16)

plt.subplot(122)
plt.scatter(x=simple_pred_train['y_train'], y = simple_pred_train['train_predictions'], alpha = 0.7, c = 'mager
plt.plot([0, 1600], [0, 1600], color = 'green', linewidth = 1.5, linestyle = 'dashed')
plt.xlabel('Actual values', fontsize = 13)
plt.ylabel('Predicted values', fontsize = 13)
plt.title('Actual vs Predicted values in train set', fontsize = 16)
plt.tight_layout();
```



The much closer the plot to the 45° line, the better the predicitions. We see that only using the variable 'DepDelay' already gives a quite good prediction for both test ans train sets.

Since we are using only 2 variables, we can do a scatterlot of the 2 variables and include the regression line:

In [28]:
```
# regression line
# we ´ll plot again the scatterplot of ArrDelay and DepDelay and we´ll include the regression line.
plt.figure(figsize=(10, 10))
# regression equation
y_simple_hat = simple_reg.coef_* x_simple + simple_reg.intercept_
#plot the regression line
plt.plot(x_simple, y_simple_hat, lw = 4, c = 'orange', label = 'regression line')
plt.scatter(x_simple, y_simple)
plt.xlabel('DepDelay',fontsize=15)
plt.ylabel('ArrDelay',fontsize=15)
plt.title('Simple linear regression', fontsize = 15)
plt.show()
```



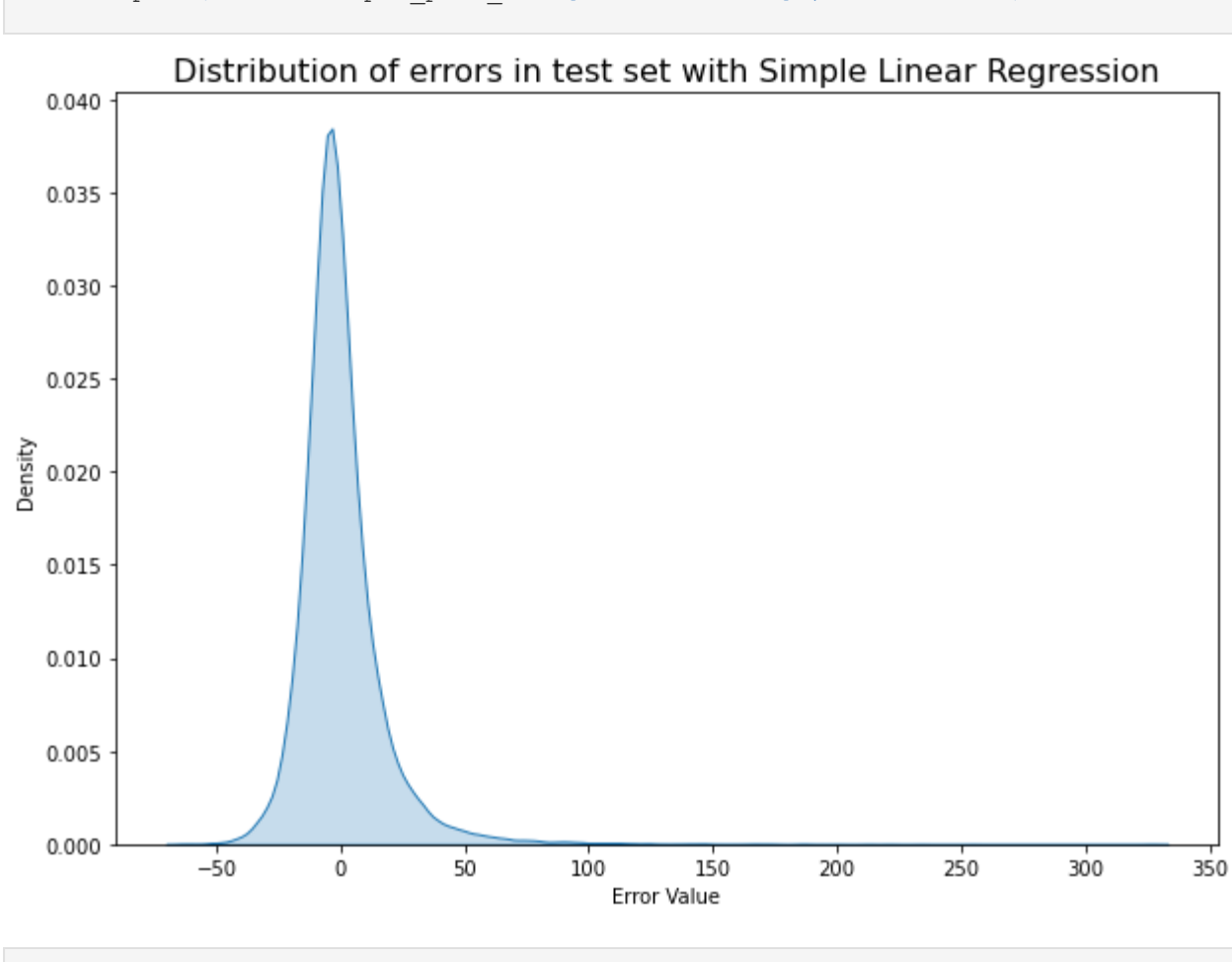
We can calculate the error and plot it too:

In [29]:
```
simple_pred_test['Error Value'] = simple_pred_test['y_test'] - simple_pred_test['test_predictions']
simple_pred_test.head()
```

Out[29]:

	y_test	test_predictions	Error Value
338265	21.0	20.864767	0.135233
601643	42.0	55.304951	-13.304951
649027	13.0	4.657622	8.342378
1281879	20.0	6.683515	13.316485
859925	17.0	19.851821	-2.851821

In [30]:
```
plt.figure(figsize=(10, 7))
plt.title('Distribution of errors in test set with Simple Linear Regression', fontsize = 16)
sns.kdeplot(data = simple_pred_test['Error Value'] , fill = True);
```



In [31]:
```
simple_pred_test['Error Value'].describe().round(2)
```

Out[31]:
```
count    57848.00
mean        -0.16
std         17.04
min        -64.72
25%         -9.23
50%         -2.70
75%          5.34
max        327.64
Name: Error Value, dtype: float64
```

The errors are centered around 0 but are a little right skewed (we see a max value for error of 327.64 minutes).

Model 2 :Ridge Regression

Now let´s compare this simple Linear Regression with Ridge Regression. In this case we´ll take into account all the available features but we are going to evaluate first multicollinearity between all features.

We saw in the previous exercise that some independent variables are higly correlated between each other, so we will use 'Variance Inflation Factor' to evaluate which featutres we can drop.

In [32]:
```
# selecting the columns we want to evaluate correlation, we dont select dependent variable ArrDelay neither du
data_sample.columns[1:22]
```

Out[32]:
```
Index(['ActualElapsedTime', 'CRSElapsedTime', 'AirTime', 'DepDelay',
       'Distance', 'Speed', 'TaxiIn', 'TaxiOut', 'CarrierDelay',
       'WeatherDelay', 'NASDelay', 'SecurityDelay', 'LateAircraftDelay',
       'DepTime', 'CRSDepTime', 'ArrTime', 'CRSArrTime', 'Month', 'DayofMonth',
       'DayOfWeek', 'DelayInterval'],
      dtype='object')
```

In [33]:
```
# import module to evaluate multicollinearity
from statsmodels.stats.outliers_influence import variance_inflation_factor

cols = ['ActualElapsedTime', 'CRSElapsedTime', 'AirTime', 'DepDelay','Distance', 'Speed', 'TaxiIn', 'TaxiOut',
        'CarrierDelay','WeatherDelay', 'NASDelay', 'SecurityDelay', 'LateAircraftDelay','DepTime', 'CRSDepTime'
        'ArrTime', 'CRSArrTime', 'Month', 'DayofMonth','DayOfWeek', 'DelayInterval']
```

In [34]:
```
# we ´ll define a function that loops across al features and show their multicollinearity
def calculate_vif(df, cols):
    variables = df[cols]
    vif = pd.DataFrame()

    vif['VIF'] = [variance_inflation_factor(variables.values, i) for i in range(variables.shape[1])]
    vif['features'] = variables.columns
    return vif
```

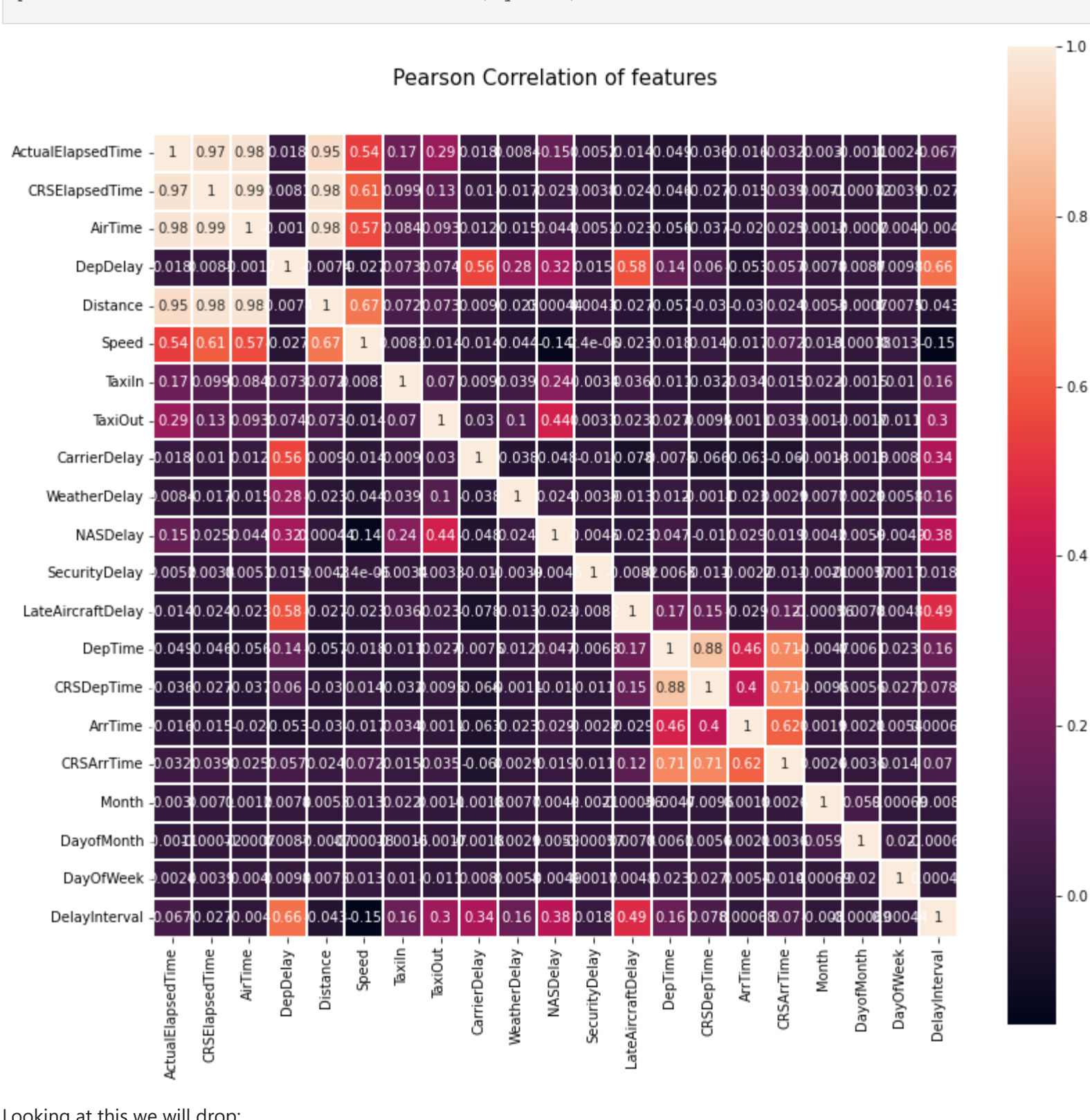
In [35]:
```
calculate_vif(data_sample, cols)
```

Out[35]:

	VIF	features
0	inf	ActualElapsedTime
1	1130.858287	CRSElapsedTime
2	inf	AirTime
3	227.018856	DepDelay
4	96.852037	Distance
5	32.232614	Speed
6	inf	TaxiIn
7	inf	TaxiOut
8	71.578302	CarrierDelay
9	16.891395	WeatherDelay
10	44.177465	NASDelay
11	1.162818	SecurityDelay
12	79.370787	LateAircraftDelay
13	64.932621	DepTime
14	65.547593	CRSDepTime
15	16.355523	ArrTime
16	39.664085	CRSArrTime
17	4.019185	Month
18	4.148999	DayofMonth
19	4.849799	DayOfWeek
20	6.202636	DelayInterval

Some of the variables return infinite values!! We will have to drop some features but we can't remove all of those with high VIF values at once, because we could be deleting important info about the model. We will look at the correlation between the features and will only remove at the same time those features that are not correlated with each other:

In [36]:
```
plt.figure(figsize = (13,13))

sns.heatmap(data_sample[cols].astype(float).corr(), linewidths=0.1,vmax=1.0, square = True,linecolor = 'white',
            annot = True)
plt.title('Pearson Correlation of features', y=1.05, size = 15);
```



Looking at this we will drop:

- ActualElapsedTime : highly correlated with CRSElapsedTime and AirTime. For now, we will only keep AirTime.
- DepDelay: we´ll keep it, we will remove this feature for Exercise 3.
- Drop TaxiIn and keep TaxiOut
- LateAircraftDelay: we´ll drop this one

In [37]:
```
data_cleaned = data_sample.copy()
```

In [38]:
```
data_cleaned.drop(['ActualElapsedTime', 'CRSElapsedTime', 'TaxiIn', 'LateAircraftDelay'], axis = 1, inplace = T
data_cleaned.shape
```

Out[38]:
```
(192825, 633)
```

With the remaining columns we check VIF again, the ideal situation would be keeping only those columns with VIF lower than 10.

In [39]:
```
cols = cols = ['AirTime', 'DepDelay','Distance', 'Speed', 'TaxiOut',
        'CarrierDelay','WeatherDelay', 'NASDelay', 'SecurityDelay','DepTime', 'CRSDepTime',
        'ArrTime', 'CRSArrTime', 'Month', 'DayofMonth','DayOfWeek', 'DelayInterval']

calculate_vif(data_sample, cols)
```

Out[39]:

	VIF	features
0	101.027046	AirTime
1	5.240997	DepDelay
2	89.990705	Distance
3	27.187316	Speed
4	3.782014	TaxiOut
5	2.049906	CarrierDelay
6	1.255059	WeatherDelay
7	1.918727	NASDelay
8	1.003144	SecurityDelay
9	64.692422	DepTime
10	65.462481	CRSDepTime
11	16.296485	ArrTime
12	39.621804	CRSArrTime
13	4.003842	Month
14	4.145941	DayofMonth
15	4.842762	DayOfWeek
16	4.807840	DelayInterval

Now we´ll drop AirTime and CRSDepTime (these 2 are not highly correlated within each other, so we can remove them at once):

In [40]:
```
data_cleaned.drop(['AirTime', 'CRSDepTime'], axis = 1, inplace = True)
data_cleaned.shape
```

Out[40]:
```
(192825, 631)
```

In [41]:
```
# check again
cols = ['DepDelay','Distance', 'Speed', 'TaxiOut', 'CarrierDelay','WeatherDelay', 'NASDelay', 'SecurityDelay','
        'ArrTime', 'CRSArrTime', 'Month', 'DayofMonth','DayOfWeek', 'DelayInterval']

calculate_vif(data_sample, cols)
```

Out[41]:

	VIF	features
0	5.124971	DepDelay
1	4.495940	Distance
2	25.347944	Speed
3	3.776428	TaxiOut
4	2.027584	CarrierDelay
5	1.249845	WeatherDelay
6	1.873349	NASDelay
7	1.003001	SecurityDelay
8	25.708232	DepTime
9	15.701616	ArrTime
10	35.975467	CRSArrTime
11	3.950177	Month
12	4.068844	DayofMonth
13	4.741692	DayOfWeek
14	4.608525	DelayInterval

'Speed' and 'CRSArrTime' are not correlated, so we can drop them at once:

In [42]:
```
data_cleaned.drop(['Speed', 'CRSArrTime'], axis = 1, inplace= True)
data_cleaned.shape
```

Out[42]:
```
(192825, 629)
```

In [43]:
```
cols = ['DepDelay','Distance','TaxiOut', 'CarrierDelay','WeatherDelay', 'NASDelay', 'SecurityDelay','DepTime',
        'ArrTime', 'Month', 'DayofMonth','DayOfWeek', 'DelayInterval']

calculate_vif(data_sample, cols)
```

Out[43]:

	VIF	features
0	5.006072	DepDelay
1	2.625796	Distance
2	3.619042	TaxiOut
3	2.007823	CarrierDelay
4	1.243499	WeatherDelay
5	1.799928	NASDelay
6	1.002818	SecurityDelay
7	14.227908	DepTime
8	11.345255	ArrTime
9	3.713597	Month
10	3.846247	DayofMonth
11	4.373165	DayOfWeek
12	4.581995	DelayInterval

Now we'll drop DepTime:

In [44]:
```
data_cleaned.drop(['DepTime'], axis = 1, inplace= True)
data_cleaned.shape
```

Out[44]:
```
(192825, 628)
```

In [45]:
```
cols = ['DepDelay','Distance','TaxiOut', 'CarrierDelay','WeatherDelay', 'NASDelay', 'SecurityDelay',
        'ArrTime', 'Month', 'DayofMonth','DayOfWeek', 'DelayInterval']

calculate_vif(data_sample, cols)
```

Out[45]:

	VIF	features
0	4.839350	DepDelay
1	2.615133	Distance
2	3.559933	TaxiOut
3	1.970225	CarrierDelay
4	1.235062	WeatherDelay
5	1.765773	NASDelay
6	1.002603	SecurityDelay
7	6.136878	ArrTime
8	3.650797	Month
9	3.769457	DayofMonth
10	4.220870	DayOfWeek
11	4.528261	DelayInterval

Now all of our features have a VIF smaller than 10, which is the recomended limit for VIF values. We have dropped 9 features. Now let´s proceed with our models:

In [46]:
```
# save this df to csv
#data_cleaned.to_csv('data_cleaned.csv', index = False)
```

In [47]:
```python
from sklearn.model_selection import train_test_split

# select dependent variable
y = data_cleaned['ArrDelay']
# independent variables
X = data_cleaned.drop(['ArrDelay'], axis = 1)
```

In [48]:
```python
print('data_cleaned.shape: ' , data_cleaned.shape)
print('y.shape: ', y.shape)
print('X.shape: ', X.shape)
```

```
data_cleaned.shape:  (192825, 628)
y.shape:  (192825,)
X.shape:  (192825, 627)
```

In [49]:
```python
# use test size of 0.3
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size= 0.3, random_state= 0)
```

In [50]:
```python
print('X_train.shape: ', X_train.shape)
print('X_test.shape: ', X_test.shape)
print('y_train.shape: ', y_train.shape)
print('y_test.shape: ', y_test.shape)
```

```
X_train.shape:  (134977, 627)
X_test.shape:  (57848, 627)
y_train.shape:  (134977,)
y_test.shape:  (57848,)
```

Now we will apply our Ridge Regression model, used when data has multicollinearity. Altough we have removed variables with high VIF we still have a lot of features in our model.

In [51]:
```python
from sklearn.linear_model import Ridge

ridge = Ridge()
ridge.fit(X_train, y_train)
```

Out[51]:
```
Ridge()
```

In [52]:
```python
ridge_test_prediction = ridge.predict(X_test)
ridge_train_prediction = ridge.predict(X_train)

print_results_test(y_test, ridge_test_prediction)
print_results_train(y_train, ridge_train_prediction)
```

```
R2 for test set :  0.9728951602159603
MSE (mean squared error) for test set:  87.54991975163803
------------------------------------------
R2 for train set :  0.9729783616559122
MSE (mean squared error) for train set:  87.65876185372439
```

We see R2 is higer than in Simple Linear Regression and MSE is lower, it makes sense because this time we are including a lot of features.

In [53]:
```python
# keep the results in a dataframe
results_df_2 = pd.DataFrame(data = [['Ridge Regression', get_results(y_test, ridge_test_prediction)[0],
                                     get_results(y_test, ridge_test_prediction)[1],
                                     get_results(y_train, ridge_train_prediction)[0],
                                     get_results(y_train, ridge_train_prediction)[1]]], columns = ['Model',
                                    'R2_test', 'MSE_test', 'R2_train', 'MSE_train'])
results_df = pd.concat([results_df, results_df_2])
results_df
```

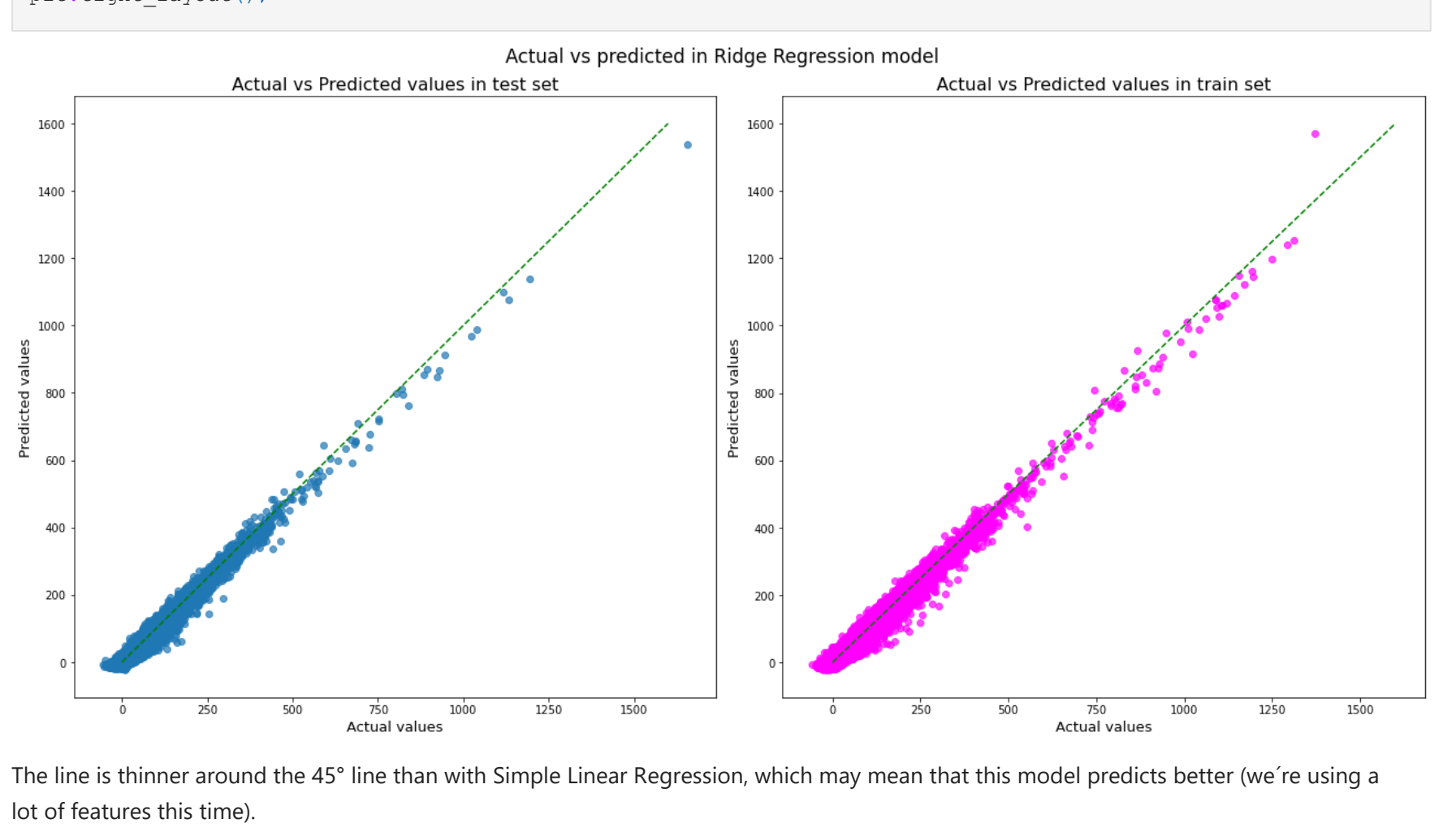
Out[53]:

	Model	R2_test	MSE_test	R2_train	MSE_train
0	Simple Linear Regression	0.909596	290.479789	0.909844	293.118977
0	Ridge Regression	0.972895	87.549920	0.972978	87.658762

Now we can plot Actual Values versus Predicted Values for both sets:

In [54]:
```python
# we´ll do a df for test predictions and another one for train predictions
ridge_pred_test = pd.DataFrame({'y_test': y_test, 'test_predictions' : ridge_test_prediction})

ridge_pred_train = pd.DataFrame({'y_train' : y_train, 'train_predictions' : ridge_train_prediction})
```

In [55]:
```python
# now we plot them
plt.figure(figsize = (18,9))
plt.suptitle('Actual vs predicted in Ridge Regression model', fontsize = 17)

plt.subplot(121)
plt.scatter(x= ridge_pred_test['y_test'], y= ridge_pred_test['test_predictions'] , alpha = 0.7)
plt.plot([0, 1600], [0, 1600], color = 'green', linewidth = 1.5, linestyle = 'dashed')
plt.xlabel('Actual values', fontsize= 13)
plt.ylabel('Predicted values', fontsize = 13)
plt.title('Actual vs Predicted values in test set', fontsize = 16)

plt.subplot(122)
plt.scatter(x=ridge_pred_train['y_train'], y = ridge_pred_train['train_predictions'], alpha = 0.7, c = 'magenta
plt.plot([0, 1600], [0, 1600], color = 'green', linewidth = 1.5, linestyle = 'dashed')
plt.xlabel('Actual values', fontsize = 13)
plt.ylabel('Predicted values', fontsize = 13)
plt.title('Actual vs Predicted values in train set', fontsize = 16)
plt.tight_layout();
```



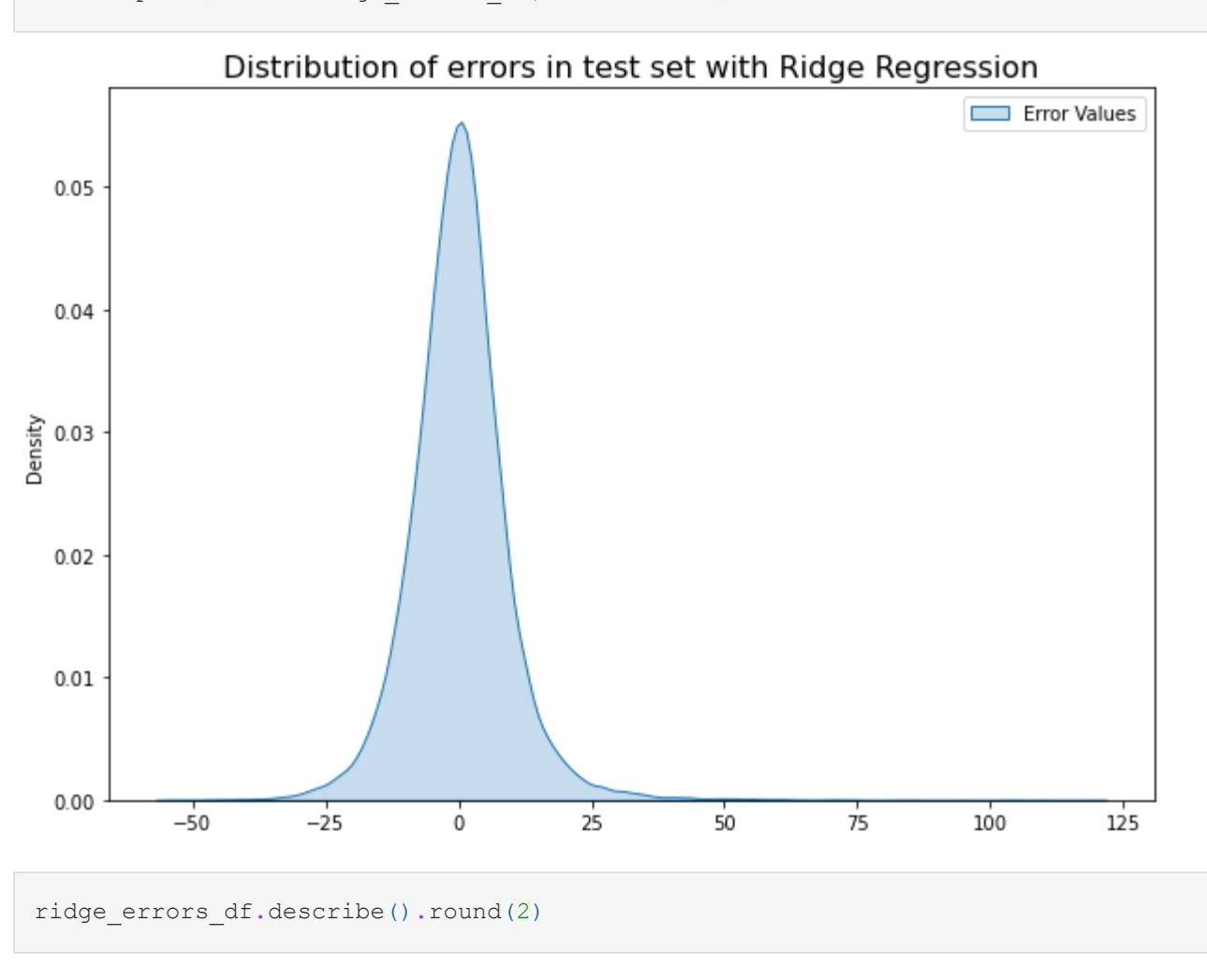
The line is thinner around the 45° line than with Simple Linear Regression, which may mean that this model predicts better (we´re using a lot of features this time).

In [56]:
```python
# now we will plot the errors of the test set
ridge_errors_df = pd.DataFrame({'Error Values' : (y_test-ridge_test_prediction)})
ridge_errors_df.head()
```

Out[56]:

	Error Values
1633320	-0.473077
1840639	-3.185111
1359883	-1.834519
1872293	6.457592
163638	13.857097

In [57]:
```python
# now we plot it
plt.figure(figsize=(10, 7))
plt.title('Distribution of errors in test set with Ridge Regression', fontsize = 16)
sns.kdeplot(data = ridge_errors_df, fill = True);
```



In [58]:
```python
ridge_errors_df.describe().round(2)
```

Out[58]:

	Error Values
count	57848.00
mean	0.05
std	9.36
min	-53.86
25%	-5.12
50%	-0.08
75%	4.77
max	118.69

Now the errors seem more concentrated around value zero than with the Simple Linear Regression. Just looking at the quartiles and the min and max values we see that this distribution is closer to normal distribution than before (altough some errors are large according to min and max values)

Model 3 : Random Forest Regression

We already have our train set and our test set from our previous regression, now we'll use the Random Forest Regressor.

In [59]:
```python
from sklearn.ensemble import RandomForestRegressor
# choose n_estimators to 50
regressor = RandomForestRegressor(n_estimators= 50, random_state= 0)

regressor.fit(X_train, y_train)
```

Out[59]:
```
RandomForestRegressor(n_estimators=50, random_state=0)
```

In [60]:
```python
forest_test_prediction = regressor.predict(X_test)
forest_train_prediction = regressor.predict(X_train)
```

In [61]:
```python
print_results_test(y_test,forest_test_prediction )
print_results_train(y_train, forest_train_prediction)
```

```
R2 for test set :  0.9881187247720432
MSE (mean squared error) for test set:  38.37708324574747
------------------------------------------
R2 for train set :  0.998282711047142
MSE (mean squared error) for train set:  5.570921401423946
```

Again test set R2 is slightly lower than for train set, but we see a high difference in MSE, MSE of train set is much lower than in test set!!

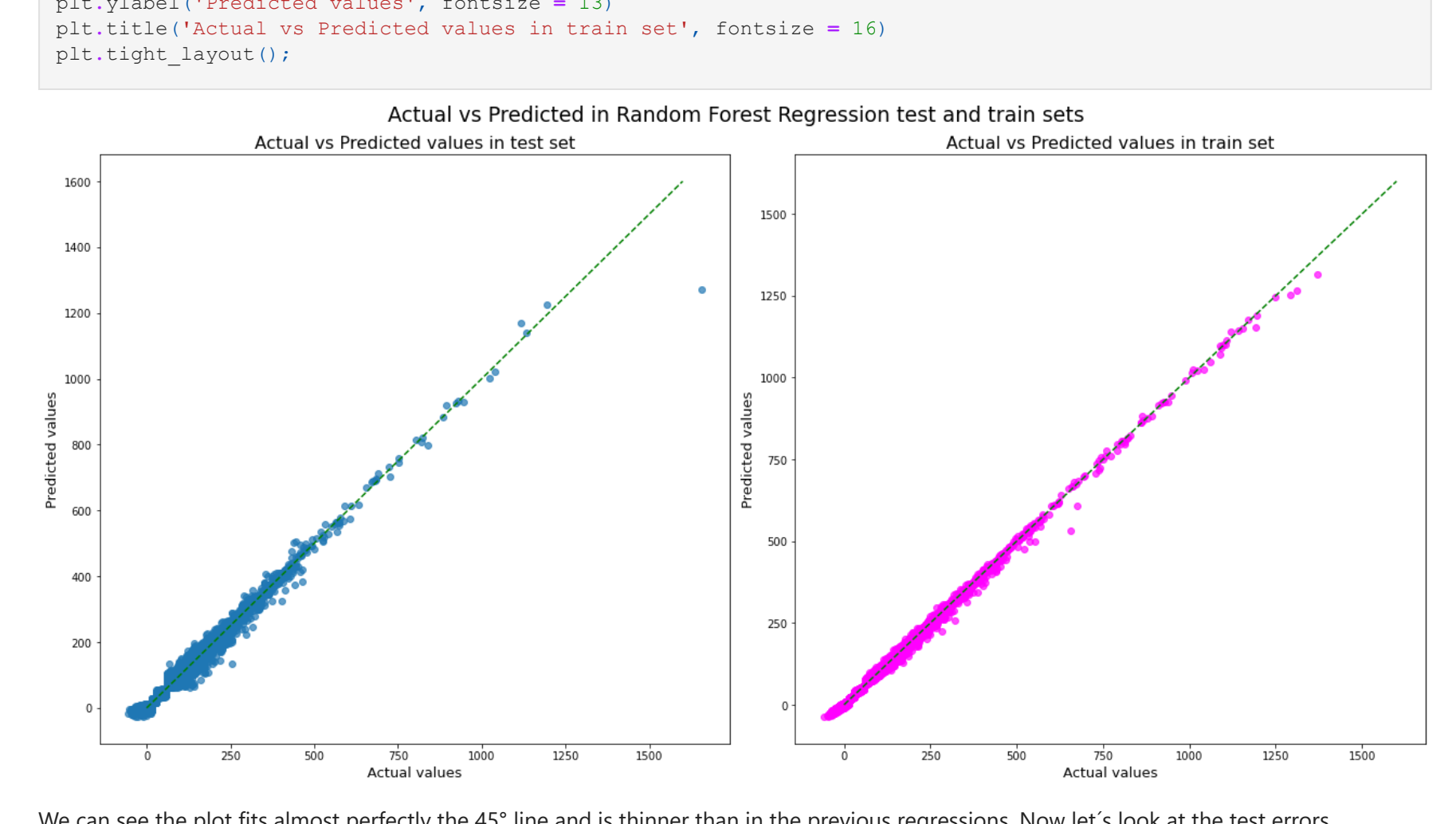
In [62]:
```python
# keep the results in a dataframe:
results_df_3 = pd.DataFrame(data = [['Random Forest Regression', get_results(y_test,forest_test_prediction)[0],
                                     get_results(y_test,forest_test_prediction)[1],
                                     get_results(y_train, forest_train_prediction)[0],
                                     get_results(y_train, forest_train_prediction)[1]]], columns =
                                     ['Model', 'R2_test', 'MSE_test', 'R2_train', 'MSE_train'])
results_df = pd.concat([results_df, results_df_3])
results_df
```

Out[62]:

	Model	R2_test	MSE_test	R2_train	MSE_train
0	Simple Linear Regression	0.909596	290.479789	0.909844	293.118977
0	Ridge Regression	0.972895	87.549920	0.972978	87.658762
0	Random Forest Regression	0.988119	38.377083	0.998283	5.570921

In [63]:
```python
# we´ll do a df for test predictions and another one for train predictions
forest_test_df = pd.DataFrame({'y_test': y_test, 'test_predictions' : forest_test_prediction})
forest_train_df = pd.DataFrame({'y_train' : y_train, 'train_predictions' : forest_train_prediction})
```

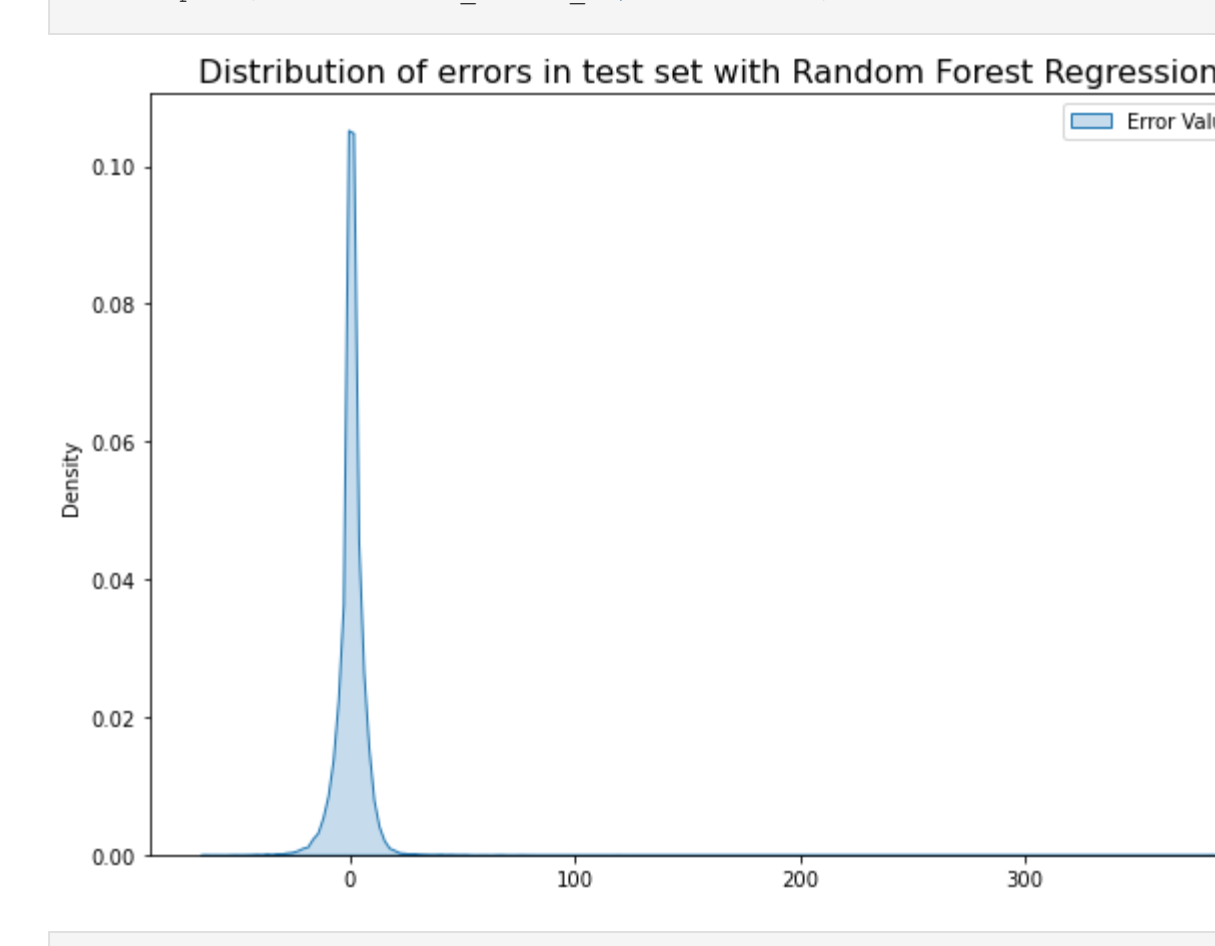
In [64]:
```python
# now we will plot actual vs predicted both on test and train sets
plt.figure(figsize= (18,9))
plt.suptitle('Actual vs Predicted in Random Forest Regression test and train sets', fontsize = 19)

plt.subplot(121)
plt.scatter(x= forest_test_df['y_test'], y = forest_test_df['test_predictions'], alpha = 0.7)
plt.plot([0, 1600], [0, 1600], color = 'green', linewidth = 1.5, linestyle = 'dashed')
plt.xlabel('Actual values', fontsize= 13)
plt.ylabel('Predicted values', fontsize = 13)
plt.title('Actual vs Predicted values in test set', fontsize = 16)

plt.subplot(122)
plt.scatter(x= forest_train_df['y_train'], y = forest_train_df['train_predictions'], alpha = 0.7, c = 'magenta'
plt.plot([0, 1600], [0, 1600], color = 'green', linewidth = 1.5, linestyle = 'dashed')
plt.xlabel('Actual values', fontsize = 13)
plt.ylabel('Predicted values', fontsize = 13)
plt.title('Actual vs Predicted values in train set', fontsize = 16)
plt.tight_layout();
```



We can see the plot fits almost perfectly the 45° line and is thinner than in the previous regressions. Now let´s look at the test errors distribution:

In [65]:
```python
forest_errors_df =  pd.DataFrame({'Error Values' : (y_test -forest_test_prediction)})
```

In [66]:
```python
# now we plot it
plt.figure(figsize=(10, 7))
plt.title('Distribution of errors in test set with Random Forest Regression', fontsize = 16)
sns.kdeplot(data = forest_errors_df, fill = True);
```



In [67]:
```python
forest_errors_df.describe().round(2)
```

Out[67]:

	Error Values
count	57848.00
mean	0.03
std	6.19
min	-64.82
25%	-1.54
50%	0.00
75%	2.16
max	382.78

Altough we see an error of 382.78 minutes (see max value), looking at the mean of errors and the quartiles we clearly see that this time errors are more concentrated around zero than in the previous regressions.

Model 4: XGBoost Regressor

Lastly, we will use the XGBoost Regression algorithm to predict ArrDelay. This algorithm is know by its good results and efficiency in its performance, let´s check how good it performs in our dataset.

In [68]:
```python
# we already have our X and y split, import the needed library
from xgboost import XGBRegressor
# instantiate the model
XGB_regressor = XGBRegressor()
# fit train set
XGB_regressor.fit(X_train, y_train)
```

Out[68]:
```
XGBRegressor(base_score=0.5, booster='gbtree', colsample_bylevel=1,
             colsample_bynode=1, colsample_bytree=1, enable_categorical=False,
             gamma=0, gpu_id=-1, importance_type=None,
             interaction_constraints='', learning_rate=0.300000012,
             max_delta_step=0, max_depth=6, min_child_weight=1, missing=nan,
             monotone_constraints='()', n_estimators=100, n_jobs=8,
             num_parallel_tree=1, predictor='auto', random_state=0, reg_alpha=0,
             reg_lambda=1, scale_pos_weight=1, subsample=1, tree_method='exact',
             validate_parameters=1, verbosity=None)
```

In [69]:
```python
XGB_test_prediction = XGB_regressor.predict(X_test)
XGB_train_prediction = XGB_regressor.predict(X_train)
```

In [70]:
```python
print_results_test(y_test,XGB_test_prediction )
print_results_train(y_train, XGB_train_prediction)
```

```
R2 for test set :  0.9882029254052389
MSE (mean squared error) for test set:  38.105111201712205
------------------------------------------
R2 for train set :  0.9913355159782089
MSE (mean squared error) for train set:  28.10776799615331
```

Again R2 for training set is a little higher and MSE a little lower. We are having a very high R2 for both test and train so it may be difficult to improve our model.

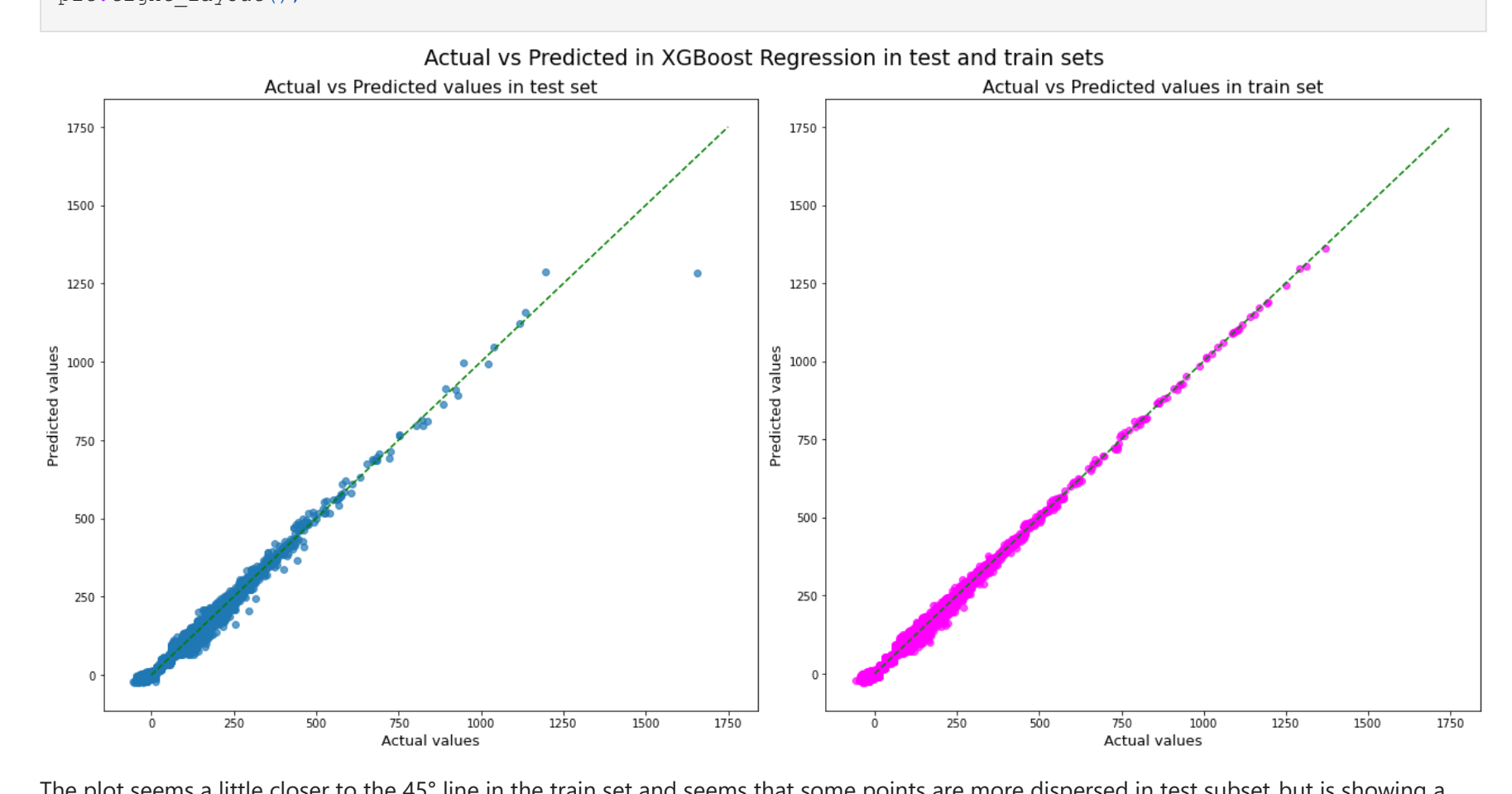
In [71]:
```python
# save the results in a df
results_df_4 = pd.DataFrame(data = [['XGBoost Regression', get_results(y_test,XGB_test_prediction)[0],
                                     get_results(y_test,XGB_test_prediction)[1], get_results(y_train,XGB_train_p
                                     get_results(y_train,XGB_train_prediction)[1]]], columns = ['Model', 'R2_tes
                                    'R2_train', 'MSE_train'])
results_df = pd.concat([results_df, results_df_4])
results_df
```

Out[71]:

	Model	R2_test	MSE_test	R2_train	MSE_train
0	Simple Linear Regression	0.909596	290.479789	0.909844	293.118977
0	Ridge Regression	0.972895	87.549920	0.972978	87.658762
0	Random Forest Regression	0.988119	38.377083	0.998283	5.570921
0	XGBoost Regression	0.988203	38.105111	0.991336	28.107768

In [72]:
```python
# df actual and predicted
XGB_test_df = pd.DataFrame({'y_test': y_test, 'test_predictions' : XGB_test_prediction})
XGB_train_df = pd.DataFrame({'y_train' : y_train, 'train_predictions' : XGB_train_prediction})
```

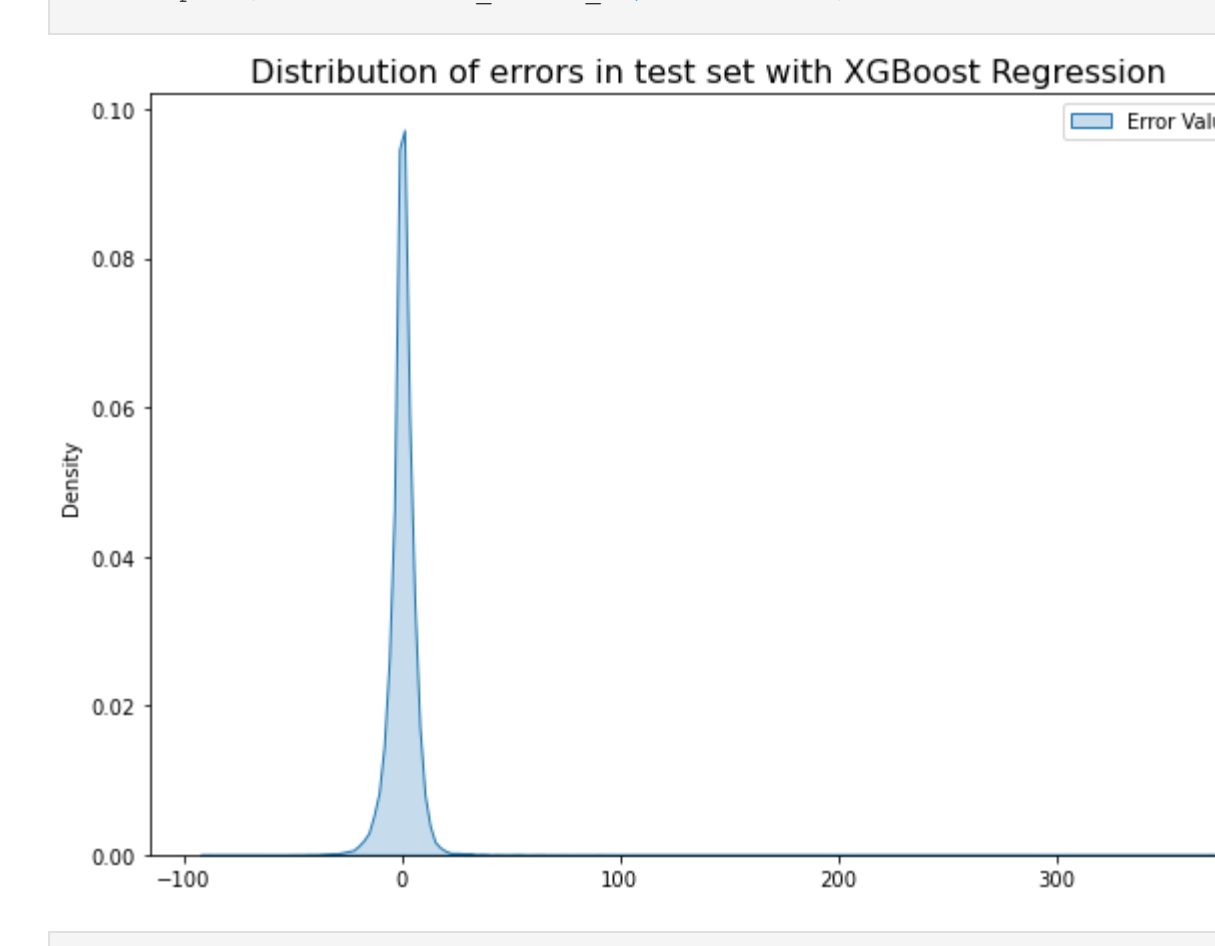
In [73]:
```python
# plot actual vs predicted
plt.figure(figsize = (18,9))
plt.suptitle('Actual vs Predicted in XGBoost Regression in test and train sets', fontsize = 19)

plt.subplot(121)
plt.scatter(x= XGB_test_df['y_test'], y = XGB_test_df['test_predictions'] , alpha = 0.7)
plt.plot([0, 1750], [0, 1750], color = 'green', linewidth = 1.5, linestyle = 'dashed')
plt.xlabel('Actual values', fontsize= 13)
plt.ylabel('Predicted values', fontsize = 13)
plt.title('Actual vs Predicted values in test set', fontsize = 16)

plt.subplot(122)
plt.scatter(x=XGB_train_df['y_train'], y = XGB_train_df['train_predictions'], alpha = 0.7, c = 'magenta')
plt.plot([0, 1750], [0, 1750], color = 'green', linewidth = 1.5, linestyle = 'dashed')
plt.xlabel('Actual values', fontsize = 13)
plt.ylabel('Predicted values', fontsize = 13)
plt.title('Actual vs Predicted values in train set', fontsize = 16)
plt.tight_layout();
```



The plot seems a little closer to the 45° line in the train set and seems that some points are more dispersed in test subset but is showing a very high predictive power in both cases.

In [74]:
```python
# create df of errors in test set
XGBoost_errors_df = pd.DataFrame({'Error Values' : (y_test -XGB_test_prediction)})
```

In [75]:
```python
# now we plot it
plt.figure(figsize=(10, 7))
plt.title('Distribution of errors in test set with XGBoost Regression', fontsize = 16)
sns.kdeplot(data = XGBoost_errors_df, fill = True);
```



In [76]:
```python
XGBoost_errors_df.describe().round(2)
```

Out[76]:

	Error Values
count	57848.00
mean	-0.01
std	6.17
min	-90.45
25%	-2.50
50%	0.09
75%	2.90
max	370.95

The distribution is very similar to the Random Forest Regresssion, it is pretty centered around zero value despite the presence of some high errors (see min and max values).

- Exercici 2

Compara'ls en base al MSE i al R2 .

To compare the 4 models we have created we can use our results_df.

In [77]:
```python
results_df
```

Out[77]:

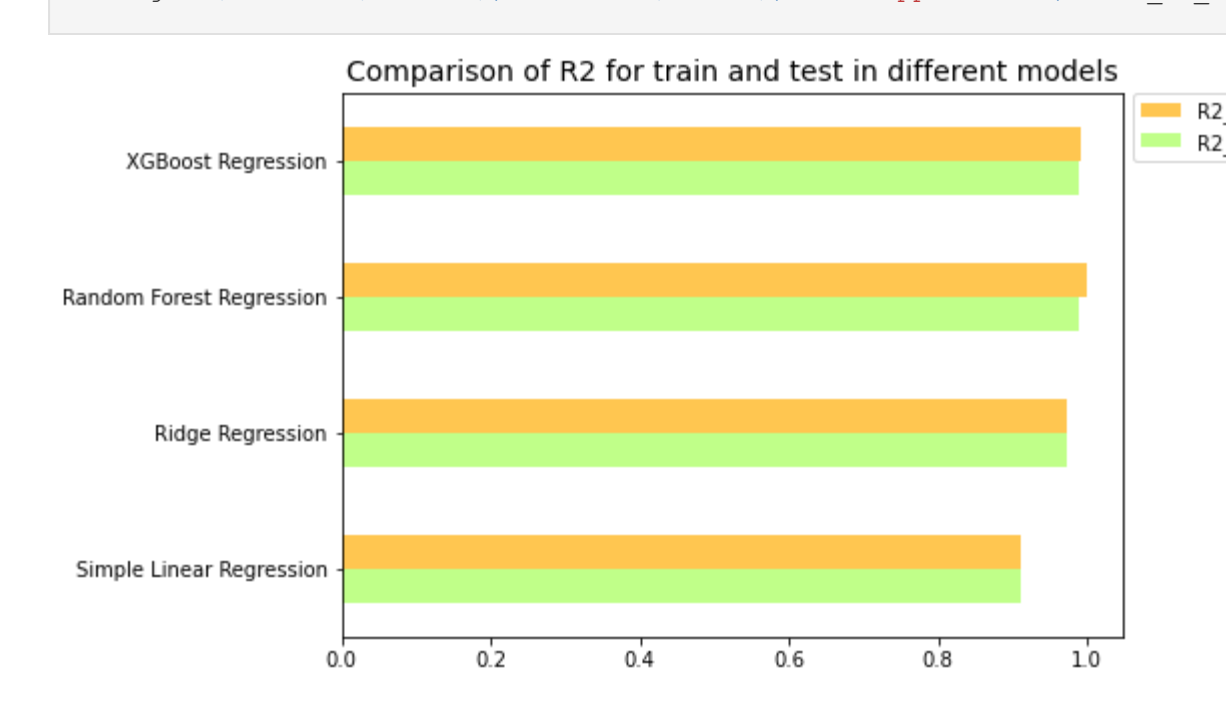
	Model	R2_test	MSE_test	R2_train	MSE_train
0	Simple Linear Regression	0.909596	290.479789	0.909844	293.118977
0	Ridge Regression	0.972895	87.549920	0.972978	87.658762
0	Random Forest Regression	0.988119	38.377083	0.998283	5.570921
0	XGBoost Regression	0.988203	38.105111	0.991336	28.107768

- Results are very similar in both train and test set, models have a higher R2 for train set but the difference is very small.
- MSE in train is a little higher in train sets in Linear Regression model compared to test set, but at the same time MSE is significantly smaller in train sets in the case of XGBoost Regression and specially in Random Forest.

In [78]:
```python
results = results_df.set_index('Model')
```

We can plot these results in a graph to do a comparison, we will look first at R2 results:

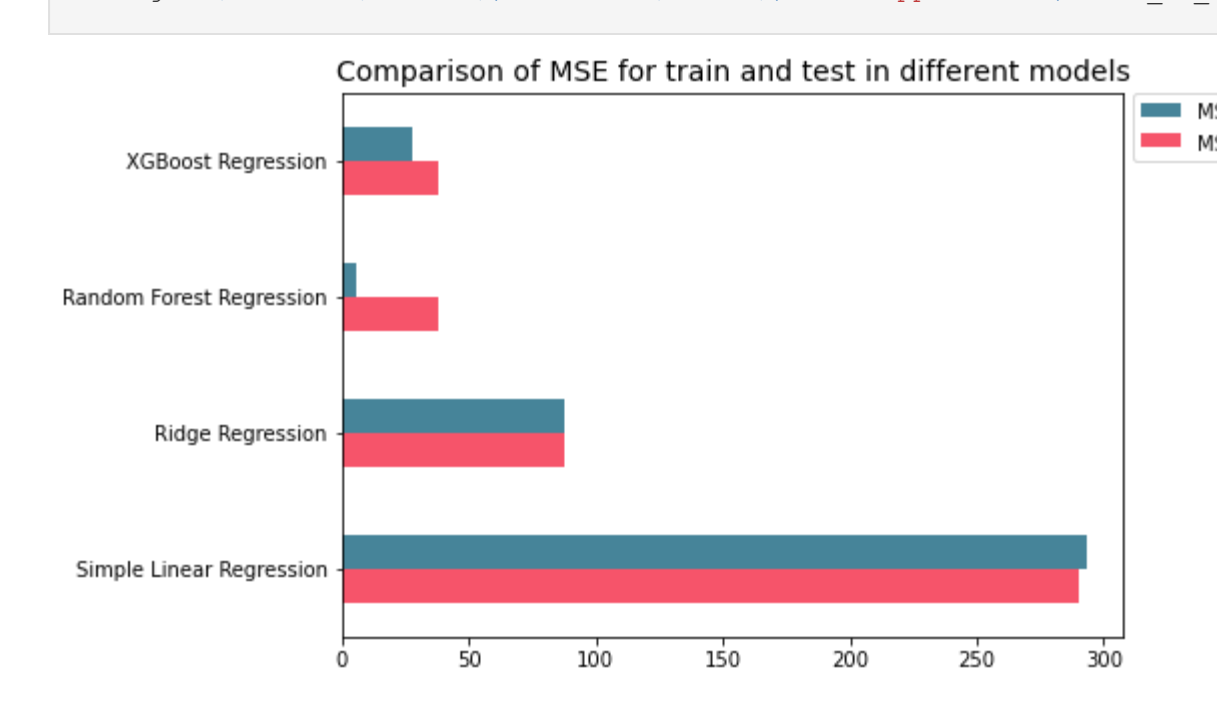
In [79]:
```python
ax = results[['R2_test', 'R2_train']].plot(kind='barh', figsize=(7, 5), color = ['#c0ff89', '#ffc650'] )
ax.set_title('Comparison of R2 for train and test in different models', fontsize = 14)
ax.set_ylabel('')
handles, labels = ax.get_legend_handles_labels()
ax.legend(reversed(handles), reversed(labels), loc='upper left', bbox_to_anchor=(1, 1.02));
```



- In all cases R2 is higher in train set but the difference with test set is very small.
- The model that has a better R2 in test set is XGBoost Regression and the lower R2 belongs to Simple Linear Regression.

Now we can do the same for MSE results:

In [80]:
```python
ax = results[['MSE_test', 'MSE_train']].plot(kind='barh', figsize=(7, 5), color = ['#f6546a', '#468499'] )
ax.set_title('Comparison of MSE for train and test in different models', fontsize = 14)
ax.set_ylabel('')
handles, labels = ax.get_legend_handles_labels()
ax.legend(reversed(handles), reversed(labels), loc='upper left', bbox_to_anchor=(1, 1.02));
```



- MSE is smaller in Random Forest and in XGBoost than in the other 2 models (these models minimize errors much more than Simple Linear Regression and Ridge Regression)
- In Simple Linear Regression MSE is a little higher in train set (but the difference is very small)
- In XGBoost Regression and specially in Random Forest Regression MSE is significantly smaller in train set

- Exercici 3

Entrena'ls utilitzant els diferents paràmetres que admeten.

Simple Linear Regression

We can check the parameters we used in the regression with the method get_params(). We' ll look at the parameters used and then change one.

In [81]:
```python
simple_reg.get_params()
```

Out[81]:
```
{'copy_X': True,
 'fit_intercept': True,
 'n_jobs': None,
 'normalize': 'deprecated',
 'positive': False}
```

We can see that the parameter 'fit_intercept' is set to True by default. The intercept(also called the constant) is the expected value (or predicted value) of y when X (or independent variable) is zero (intercept is the constant of the regression equation). In our model the intecept was:

In [82]:
```python
simple_reg.intercept_
```

Out[82]:
```
-1.4200579480792328
```

In our Simple Regression we only used one feature, DepDelay (delay in the departure of the flight) as independent variable, this intercept means that in the cases where DepDelay equals 0 the Arrival Delay is expected to be -1,42 (the flight arrives 1,4 minutes earlier if the flight departs on time).

Let´s check how our model changes if we set fit_intercep = False:

In [83]:
```python
simple_reg_no_intercept = LinearRegression(fit_intercept= False)
simple_reg_no_intercept.fit(simple_x_train, simple_y_train)
```

Out[83]:
```
LinearRegression(fit_intercept=False)
```

In [84]:
```python
# predictions for test set
simple_pred_test_no_intercept = simple_reg_no_intercept.predict(simple_x_test)

# predictions for train test
simple_pred_train_no_intercept = simple_reg_no_intercept.predict(simple_x_train)

print_results_test(simple_y_test, simple_pred_test_no_intercept)
print_results_train(simple_y_train, simple_pred_train_no_intercept )
```

```
R2 for test set :  0.9090716633878027
MSE (mean squared error) for test set:  292.166020007475
------------------------------------------
R2 for train set :  0.9094669729505063
MSE (mean squared error) for train set:  294.3435059513098
```

R2 is now a little lower, and MSE a little higher, it seems removing the intercept has decreased the predictive power of our model.

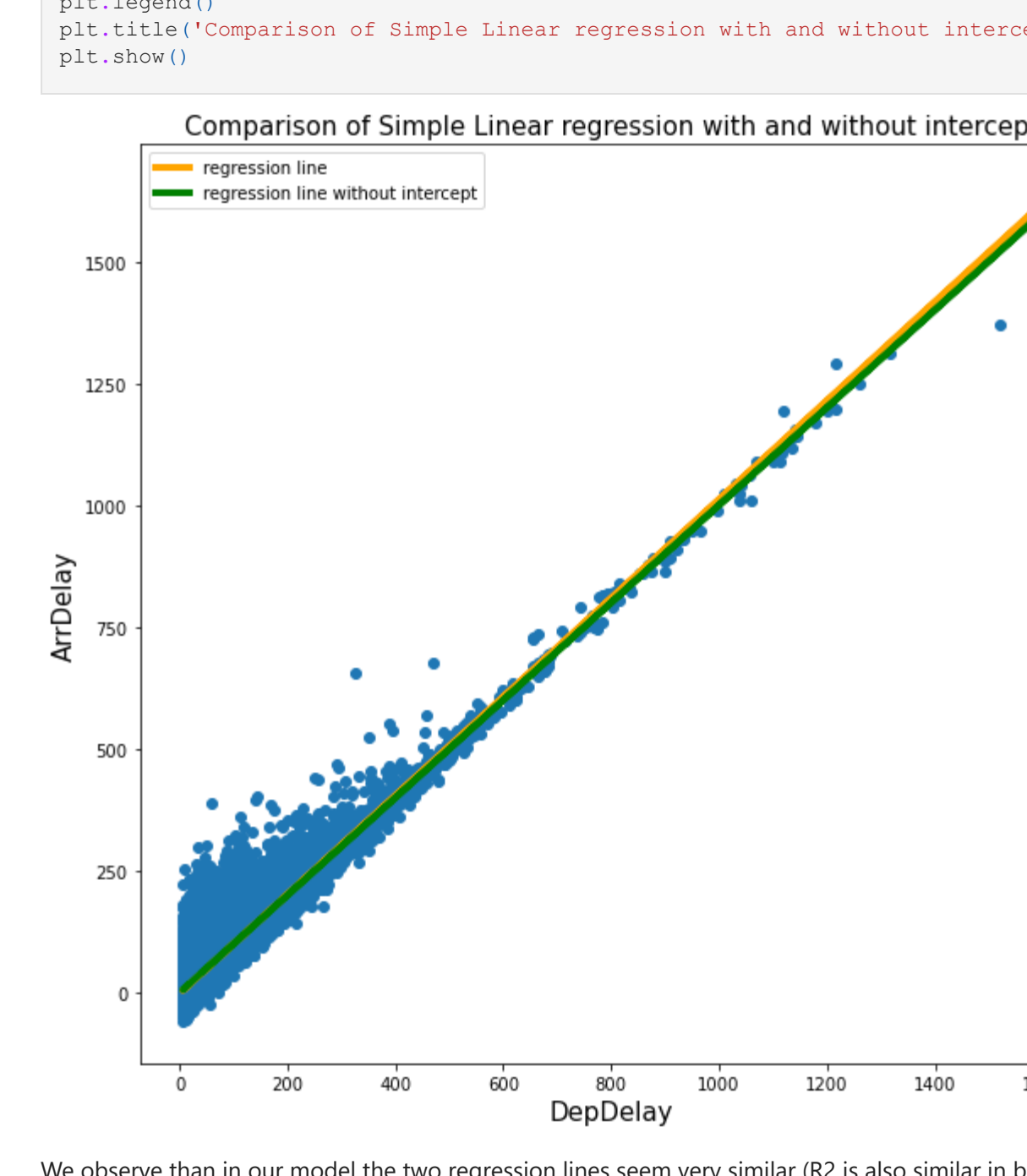
In [85]:
```python
# save the results
results_df_5 = pd.DataFrame(data= [['Simple Linear Regression no intercept',
                            get_results(simple_y_test, simple_pred_test_no_intercept)[0],
                            get_results(simple_y_test, simple_pred_test_no_intercept)[1],
                            get_results(simple_y_train, simple_pred_train_no_intercept)[0],
                            get_results(simple_y_train, simple_pred_train_no_intercept)[1]]],
                            columns = ['Model', 'R2_test', 'MSE_test', 'R2_train', 'MSE_train'])
results_df = pd.concat([results_df, results_df_5])
results_df
```

Out[85]:

	Model	R2_test	MSE_test	R2_train	MSE_train
0	Simple Linear Regression	0.909596	290.479789	0.909844	293.118977
0	Ridge Regression	0.972895	87.549920	0.972978	87.658762
0	Random Forest Regression	0.988119	38.377083	0.998283	5.570921
0	XGBoost Regression	0.988203	38.105111	0.991336	28.107768
0	Simple Linear Regression no intercept	0.909072	292.166020	0.909467	294.343506

We will do a scatterplot of ArrDelay And DepDelay and we will draw the 2 regression lines, the one with intercept and the one without intercept.

In [86]:
```python
plt.figure(figsize=(10, 10))
# regression equation
y_simple_hat = simple_reg.coef_* x_simple + simple_reg.intercept_ # regression line with intercept
y_simple_hat_no_intercept = simple_reg_no_intercept.coef_*x_simple # regression line without intercept
#plot the regression line
plt.plot(x_simple, y_simple_hat, lw = 4, c = 'orange', label = 'regression line')
plt.plot(x_simple, y_simple_hat_no_intercept, lw =4, c = 'green', label= 'regression line without intercept')
plt.scatter(x_simple, y_simple)
plt.xlabel('DepDelay',fontsize=15)
plt.ylabel('ArrDelay',fontsize=15)
plt.legend()
plt.title('Comparison of Simple Linear regression with and without intercept', fontsize = 15)
plt.show()
```



We observe than in our model the two regression lines seem very similar (R2 is also similar in both cases, 0.909).

In our original regression intercept was -1.42 (ArrDelay was -1.42 min when DepDelay was 0). We can calculate the p-value of the intercept of our previous model (the model with interceot) to see if the intercept is significant for the model:

In [87]:
```python
# to calculate the p values we will use statsmodel module
import statsmodels.api as sm
# define the intercept
x = sm.add_constant(simple_x_train)
# do the regression with intercept
regression = sm.OLS(simple_y_train, x )
regression = regression.fit()
```

In [88]:
```python
regression.summary()
```

Out[88]:

OLS Regression Results

Dep. Variable:	ArrDelay	R-squared:	0.910
Model:	OLS	Adj. R-squared:	0.910
Method:	Least Squares	F-statistic:	1.362e+06
Date:	Thu, 21 Apr 2022	Prob (F-statistic):	0.00
Time:	14:24:10	Log-Likelihood:	-5.7490e+05
No. Observations:	134977	AIC:	1.150e+06
Df Residuals:	134975	BIC:	1.150e+06
Df Model:	1		
Covariance Type:	nonrobust		

	coef	std err	t	P>|t|	[0.025	0.975]
const	-1.4201	0.060	-23.746	0.000	-1.537	-1.303
x1	1.0129	0.001	1167.110	0.000	1.011	1.015

Omnibus:	82571.611	Durbin-Watson:	2.001
Prob(Omnibus):	0.000	Jarque-Bera (JB):	1751003.095
Skew:	2.569	Prob(JB):	0.00
Kurtosis:	19.880	Cond. No.	88.4

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.

- We observe doing the Regression with statsmodel returns the same results as using sklearn: R2 is the same as in model (0.910, 0.909844 with SKLearn) and the intercept is the same too.
- According to the p-value the intercept is significant in our model, since p value is zero (here the null hypothesis is that intercept has no predictive power)

Ridge Regression

In [89]:
```python
# look at the parameters used in the previous model
ridge.get_params()
```

Out[89]:
```
{'alpha': 1.0,
 'copy_X': True,
 'fit_intercept': True,
 'max_iter': None,
 'normalize': 'deprecated',
 'positive': False,
 'random_state': None,
 'solver': 'auto',
 'tol': 0.001}
```

We can change the value of alpha : According to sklearn page: " Regularization strength; must be a positive float. Regularization improves the conditioning of the problem and reduces the variance of the estimates. Larger values specify stronger regularization". We will use GridDSearch to look which alpha value is best to maximize R2.

In [90]:
```python
from sklearn.model_selection import GridSearchCV
# define the params we want to evaluate
parameters = {'alpha' : [0.75, 1.25, 1.75] }

tuned_ridge = Ridge()

clf = GridSearchCV(estimator = tuned_ridge, param_grid=parameters, scoring = 'r2', verbose = 1)
clf.fit(X_train,y_train)

print("Best parameters:", clf.best_params_)
```

```
Fitting 5 folds for each of 3 candidates, totalling 15 fits
Best parameters: {'alpha': 1.75}
```

In [91]:
```python
# best parameters return an alpha of 1.75, so we will try this parameter in our model

ridge_tuned = Ridge(alpha = 1.75)
ridge_tuned.fit(X_train, y_train)
```

Out[91]:
```
Ridge(alpha=1.75)
```

In [92]:
```
ridge_tuned_test_prediction = ridge_tuned.predict(X_test)
ridge_tuned_train_prediction = ridge_tuned.predict(X_train)

print_results_test(y_test, ridge_tuned_test_prediction)
print_results_train(y_train, ridge_tuned_train_prediction)
```

```
R2 for test set :  0.9728971632080551
MSE (mean squared error) for test set:  87.54344999204696
------------------------------------------
R2 for train set :  0.972976916178329
MSE (mean squared error) for train set:  87.66345101333845
```

R2 is sligtly higher in this case, and MSE a little lower compared to the case when we used alpha =0.1. It seems changing this parameter has worked well for our model. The results we got before where:

In [93]:
```
# see results with initial parameters
results_df[1:2]
```

Out[93]:

	Model	R2_test	MSE_test	R2_train	MSE_train
0	Ridge Regression	0.972895	87.54992	0.972978	87.658762

In [94]:
```
# we will save this results
results_df_6 = pd.DataFrame(data=[['Tuned Ridge Regression', get_results(y_test, ridge_tuned_test_prediction)[(
                                   get_results(y_test, ridge_tuned_test_prediction)[1],
                                   get_results(y_train, ridge_tuned_train_prediction)[0],
                                   get_results(y_train, ridge_tuned_train_prediction)[1]]] , columns =['Model',
                                   'R2_test', 'MSE_test', 'R2_train', 'MSE_train'])
results_df = pd.concat([results_df, results_df_6])
```

In [95]:
```
results_df
```

Out[95]:

	Model	R2_test	MSE_test	R2_train	MSE_train
0	Simple Linear Regression	0.909596	290.479789	0.909844	293.118977
0	Ridge Regression	0.972895	87.549920	0.972978	87.658762
0	Random Forest Regression	0.988119	38.377083	0.998283	5.570921
0	XGBoost Regression	0.988203	38.105111	0.991336	28.107768
0	Simple Linear Regression no intercept	0.909072	292.166020	0.909467	294.343506
0	Tuned Ridge Regression	0.972897	87.543450	0.972977	87.663451

Random Forest Regression

Now we´ll change parameters of our Random Forest Regression, altough default parameter for n_estimators is 100, in the previous model I changed it to 50 to speed up the model, let´s see if we got better results setting n_estimators to 100.

In [96]:
```
# look for params of our previous model
regressor.get_params()
```

Out[96]:
```
{'bootstrap': True,
 'ccp_alpha': 0.0,
 'criterion': 'squared_error',
 'max_depth': None,
 'max_features': 'auto',
 'max_leaf_nodes': None,
 'max_samples': None,
 'min_impurity_decrease': 0.0,
 'min_samples_leaf': 1,
 'min_samples_split': 2,
 'min_weight_fraction_leaf': 0.0,
 'n_estimators': 50,
 'n_jobs': None,
 'oob_score': False,
 'random_state': 0,
 'verbose': 0,
 'warm_start': False}
```

We will now train our model with max_depth :7 and n_stimators = 100 (before it was None and 50).

- Max_depth refers to the minimum number of samples each branch must have after splitting a node.
- n_stimator refers to the number of trees in the forest. Before we set it to 50 to speed the model but the default mode is 100 so we will do now 100 trees.

In [97]:
```
# instantiate and fit our model with the new parameters
regressor_changed = RandomForestRegressor(n_estimators = 100, max_depth = 7, random_state=0)
regressor_changed.fit(X_train, y_train)
```

Out[97]:
```
RandomForestRegressor(max_depth=7, random_state=0)
```

In [98]:
```
forest_changed_test_prediction = regressor_changed.predict(X_test)
forest_changed_train_prediction = regressor_changed.predict(X_train)

print_results_test(y_test, forest_changed_test_prediction)
print_results_train(y_train, forest_changed_train_prediction)
```

```
R2 for test set :  0.9782949798048104
MSE (mean squared error) for test set:  70.10824603418195
------------------------------------------
R2 for train set :  0.97961801386437
MSE (mean squared error) for train set:  66.11959075235038
```

R2 is lower and mse is higher than before!!! Maybe the max_depth parameter was not worth changing, we 'll repeat leaving the default and repeat the model only changing number of estimators (number of trees)

In [99]:
```
regressor_changed2 = RandomForestRegressor(n_estimators= 100, random_state= 0)
regressor_changed2.fit(X_train, y_train)
```

Out[99]:
```
RandomForestRegressor(random_state=0)
```

In [100…
```
forest_changed2_test_prediction = regressor_changed2.predict(X_test)
forest_changed2_train_prediction = regressor_changed2.predict(X_train)
```

In [101…
```
print_results_test(y_test, forest_changed2_test_prediction)
print_results_train(y_train, forest_changed2_train_prediction)
```

```
R2 for test set :  0.9882930131220383
MSE (mean squared error) for test set:  37.81412359805006
------------------------------------------
R2 for train set :  0.9983593767169089
MSE (mean squared error) for train set:  5.3222163598242656
```

Now we have improved the results of our model, R2 both for test and train is higher than before and MSE is a little lower (let´s look at the results we got before):

In [102…
```
# looking at initial results
results_df[2:3]
```

Out[102…

	Model	R2_test	MSE_test	R2_train	MSE_train
0	Random Forest Regression	0.988119	38.377083	0.998283	5.570921

In any case, the improvement is very little (we already have a very high R2 so it may be difficult to increase it more). Maybe it´s not worth it considering than before we did the regression with half of estimators (much less computational power needed, the execution time in this model is much higher than before!!) and got very close results. We will keep this results in our dataframe:

In [103…
```
results_df_7= pd.DataFrame(data = [['Random Forest Doubled Trees', get_results(y_test, forest_changed2_test_pre
                                   get_results(y_test, forest_changed2_test_prediction)[1],
                                   get_results(y_train, forest_changed2_train_prediction)[0],
                                   get_results(y_train, forest_changed2_train_prediction)[1]
                                   ]], columns = ['Model', 'R2_test', 'MSE_test', 'R2_train', 'MSE_train'])
results_df = pd.concat([results_df, results_df_7])
results_df
```

Out[103…

	Model	R2_test	MSE_test	R2_train	MSE_train
0	Simple Linear Regression	0.909596	290.479789	0.909844	293.118977
0	Ridge Regression	0.972895	87.549920	0.972978	87.658762
0	Random Forest Regression	0.988119	38.377083	0.998283	5.570921
0	XGBoost Regression	0.988203	38.105111	0.991336	28.107768
0	Simple Linear Regression no intercept	0.909072	292.166020	0.909467	294.343506
0	Tuned Ridge Regression	0.972897	87.543450	0.972977	87.663451
0	Random Forest Doubled Trees	0.988293	37.814124	0.998359	5.322216

XGBoost Regression

Let´s check the params used in our previous model in XGBoost Regression:

In [104…
```
XGB_regressor.get_params()
```

Out[104…
```
{'objective': 'reg:squarederror',
 'base_score': 0.5,
 'booster': 'gbtree',
 'colsample_bylevel': 1,
 'colsample_bynode': 1,
 'colsample_bytree': 1,
 'enable_categorical': False,
 'gamma': 0,
 'gpu_id': -1,
 'importance_type': None,
 'interaction_constraints': '',
 'learning_rate': 0.300000012,
 'max_delta_step': 0,
 'max_depth': 6,
 'min_child_weight': 1,
 'missing': nan,
 'monotone_constraints': '()',
 'n_estimators': 100,
 'n_jobs': 8,
 'num_parallel_tree': 1,
 'predictor': 'auto',
 'random_state': 0,
 'reg_alpha': 0,
 'reg_lambda': 1,
 'scale_pos_weight': 1,
 'subsample': 1,
 'tree_method': 'exact',
 'validate_parameters': 1,
 'verbosity': None}
```

This time, to find out which parameters we can change we can use Grid Search again, we will look for the combination of parameters that optimizes MSE (before we used GridSearch to maximize R2). We have choosed 3 parameters and two values for each one and we will find out if we can have some improvement in MSE:

In [105…
```
from sklearn.model_selection import GridSearchCV
```

In [106…
```
import xgboost as xgb
# we define the parameters we want to evaluate:
params = { 'max_depth': [3,8], 'learning_rate': [0.05, 0.1], 'colsample_bytree': [0.3, 0.7]}

tuned_xgb = xgb.XGBRegressor()

clf = GridSearchCV(estimator= tuned_xgb,
                   param_grid=params,
                   scoring='neg_mean_squared_error',
                   verbose=1)
clf.fit(X_train, y_train)
print("Best parameters:", clf.best_params_)
print("Lowest RMSE: ", (-clf.best_score_)**(1/2.0))
```

```
Fitting 5 folds for each of 8 candidates, totalling 40 fits
Best parameters: {'colsample_bytree': 0.7, 'learning_rate': 0.1, 'max_depth': 8}
Lowest RMSE:  6.216730134758261
```

In [107…
```
# Output:

# Fitting 5 folds for each of 8 candidates, totalling 40 fits
# Best parameters: {'colsample_bytree': 0.7, 'learning_rate': 0.1, 'max_depth': 8}
# Lowest RMSE:  6.216730134758261
```

Now let´s apply the model with the new parameters:

In [108…
```
XGB_tuned_regressor = XGBRegressor(colsample_bytree= 0.7, learning_rate= 0.1, max_depth= 8)
# fit train set
XGB_tuned_regressor.fit(X_train, y_train)
```

Out[108…
```
XGBRegressor(base_score=0.5, booster='gbtree', colsample_bylevel=1,
             colsample_bynode=1, colsample_bytree=0.7, enable_categorical=False,
             gamma=0, gpu_id=-1, importance_type=None,
             interaction_constraints='', learning_rate=0.1, max_delta_step=0,
             max_depth=8, min_child_weight=1, missing=nan,
             monotone_constraints='()', n_estimators=100, n_jobs=8,
             num_parallel_tree=1, predictor='auto', random_state=0, reg_alpha=0,
             reg_lambda=1, scale_pos_weight=1, subsample=1, tree_method='exact',
             validate_parameters=1, verbosity=None)
```

In [109…
```
XGBtuned_test_prediction = XGB_tuned_regressor.predict(X_test)
XGBtuned_train_prediction = XGB_tuned_regressor.predict(X_train)
```

In [110…
```
print_results_test(y_test, XGBtuned_test_prediction )
print_results_train(y_train, XGBtuned_train_prediction)
```

```
R2 for test set :  0.9882761569466629
MSE (mean squared error) for test set:  37.868569845037634
------------------------------------------
R2 for train set :  0.9914808862918554
MSE (mean squared error) for train set:  27.636183647999896
```

In [111…
```
# results of the model with default parameters:
results_df[3:4]
```

Out[111…

	Model	R2_test	MSE_test	R2_train	MSE_train
0	XGBoost Regression	0.988203	38.105111	0.991336	28.107768

Comparing the results with our previous model we see a little improvement for both R2 and MSE for both train and test!! (The improvement is small because results where already very good).

In [112…
```
# keep results in df
results_df_8 = pd.DataFrame( data = [['XGBoost Tuned Regression', get_results(y_test, XGBtuned_test_prediction)
                                    get_results(y_test, XGBtuned_test_prediction)[1],
                                    get_results(y_train, XGBtuned_train_prediction)[0],
                                    get_results(y_train, XGBtuned_train_prediction)[1]]], columns = ['Model',
                                   'R2_test', 'MSE_test', 'R2_train', 'MSE_train'])
results_df = pd.concat([results_df, results_df_8])
results_df
```

Out[112…

	Model	R2_test	MSE_test	R2_train	MSE_train
0	Simple Linear Regression	0.909596	290.479789	0.909844	293.118977
0	Ridge Regression	0.972895	87.549920	0.972978	87.658762
0	Random Forest Regression	0.988119	38.377083	0.998283	5.570921
0	XGBoost Regression	0.988203	38.105111	0.991336	28.107768
0	Simple Linear Regression no intercept	0.909072	292.166020	0.909467	294.343506
0	Tuned Ridge Regression	0.972897	87.543450	0.972977	87.663451
0	Random Forest Doubled Trees	0.988293	37.814124	0.998359	5.322216
0	XGBoost Tuned Regression	0.988276	37.868570	0.991481	27.636184

In [113…
```
# save this results_df
results_df.to_csv('results_df.csv', index = False)
```

- Exercici 4

Compara el seu rendiment utilitzant l'aproximació traint/test o utilitzant totes les dades (validació interna)

We will do Cross-Validation of the 4 models we have used. Since some of the models take a lot of computing time, we will use cv = 5 instead of cv = 10.

Simple Linear Regression

In [114…
```
from sklearn.model_selection import cross_val_score
```

In [115…
```
lr = LinearRegression()

# apply cross validation for r2
r2_scores_lr = cross_val_score(lr, x_simple, y_simple, cv = 10, scoring = 'r2')
r2_lr =np.mean(r2_scores_lr).round(4)
r2_lr
```

Out[115…
```
0.9077
```

In [116…
```
mse_scores_lr = cross_val_score(lr, x_simple, y_simple, cv = 10 , scoring = 'neg_mean_squared_error')
mse_lr = abs(np.mean(mse_scores_lr)).round(4)
mse_lr
```

Out[116…
```
293.3321
```

In [117…
```
# we are going to create a dataframe for the results
cv_results = pd.DataFrame(data = [['Simple Linear Regression', r2_lr, mse_lr]], columns = ['Model', 'R2', 'MSE'
cv_results
```

Out[117…

	Model	R2	MSE
0	Simple Linear Regression	0.9077	293.3321

Ridge regression

Now we´ll do the same with Ridge Regression

In [118…
```
# now we apply CV to X and y with ridge model
# we apply CV to X and y (not splitted)
ridge = Ridge()
ridge_r2_scores = cross_val_score(ridge, X, y, cv =5)
ridge_r2_scores
```

Out[118…
```
array([0.97113636, 0.96375803, 0.97460197, 0.96741267, 0.97064173])
```

In [119…
```
r2_cv_ridge = np.mean(ridge_r2_scores)
r2_cv_ridge
```

Out[119…
```
0.96951015141
```

In [120…
```
ridge_mse_scores = cross_val_score(ridge, X, y, cv =5,  scoring = 'neg_mean_squared_error')
```

In [121…
```
mse_cv_ridge = abs(np.mean(ridge_mse_scores))
mse_cv_ridge
```

Out[121…
```
97.4153010417725
```

In [122…
```
ridge_results = pd.DataFrame(data = [['Ridge Regression', r2_cv_ridge, mse_cv_ridge]],
                             columns = ['Model', 'R2', 'MSE'])
cv_results = pd.concat([cv_results, ridge_results])
cv_results
```

Out[122…

	Model	R2	MSE
0	Simple Linear Regression	0.90770	293.332100
0	Ridge Regression	0.96951	97.415301

Random Forest Regression

In [123…
```
forest = RandomForestRegressor(n_estimators= 50, random_state= 0)
forest_r2_scores = cross_val_score(forest, X, y, cv = 5)
```

In [124…
```
r2_cv_forest = np.mean(forest_r2_scores)
r2_cv_forest
```

Out[124…
```
0.9875035113459513
```

In [125…
```
forest_mse_scores = cross_val_score(forest, X, y, cv = 5,scoring = 'neg_mean_squared_error' )
forest_mse_scores
```

Out[125…
```
array([-51.6013453 , -39.2487797 , -40.37977414, -38.04800514,
       -31.36632787])
```

In [126…
```
mse_cv_forest  = abs(np.mean(forest_mse_scores))
mse_cv_forest
```

Out[126…
```
40.12884643173862
```

In [127…
```
# save it to a dataframe
forest_results = pd.DataFrame(data = [['Random Forest Regression', r2_cv_forest, mse_cv_forest]],
                              columns = ['Model', 'R2', 'MSE'])

cv_results = pd.concat([cv_results, forest_results])
```

XGBoost Regression

In [128…
```
xgb_regressor = XGBRegressor()
xgb_r2_scores = cross_val_score(xgb_regressor, X, y, cv = 5)
xgb_r2_scores
```

Out[128…
```
array([0.98736239, 0.9869738 , 0.98933323, 0.98577245, 0.98783103])
```

In [129…
```
r2_cv_xgb = np.mean(xgb_r2_scores)
r2_cv_xgb
```

Out[129…
```
0.9874545798528283
```

In [130…
```
xgb_mse_scores = cross_val_score(xgb_regressor, X, y, cv = 5, scoring = 'neg_mean_squared_error')
xgb_mse_scores
```

Out[130…
```
array([-49.51210968, -40.63479463, -39.81449616, -37.4899658 ,
       -33.27155275])
```

In [131…
```
mse_cv_xgb = abs(np.mean(xgb_mse_scores))
mse_cv_xgb
```

Out[131…
```
40.144583804872454
```

In [132…
```
# save results to dataframe
xgb_results = pd.DataFrame(data = [['XGBoost Regression', r2_cv_xgb, mse_cv_xgb ]],
                           columns = ['Model', 'R2', 'MSE'])

cv_results = pd.concat([cv_results, xgb_results])
```

In [133…
```
cv_results
```

Out[133…

	Model	R2	MSE
0	Simple Linear Regression	0.907700	293.332100
0	Ridge Regression	0.969510	97.415301
0	Random Forest Regression	0.987504	40.128846
0	XGBoost Regression	0.987455	40.144584

In [4]:
```
# loof at the df with the results of our models using train/test split
results_df = pd.read_csv('results_df.csv')
results_df
```

Out[4]:

	Model	R2_test	MSE_test	R2_train	MSE_train
0	Simple Linear Regression	0.909596	290.479789	0.909844	293.118977
1	Ridge Regression	0.972895	87.549920	0.972978	87.658762
2	Random Forest Regression	0.988119	38.377083	0.998283	5.570921
3	XGBoost Regression	0.988203	38.105111	0.991336	28.107768
4	Simple Linear Regression no intercept	0.909072	292.166020	0.909467	294.343506
5	Tuned Ridge Regression	0.972897	87.543450	0.972977	87.663451
6	Random Forest Doubled Trees	0.988293	37.814124	0.998359	5.322216
7	XGBoost Tuned Regression	0.988276	37.868570	0.991481	27.636184

If we compare the df with the results of our Cross Validation and the df with our train/test results :

- MSE is a little higer for all the models (compared with train/test split) specially in the models that got better results: Random Forest and XGBoost.
- R2 is a little lower in Cross Validation but the difference is not worrying.
- We could say that our model does not suffer from overfitting, because altought the results are worse than with train/test, this difference is very small and Cross Validation still shows very good results.

The exercise is continued in another Notebook in the same Github link.

In [134…
```
# save file to csv
cv_results.to_csv('cv_results', index = False)
```