Exercise Set 1

Problem 1

Task a and Task b

Task a and *Task b* are trivial, hence the code is not reported. After dataset loading, though, the dataframe I obtained has the following shape: `458 rows × 103 columns`.

Task c

With regards to *Task c*, applying the `describe()` function gave a dataframe with shape equals to `8 rows x 101 columns`; the rows coincide with the typical description variables: `count`, `mean`, `std`, `min`, `25%`, `50%`, `75%`, `max`.

Then, I applied the function `pairplot` from seaborn library:

```
sns.pairplot(npf, hue='class4', vars=npf.columns[2:12], kind='reg')
```

This returned the following result:

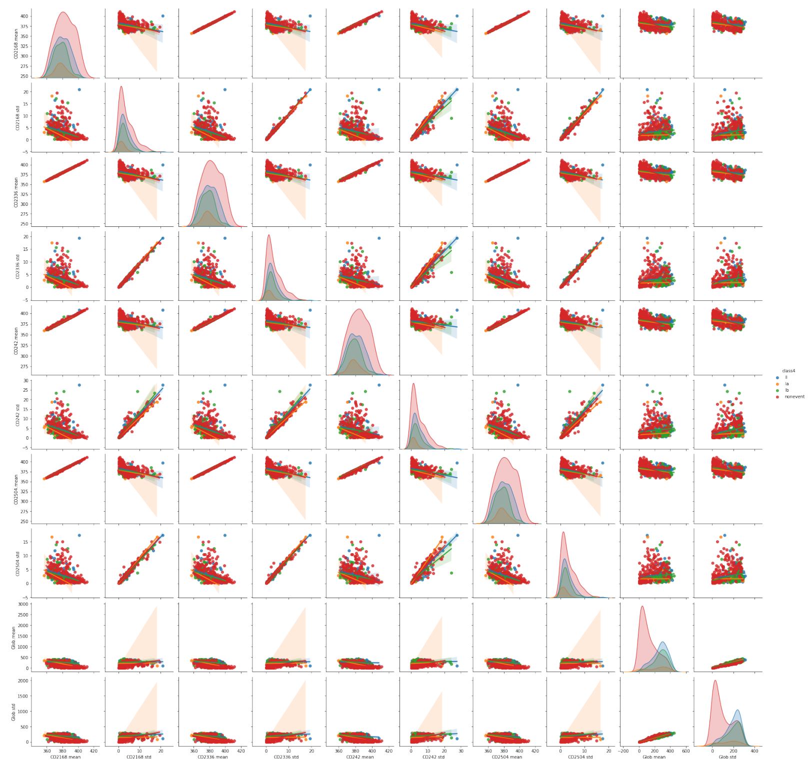


Figure 1: Result of pariplot function

Secondarily, I applied the function `boxplot` from seaborn library:

```
sns.boxplot(x='class2', y='CS.mean', data=npf)
```

This returned the following result:

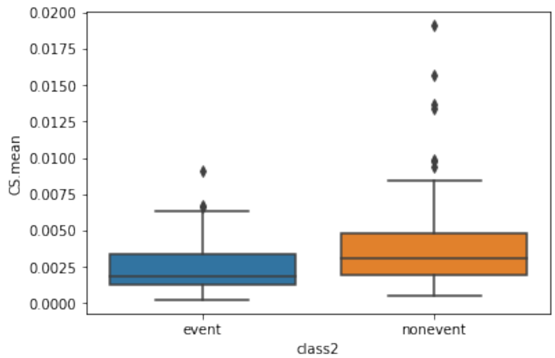


Figure 2: Result of first boxplot function

Finally, I created a new qualitative variable as asked. The `describe` command reports a number of 458 *event days*, and the last boxplot function (`sns.boxplot(x='class2', y='CS.mean', data=npf)`) returns this output:

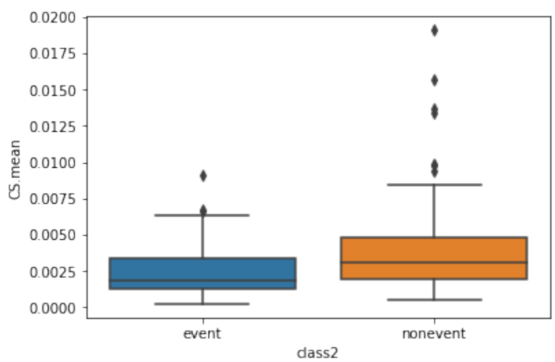


Figure 3: Result of second boxplot function

Coming to the personal implementation of histograms, I used `matplotlib` to plot four histograms on quantitative variables with different number of bins. The following code

```
fig, axs = plt.subplots(2, 2, sharey=True, sharex=True, tight_layout=True)
axs[0][0].hist(npf['T168.mean'], bins=10)
axs[0][1].hist(npf['RHIRGA672.mean'], bins=6)
axs[1][0].hist(npf['O3168.mean'], bins=16)
axs[1][1].hist(npf['NOx336.mean'], bins=6)
```

plots these four histograms:

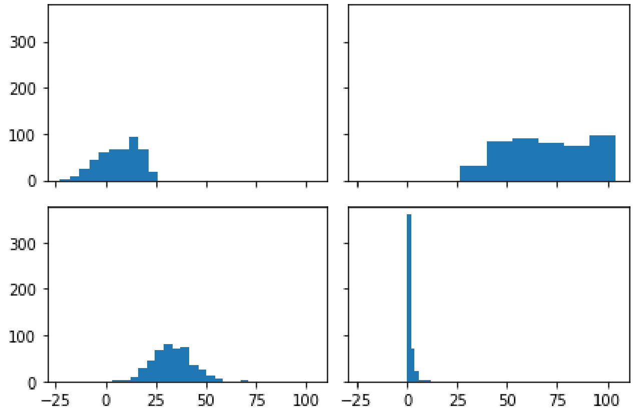


Figure 4: Histograms with matplotlib

Doing other *exploratory data analysis* on the given dataset, I found out that many of the variables have little-to-no variance, while there are mainly four of them that have a huge variance in the dataset; these variables are:

- PAR
- NET
- GLOB
- SWS

This phenomenon can be seen also in the following pie chart:

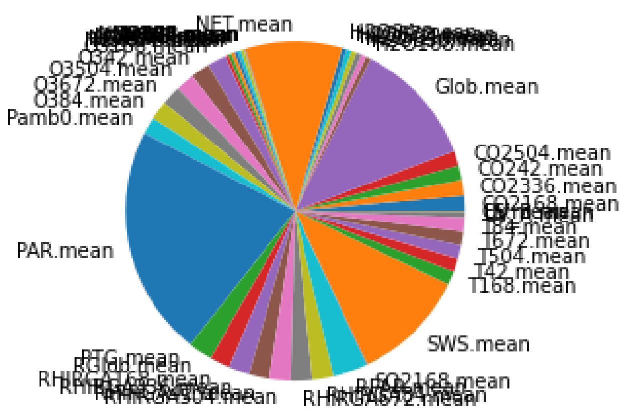


Figure 5: Example of pie chart

In order to obtain this pie chart, I used the following code:

```
diff = []
labels = []
for i in npf:
    if(npf[i].dtype.name != 'category' and 'std' not in i):
        diff.append(npf[i].max() - npf[i].min())
        labels.append(i)

diff = diff[1:]
```

```
labels = labels[1:]
plt.pie(diff, labels=labels)
```

Problem 2

Task a

I used `numpy` and `pandas` in order to create the three sets; I used the following function in order to calculate them as requested (note: `np` stands for `numpy` and `pd` stands for `pandas`):

```
def create_dataset(n):
    x = np.random.uniform(low=-3, high=3, size=n)
    eps = np.random.normal(loc=0, scale=0.4, size=n)
    y = []
    for i in range(0, len(x)):
        y.append((1+x[i]-(x[i]**2)/2) + eps[i])
    d = {'x':x,'y':y}
    return pd.DataFrame(d)
```

Then, I called the function for three times:

```
training = create_dataset(20)
validation = create_dataset(20)
test = create_dataset(1000)
```

Task b and Task c

I implemented from scratch linear regression functions; these are the following:

```
def transform_x(x, degree):
    X = []
    for xi in x:
        row = [xi**d for d in range(0,degree+1)]
        X.append(row)
    return X

def ols(x, y, deg):
    X = np.matrix(transform_x(x, deg))
    betas = -np.matmul(
      np.matmul(np.linalg.inv(np.matmul(X.transpose(), X)),
      X.transpose()), y
      )
    return betas

def f(x, betas):
    y = betas[0]
    for i in range(1,len(betas)):
        y+=betas[i]*(x**i)
    return -y
```

I then applied these functions with the following code:

```
degrees = range(0,11)
for degree in degrees:
    betas = ols(training['x'], training['y'], degree)
    line_x = np.linspace(start=-3, stop=3, num=256)
```

```
    line_y = np.array([f(xi, betas) for xi in line_x])
    plt.scatter(training['x'], training['y'])
    plt.plot(line_x, line_y)
    plt.show()
```

Respectively, in the first code block the first function transforms the array x into the input matrix **X**, used to fitting the polynomial (cfr. lecture slides). The function `ols` fits the polynomial given `x` the previous transformed matrix, `y` the targets vector and `deg` the degree of the polynomial. `f` then applies the function over a point `x`. In the second code block these functions are applied, and at the same time data is plotted.

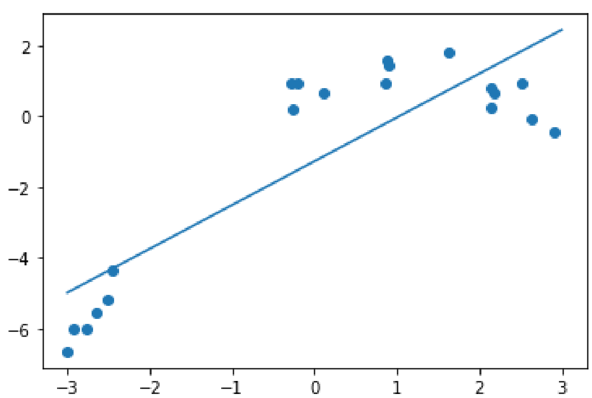
In order to calculate the MSE I used the following code:

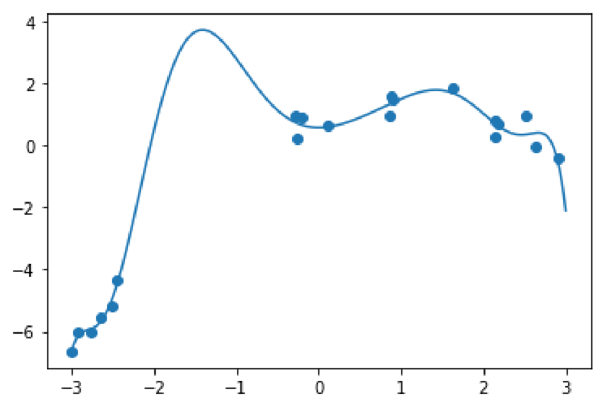
```
def calculate_mse(degree, betas, tr):
    pred = []
    for i in range(0, len(tr)):
        pred.append(f(tr['x'][i], betas))
    mse = np.sum((tr['y']-pred)**2)
    mse/=len(tr)
    return mse

mses = []
for degree in degrees:
    betas = ols(training['x'], training['y'], deg=degree)
    mses.append(calculate_mse(degree, betas, training))
```

This code calculates the MSE with the function `calculate_mse` for every degree from 0 to 10. I applied the same code for Task c, just substituting `training` variable with `validation` and `test`.

I'm not reporting every graph due to brevity, but these are the two graphs for, respectively, degree=1 and degree=10 on the training set.





The MSE results are reported at the end of this exercise's section.

Task d and Task e

In order to calculate the cross-validation loss I used the following code:

```
from copy import deepcopy

tv_combined = training.append(validation).reset_index()

def cv_split(tosplit, folds):
    split = []
```

```python
    copy = deepcopy(tosplit).to_numpy()
    for i in range(0, folds):
        t = []
        while len(t) < int(len(tosplit) / folds):
            toremove = np.random.randint(0, len(copy))
            t.append([copy[toremove][1], copy[toremove][2]])
            copy = np.delete(copy, toremove, 0)
        split.append(t)
    return split

splits = cv_split(tv_combined, 10)
for degree in range(0,10):
    cv = 0
    for i in range(0, 10):
        validat_set = pd.DataFrame(splits[i], columns=['x','y'])
        train_set = pd.DataFrame(columns=['x','y'])
        for j in range(0,10):
            if(j!=i):
                sp = pd.DataFrame(splits[j], columns=['x','y'])
                train_set = train_set.append(sp, ignore_index=True)

        min_mse = float('inf')
        betas = ols(training['x'], training['y'], deg=degree)
        mse = calculate_mse(degree, betas, train_set)
        cv+=mse
        if mse < min_mse:
            min_mse = mse
            min_mse_index = i
    cv/=10
```

The `cv_split` function splits the data into `folds` folds, and returns the splits as a list. Then, I used the function and I computed the cross validation loss for every degree from 0 to 10; I got the best result with a polynomial with degree equal to two (cross validation loss equal to 0.111). This was predictable, since the artificial data has been generated with a quadratic function. The other results are reported in the table in the section below.

Table of results

Polynomial Degree	MSE training set	MSE test set	MSE validation set	Cross validation loss	MSE validation+test on test
0	8.986222	5.750446	3.223248	7.5607017	2.545747
1	2.473259	2.924710	2.159980	2.8998730	1.660668
2	0.112000	0.197443	0.176187	0.1118274	0.143234
3	0.111406	0.259663	0.201487	0.1141089	0.152570
4	0.111250	0.201979	0.186965	0.1147524	0.144825
5	0.108734	0.340275	0.445334	0.1086647	0.288850
6	0.101122	12.401310	17.365585	0.1736703	9.673253
7	0.098209	9.787755	13.593989	6.8223801	7.577771
8	0.079053	99.970575	150.368588	75.2089	83.56379
9	0.078774	2092.939926	3354.972441	1677.5100	1863.8999
10	0.072277	6718.510395	11094.152098	5547.0997	6163.443

Task f

Using the table constructed, it is pretty clear that the best model is the polynomial with degree equals to two; this, as said in the previous section, was predictable, since the data was generated by a quadratic function ($f(x) = 1 + x - \frac{x^2}{2}$).

Problem 3

Task a and Task b

I chose Ridge as the other regression model implemented, though it is not so much different from simple linear regression for a dataset like this (there's no high dimensionality of data, since there are only 22 columns and 7590 rows). I implemented these methods using the `scikit-learn` library. I'm not reporting the entire code due to brevity, but it is pretty similar to the regression example below:

```
training_set = bcnp.sample(n=100)
test_set = pd.concat([bcnp, training_set]).drop_duplicates(keep=False)

# linear regression
reg = LinearRegression().fit(
  training_set[training_set.columns.difference(['Next_Tmax'])],
  training_set['Next_Tmax']
  )
y_pred = reg.predict(
  test_set[test_set.columns.difference(['Next_Tmax'])]
  )
rmse = np.sqrt(
  mean_squared_error(test_set['Next_Tmax'], y_pred)
  )
y_pred_t = reg.predict(
  training_set[test_set.columns.difference(['Next_Tmax'])]
  )
rmse_train = np.sqrt(
  mean_squared_error(training_set['Next_Tmax'], y_pred_t)
  )
```

For each model I calculated the RMSE both on test and train set; the results are reported in the table at the end of this exercise's section.

Task c

I implemented the 10-fold cross-validation losses joining the code from Exercise 2 and the code here above; I could have also used pre-implemented functions from `scikit-learn`, but since I already had this code I used it. Also in this case, the code is pretty similar to the regression example below:

```
kf = KFold(n_splits=10)

cv = 0
for tr, val in kf.split(training_set):
    reg = LinearRegression().fit(
      training_set.iloc[tr][training_set.columns.difference(
        ['Next_Tmax'])], training_set.iloc[tr]['Next_Tmax']
        )
    y_pred = reg.predict(
      training_set.iloc[val][training_set.columns.difference(['Next_Tmax'])])
    mse = mean_squared_error(training_set.iloc[val]['Next_Tmax'], y_pred)
```

```
    cv+=mse
cv/=10
```

The results are reported in the table at the end of this exercise's section as well.

Table of results

Regressor	RMSE on test set	RMSE on training set	Cross validation loss
Linear regression	1.8698695351417394	1.1616132699948303	2.365633087039427
Regression Tree	2.206974319635378	6.153480596427405e-16	3.2495000000000003
Random Forest	1.7152949723559454	0.5578841187917046	2.264977390000001
SVM	3.211369069051392	3.014713257799681	11.058880968944521
Ridge	1.8065227008021323	1.197506935478486	2.2091122109416226

Task d

As I can see from the results, the best regressor overall is random forest, since both RMSE on test set and cross validation loss are very low. The RMSE on training data is lower in every examined case; this was quite predictable, since it's clear that the model trained on the training set is not perfectly suitable also for data on the test set. It's a good sign, though, that for the most part of the regressor it's lower but not too much: this means that a correct tradeoff between bias and variance has been found.

In order to make these models perform better, a good idea is to tweak the models hyperparameters. I used, in fact, the models in a plain fashion, but more work can be done modifying general parameters like regularization strenght, or more specific ones like the maximum depth of the regression trees for the simple regression tree and the random forest models.

Problem 4

Task a

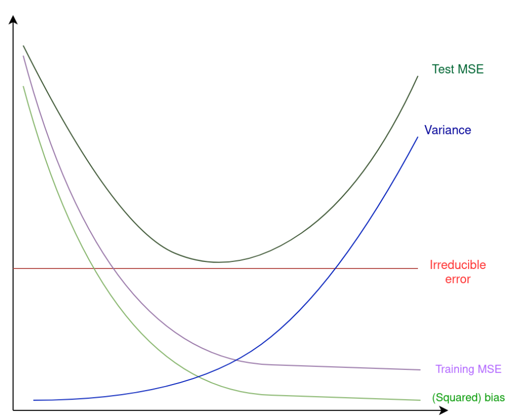


Figure 6: Curves: x-axis is the flexibility, y-axis are the "hypotetical values"

Explanation

- **Irreducible error**: the irreducible error is a constant and it's always lower than the test MSE.
- **Squared bias and Variance**: known for the "bias-variance tradeoff" issue, the variance increases when the model becomes more flexible, while the bias decreases. This happens because a more flexible model is a function that better fits the observations, hence if one or more points are different on another

training set, the function won't be able to fit them as well, and then the variance gets higher; at the same time, since the bias is how far the estimated value is from the real value, a function that tends to perfectly fit the observation has bias tending to zero.

- **Training and Test MSE**: as said, a more flexible model is a function that better fits the observations; since the observations come from the training set, it's trivial that the training MSE get lower with more flexibility. For the same reason, the test MSE tends to decrease (though it never gets lower than the irreducible error) since the "best tradeoff" is found, and then it starts increasing.

Task b

Problem 5

Task a

We know that $MSE = E[(\hat{\beta} - \beta)^2] = bias^2 + variance$, and we know that the generalization error for the OLS regression is

$$\frac{\sum_{i \in test}^{m} (y_i - \hat{y}_i)^2}{m}$$

for m number of samples in the test set. Since y_i are actually observations in the test set, the last formula is exactly the variance of the model, that is L_{test}. Thus, since $MSE = bias^2 + variance$, bias has to be equal to zero, and then L_{test} is an unbiased estimate of the generalization error for the OLS regression.

Task b

We know that

$$E[L_{train}] = E\left[\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{\beta}^T \bar{\mathbf{x}}_i)^2\right]$$

and, since it's biased, it is equal to

$$\left(1 - \frac{1}{n}\right)\sigma^2$$

$E[L_{test}]$, on the other hand, corresponds with the variance, i.e. σ^2. It's trivial to see then that

$$\left(1 - \frac{1}{n}\right)\sigma^2 \leq \sigma^2$$

Task c

The result of task b says that the expectation of the train MSE is at most equal to the test MSE, but it's usually lower. This relates to the generalization problem in machine learning since it means that a tradeoff has to be found between bias and variance so that the model is neither too fitting to training data (overfitting), nor too general (underfitting).