Solution 1: HRO in sklearn

a)

Model classes representing a certain **hypothesis** are stored in subpackages of sklearn. You can reach it with importing the desired class with e.g.

[1]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
from sklearn.datasets import load_iris
import seaborn as sns
from sklearn.tree import DecisionTreeRegressor
import math
from sklearn.linear_model import LinearRegression
from sklearn.metrics import mean_absolute_error
import sklearn.metrics as metrics
```

It is good practice to import everything in the beginning of your code.

You initialize your "learner" or model with its properties, defined by the parameters, e.g.

[2]:
```
model = LinearRegression(fit_intercept = True)
model
```

[2]:
```
LinearRegression()
```

Before training them on actual data, they just contain information on the functional form of f. Once a learner has been trained we can examine the parameters of the resulting model. The empirical **risk** can be assessed after training by several performance measures (e.g., based on L2 loss). **Optimization** happens rather implicitly as sklearn only acts as a wrapper for existing implementations and calls package-specific optimization procedures.

b)

[6]:
```
        iris = load_iris() # function to import iris data set as type "utils.
↪Bunch" with sklearn
        X = iris.data
        y = iris.target
        feature_names = iris.feature_names
        target_names = iris.target_names
        print("Feature names:", feature_names)
        print("Target names:", target_names)
        print("\nShape of X and y\n", X.shape, y.shape)
        print("\nType of X and y\n", type(X), type(y))
```

```
Feature names: ['sepal length (cm)', 'sepal width (cm)', 'petal length (cm)',
'petal width (cm)']
Target names: ['setosa' 'versicolor' 'virginica']

Shape of X and y
(150, 4) (150,)

Type of X and y
<class 'numpy.ndarray'> <class 'numpy.ndarray'>
```

We obtain the following information:

- `iris` has categorical targets `['setosa' 'versicolor' 'virginica']`
- It has 150 observations of 5 variables, one of which is the target.
- both, X and y, are of type `'numpy.ndarray'`, thus numerical. The 3 classes in target y are stored as numbers 0, 1, 2.

c)

`sklearn` offers many different models. Let's look at **regression trees**:

Roughly speaking, regression trees create small, homogeneous subsets ("nodes") by repeatedly splitting the data at some cut-off (e.g., for iris: partition into observations with Sepal.Width ≤ 3 and > 3), and predict the mean target value within each final group.

[8]:
```
# help(DecisionTreeRegressor)
```

Prints documentary in console, or visit scikit-learn.org –> select right version –> go to right class, here sklearn.tree.DecisionTreeRegressor.

[9]:
```
rtree = DecisionTreeRegressor() #default setting
print(rtree.get_params())
print(rtree.get_depth()) # not working because no tree was fitted yet
print(rtree.get_n_leaves()) # not working because no tree was fitted yet
```

```
{'ccp_alpha': 0.0, 'criterion': 'squared_error', 'max_depth': None,
'max_features': None, 'max_leaf_nodes': None, 'min_impurity_decrease': 0.0,
'min_samples_leaf': 1, 'min_samples_split': 2, 'min_weight_fraction_leaf': 0.0,
'random_state': None, 'splitter': 'best'}
```

```
---------------------------------------------------------------------------
NotFittedError                            Traceback (most recent call last)
~\AppData\Local\Temp\ipykernel_16280\3357154144.py in <module>
      1 rtree = DecisionTreeRegressor() #default setting
      2 print(rtree.get_params())
----> 3 print(rtree.get_depth()) # not working because no tree was fitted yet
      4 print(rtree.get_n_leaves()) # not working because no tree was fitted yet

~\anaconda3\envs\I2ML_env\lib\site-packages\sklearn\tree\_classes.py in␣
 ↪get_depth(self)
    134             The maximum depth of the tree.
    135         """
```

```
--> 136         check_is_fitted(self)
    137         return self.tree_.max_depth
    138

~\anaconda3\envs\I2ML_env\lib\site-packages\sklearn\utils\validation.py in␣
 ↪check_is_fitted(estimator, attributes, msg, all_or_any)
   1220
   1221     if not fitted:
-> 1222         raise NotFittedError(msg % {"name": type(estimator).__name__})
   1223
   1224

NotFittedError: This DecisionTreeRegressor instance is not fitted yet. Call 'fit'␣
 ↪with appropriate arguments before using this estimator.
```

In general: DecisionTreeRegressor inherits from class sklearn.tree as it is used for regression, it predicts regression value for input X.

Important parameters
criteria: choose between L2, L1, and others as Loss function
splitter: strategy for choosing the split, default "best"
max-depth: The maximum depth of the tree other complexity related params
random_state: Controls the randomness of the estimator. To obtain a deterministic behaviour during fitting, random_state has to be fixed to an integer.

Solution 2: Loss Function for Regression Task

See R solution sheet.

Solution 3: Polynomial Regression

a)

See R solution sheet.

b)

Choose 3 different parameterizations and plot the resulting polynomials:

[7]:
```
x = np.linspace(-3,3, num = 60) # 3 included
```

[11]:
```
def fun_y(x_in):
"""
    Method to produce named sinus function
    Input: data as numpy array
    Output: Function -3 + 5*sin(0.4 * pi * x_in) as numpy array
    """
erg = -3 + 5* np.sin(0.4 * math.pi * x_in)
return erg

def fun_poly3(x_in, beta):
"""
```

```
        Method to produce poynomial degree 3 with coefficents in numpy array␣
↪beta for input data x_in
        Input: x_in as numpy array, beta as numpy array
        Output: function value as numpy array
        """
    erg = beta[0] + beta[1] * x_in + beta[2] * x_in*x_in + beta[3] *␣
↪x_in*x_in*x_in
    return erg
```

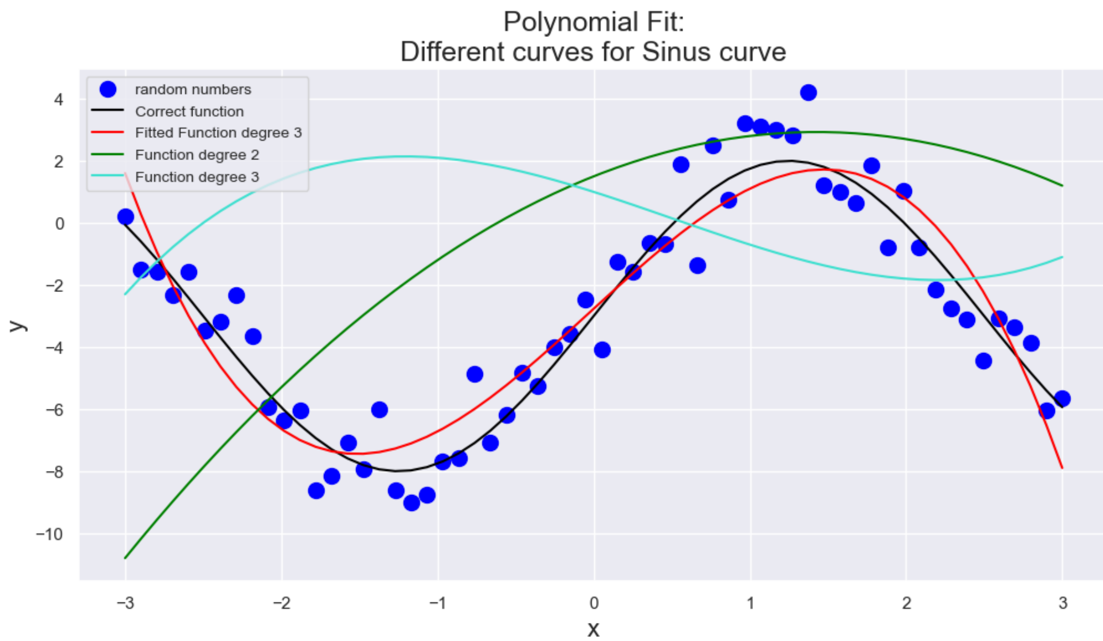
[12]:
```
    np.random.seed(43)
    y = fun_y(x) + np.random.normal(size = 60)
```

[13]:
```
    poly3d = np.poly1d(np.polyfit(x,y,3)) # Polyfit function for polynomial␣
↪functions
    print(np.polyfit(x,y,3)) # coefficients
```

```
[-0.68708783 -0.04208217  4.60056399 -2.76629061]
```

Create plot from mathplotlib.pyplot

[14]:
```
    plt.figure(figsize=(12, 6))
    plt.grid(True)
    plt.plot(x, y, color='blue', linestyle='none',marker='o',markersize=10,␣
↪label = 'random numbers')
    plt.plot(x, fun_y(x), color='black', linestyle='solid', label = 'Correct␣
↪function')
    plt.plot(x, poly3d(x), color='red', linestyle='solid', label = 'Fitted␣
↪Function degree 3')
    plt.plot(x, fun_poly3(x,np.array([1.5,2,-0.7,0])), color='green',␣
↪linestyle='solid', label = 'Function degree 2')
    plt.plot(x, fun_poly3(x,np.array([1,-1.6,-0.3,0.2])), color='turquoise',␣
↪linestyle='solid', label = 'Function degree 3')
    # title & label axes
    plt.title('Polynomial Fit:\nDifferent curves for Sinus curve', size=18)
    plt.xlabel('x', size=16)
    plt.ylabel('y', size=16)
    plt.legend(loc='upper left', prop={'size': 10})
    plt.show()
```



We see that our hypothesis space is simply a family of curves. The 3 examples plotted here already hint at the amount of flexibility third-degree polynomials offer over simple linear functions.

c, d, e, f)

See R solution sheet.

Solution 4: Predicting abalone

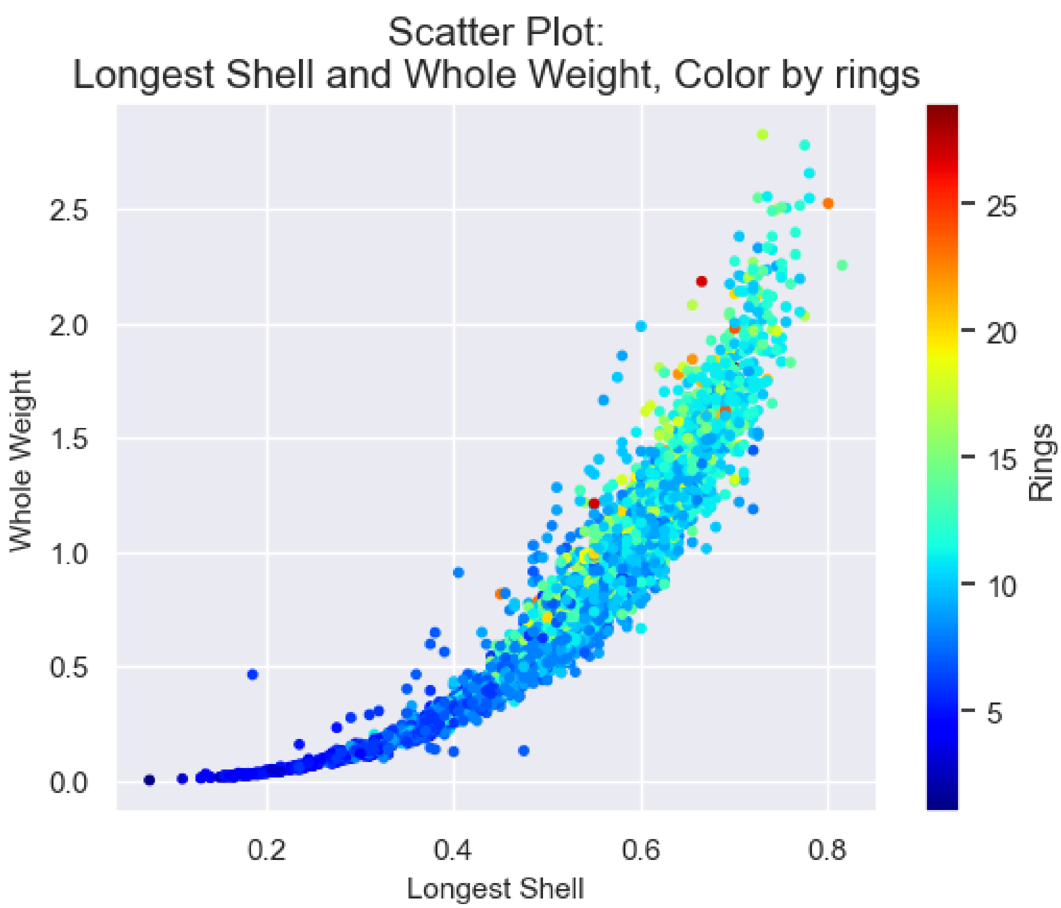
[15]:
```
# Exercise 4 Prep: load data from url

url = "https://archive.ics.uci.edu/ml/machine-learning-databases/abalone/abalone.
 ↪data"
abalone = pd.read_csv(url, sep=',', names=['sex', "longest_shell", "diameter",␣
 ↪"height", "whole_weight",
  "shucked_weight", "visceral_weight", "shell_weight", "rings"])

abalone = abalone[['longest_shell', 'whole_weight', 'rings']]
print(abalone.head)
```

```
<bound method NDFrame.head of       longest_shell  whole_weight  rings
0             0.455        0.5140     15
1             0.350        0.2255      7
2             0.530        0.6770      9
3             0.440        0.5160     10
4             0.330        0.2050      7
...             ...           ...    ...
4172          0.565        0.8870     11
4173          0.590        0.9660     10
4174          0.600        1.1760      9
```

```
4175           0.625        1.0945     10
4176           0.710        1.9485     12

[4177 rows x 3 columns]>
```

a)

```
[16]: plt.grid(True)
plt.scatter(abalone.longest_shell, abalone.whole_weight, s=10, c= abalone.rings,␣
 ↪cmap = 'jet') #choose appropriate color map
plt.colorbar(label = 'Rings') # add color bar
# title & label axes
plt.title('Scatter Plot:\nLongest Shell and Whole Weight, Color by rings',␣
 ↪size=15)
plt.xlabel('Longest Shell', size=11)
plt.ylabel('Whole Weight', size=11)
plt.show()
```



We see that weight scales exponentially with shell length and that larger/heavier animals tend to have more rings.

b)

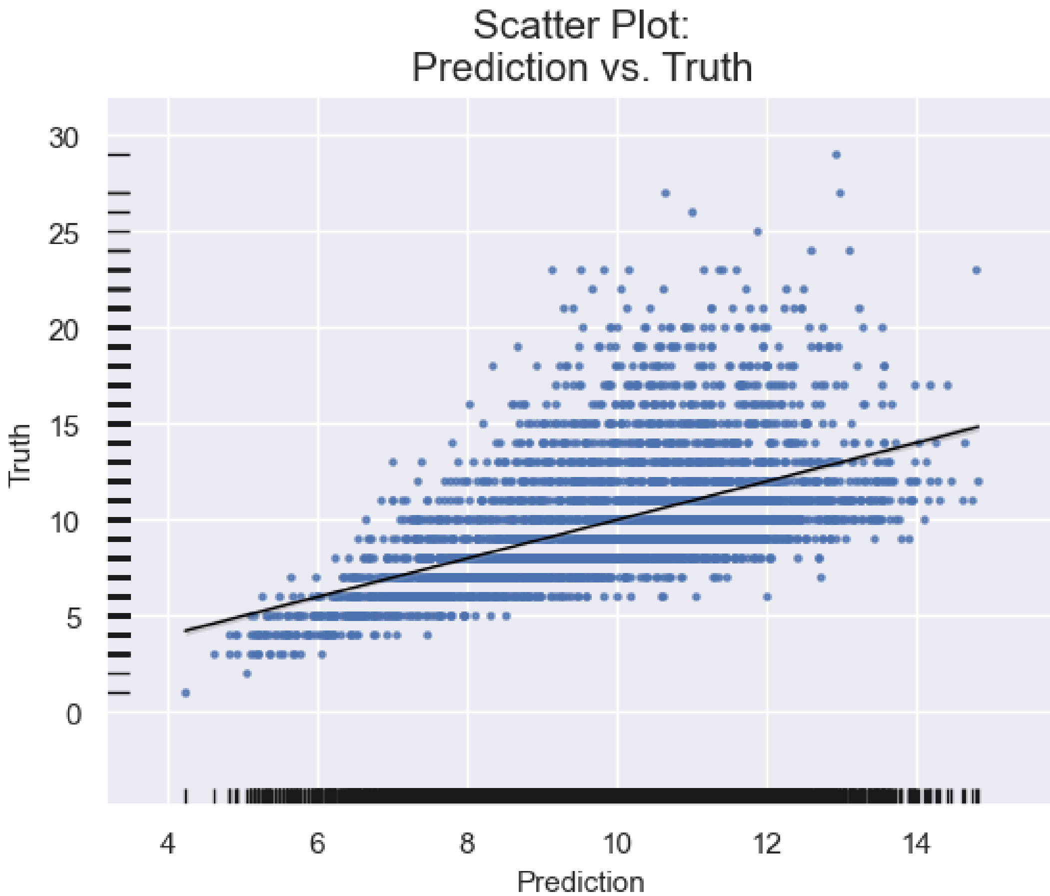
[17]:
```python
X_lm = abalone.iloc[:, 0:2].values
y_lm = abalone.rings

lm = LinearRegression().fit(X_lm,y_lm)

pred_lm = lm.predict(X_lm)

results_dic = {'prediction' : pred_lm,
            'truth': y_lm}

results = pd.DataFrame(results_dic)

results.head()
```

[17]:

	prediction	truth
0	8.840042	15
1	7.395659	7
2	9.821995	9
3	8.683616	10
4	7.160333	7

c)

[18]:
```python
plt.grid(True)
#plt.scatter(pred_lm, y_lm, s=5)
sns.regplot(x = pred_lm, y = y_lm, ci = 95, scatter_kws={'s':5}, 
 ↪line_kws={"color": "black", 'linewidth':1})
sns.rugplot(x = pred_lm, y = y_lm, height=0.025,  color='k')
# title & label axes
plt.title('Scatter Plot:\nPrediction vs. Truth', size=15)
plt.xlabel('Prediction', size=11)
plt.ylabel('Truth', size=11)
plt.show()
```



We see a scatterplot of prediction vs true values, where the small bars along the axes (a so-called rugplot) indicate the number of observations that fall into this area. As we might have suspected from the first plot, the underlying relationship is not exactly linear (ideally, all points and the resulting line should lie on the diagonal). With a linear model we tend to underestimate the response.

d)

[19]:
```
#import function from sklearn
MAE = mean_absolute_error(pred_lm, y_lm)
print(MAE)
```

```
1.9506602873468448
```

*) Additional model assessing

There exists no R type regression summary report in sklearn. The main reason is that sklearn is used for predictive modelling / machine learning and the evaluation criteria are based on performance on previously unseen data (such as predictive r^2 for regression).

For the statistical view on Linear Regression you can use the package

[20]:
```
import statsmodels.formula.api as smf
```

The function OLS performs Ordinary least square fit (Linear regression) and has a summary() function.
Nevertheless, self-defined functions can be used for assessing models from sklearn:

[21]:
```
def regression_results(y_true, y_pred):
    """
    Method to produce model metrics for training data
    Input: training response vector as array, prediction vector as array
    Output: -
    """
    # Regression metrics
    explained_variance=metrics.explained_variance_score(y_true, y_pred)
    mean_absolute_error=metrics.mean_absolute_error(y_true, y_pred)
    mse=metrics.mean_squared_error(y_true, y_pred)
    mean_squared_log_error=metrics.mean_squared_log_error(y_true, y_pred)
    median_absolute_error=metrics.median_absolute_error(y_true, y_pred)
    r2=metrics.r2_score(y_true, y_pred)

    print('explained_variance: ', round(explained_variance,4))
    print('mean_squared_log_error: ', round(mean_squared_log_error,4))
    print('r2: ', round(r2,4))
    print('MAE: ', round(mean_absolute_error,4))
    print('MSE: ', round(mse,4))
    print('RMSE: ', round(np.sqrt(mse),4))
    print('Median Absolut Error: ', round(median_absolute_error,4))
```

[22]:
```
regression_results(y_lm, pred_lm)
```

```
explained_variance:  0.3144
mean_squared_log_error:  0.0471
r2:  0.3144
MAE:  1.9507
MSE:  7.1255
RMSE:  2.6694
Median Absolut Error:  1.5254
```