Linear regression with sklearn API

The objective of this colab is to demonstrate how to build a linear regression model with `sklearn`. We will be using the following set up:

1. Dataset: California housing
2. Linear regression API: `LinearRegression`
3. Training: `fit` (normal equation) and `cross_validate` (normal equation with cross validation).
4. Evaluation: `score` (r2 score) and `cross_val_score` with different scoring parameters.

We will study the model dignosis with `LearningCurve` and learn how to examine the learned model or weight vector.

```
# Imports
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns

from sklearn.datasets import fetch_california_housing
from sklearn.linear_model import LinearRegression

from sklearn.model_selection import cross_validate
from sklearn.model_selection import cross_val_score
from sklearn.model_selection import learning_curve
from sklearn.model_selection import ShuffleSplit

from sklearn.metrics import mean_squared_error

from sklearn.pipeline import Pipeline
from sklearn.preprocessing import StandardScaler


np.random.seed(306)
plt.style.use('seaborn')
```

We will use `ShuffleSplit` cross validation with:

- 10 folds (`n_splits`) and
- set aside 20% examples as test examples (`test_size`).

```
shuffle_split_cv = ShuffleSplit(n_splits=10, test_size=0.2, random_state=0)
```

Creates 10 folds through shuffle split by keeping aside 20% examples as test in each fold.

STEP #1: Load the dataset

The first step is to load the dataset. We have already discussed how to load California housing dataset in the last colab demonstration.

```
features, labels = fetch_california_housing(as_frame=True, return_X_y=True)
```

The feature matrix is loaded in `features` dataframe and the labels in `labels` dataframe. Let's examine the shapes of these two dataframes.

```
print ("Shape of feature matrix:", features.shape)
print ("Shape of label vector:", labels.shape)
```

```
Shape of feature matrix: (20640, 8)
Shape of label vector: (20640,)
```

As a sanity check, make sure that the number of rows in feature matrix and labels match.

```
assert (features.shape[0] == labels.shape[0])
```

STEP #2. Data exploration

Data exploration has been covered in [california housing data exploration]() colab.

STEP #3. Preprocessing and model building

3.1 Train test split

The first step is to split the training data into training and test set. We do not access the test data till the end. All data exploration and tuning is performed on the training set and by setting aside a small portion of training as a dev or validation set.

The following code snippet divides the data into training and test sets.

```
from sklearn.model_selection import train_test_split
train_features, test_features, train_labels, test_labels = train_test_split(
    features, labels, random_state=42)
```

Let's examine shapes of training and test sets

```
print ("# trainings samples:", train_features.shape[0])
print ("# test samples:", test_features.shape[0])
```

```
# trainings samples: 15480
# test samples: 5160
```

It's time to perform another sanity check - here we check if the training feature matrix has the same number of rows as the training label vector. We perform the same check on the test set too.

```
assert (train_features.shape[0] == train_labels.shape[0])
assert (test_features.shape[0] == test_labels.shape[0])
```

3.2 Pipeline: preprocessing + model

As a first step, build linear regression models with default parameter setting of `LinearRegression` APIs.

> We will make use of `Pipeline` API for combining data preprocessing and model building.

We will use `StandardScaler` feature scaling to bring all features on the same scale followed by a `LinearRegression` model.

The `pipeline` object has two components:

1. `StandardScaler` as step 1
2. `LinearRegression` as step 2

After constructing the pipeline object, let's train it with training set.

```
# set up the linear regression model.
lin_reg_pipeline = Pipeline([("feature_scaling", StandardScaler()),
                             ("lin_reg", LinearRegression())])

# train linear regression model with normal equation.
lin_reg_pipeline.fit(train_features, train_labels)
```

```
Pipeline(steps=[('feature_scaling', StandardScaler()),
                ('lin_reg', LinearRegression())])
```

Now that we have trained the model, let's check the learnt/estimated weight vectors (`intercept_` and `coef_`).

```
print("intercept (w_0):", lin_reg_pipeline[-1].intercept_)
```

```
print("weight vector (w_1, ..., w_m):", lin_reg_pipeline[-1].coef_)
```

```
intercept (w_0): 2.0703489205426377
weight vector (w_1, ..., w_m): [ 0.85210815  0.12065533 -0.30210555  0.34860575 -0.06
 -0.89314697 -0.86784046]
```

A couple of things to notice:

- We accessed the `LinearRegression` object as `lin_reg_pipeline[-1]` which is the last step in the pipeline.
- The intercept can be obtained via `intercept_` member variable and
- The weight vector corresponding to features via `coef_`.

STEP #4. Model evaluation

`score`

Let's use `score` method to obtain train and test errors with twin objectives

> - Estimation of model performance as provided by test error.
> - Comparison of errors for model dignostic purpose (under/over/just right fit).

```
# evaluate model performance on the test set.
test_score = lin_reg_pipeline.score(test_features, test_labels)
print ("Model performance on test set: ", test_score)

train_score = lin_reg_pipeline.score(train_features, train_labels)
print ("Model performance on train set: ", train_score)
```

```
Model performance on test set:  0.5910509795491352
Model performance on train set:  0.609873031052925
```

The `score` method returns `r2` score whose best value is 1. The `r2` scores on training and test are comparable but they are not that high. It points to underfitting issue in model training.

Cross validated score (`cross_val_score`)

Since the `score` was computed on one fold that was selected as a test set, it may not be all that robust. In order to obtain robust estimate of the performance, we use `cross_val_score` that calculates `score` on different test folds through cross validation.

```
lin_reg_score = cross_val_score(lin_reg_pipeline,
```

```
                                   train_features,
                                   train_labels,
                                   scoring='neg_mean_squared_error',
                                   cv=shuffle_split_cv)

# This will return 10 different scores, one for
# each fold.
print (lin_reg_score)

# We can take mean and standard deviation of the
# score and report it.
print(f"\nScore of linear regression model on the test set:\n"
      f"{lin_reg_score.mean():.3f} +/- {lin_reg_score.std():.3f}")
```

```
[-0.50009976 -0.52183352 -0.55931218 -0.52110499 -0.56059203 -0.50510767
 -0.52386194 -0.54775518 -0.5007161  -0.54713448]

Score of linear regression model on the test set:
-0.529 +/- 0.022
```

Here we got the negative mean squared error as a score. We can convert that to error as follows:

```
lin_reg_mse = -lin_reg_score
print(f"MSE of linear regression model on the test set:\n"
      f"{lin_reg_mse.mean():.3f} +/- {lin_reg_mse.std():.3f}")
```

```
MSE of linear regression model on the test set:
0.529 +/- 0.022
```

We can use other `scoring` parameters and obtain cross validated scores based on that parameter. The following choices are available for `scoring`:

- `explained_variance`
- `max_error`
- `neg_mean_absolute_error`
- `neg_root_mean_squared_error`
- `neg_mean_squared_log_error`
- `neg_median_absolute_error`
- `neg_mean_absolute_percentage_error`
- `r2`

Cross validation

We just calculated `cross_val_score` based on the cross validation. It however returns only scores for each fold. What if we also need to access the models trained in each fold along with some other statistics like train error for that fold?

> `cross_validate` API enables us to obtain them.

```
lin_reg_cv_results = cross_validate(lin_reg_pipeline,
                                    train_features,
                                    train_labels,
                                    cv=shuffle_split_cv,
                                    scoring="neg_mean_squared_error",
                                    return_train_score=True,
                                    return_estimator=True)
```

The `lin_reg_cv_result` is a dictionary with the following contents:

- trained `estimators`,
- time taken for fitting (`fit_time`) and scoring (`score_time`) the models in cross validation,
- training score (`train_score`) and
- test scores (`test_score`)

Let's print the contents of the dictionary for us to examine.

```
lin_reg_cv_results
```

```
{'estimator': [Pipeline(steps=[('feature_scaling', StandardScaler()),
                 ('lin_reg', LinearRegression())]),
  Pipeline(steps=[('feature_scaling', StandardScaler()),
                 ('lin_reg', LinearRegression())]),
  Pipeline(steps=[('feature_scaling', StandardScaler()),
                 ('lin_reg', LinearRegression())]),
  Pipeline(steps=[('feature_scaling', StandardScaler()),
                 ('lin_reg', LinearRegression())]),
  Pipeline(steps=[('feature_scaling', StandardScaler()),
                 ('lin_reg', LinearRegression())]),
  Pipeline(steps=[('feature_scaling', StandardScaler()),
                 ('lin_reg', LinearRegression())]),
  Pipeline(steps=[('feature_scaling', StandardScaler()),
                 ('lin_reg', LinearRegression())]),
  Pipeline(steps=[('feature_scaling', StandardScaler()),
                 ('lin_reg', LinearRegression())]),
  Pipeline(steps=[('feature_scaling', StandardScaler()),
                 ('lin_reg', LinearRegression())]),
  Pipeline(steps=[('feature_scaling', StandardScaler()),
                 ('lin_reg', LinearRegression())])],
 'fit_time': array([0.03175783, 0.03753352, 0.04121518, 0.03762102, 0.02221799,
        0.02387691, 0.0383749 , 0.0338521 , 0.03492212, 0.04238749]),
 'score_time': array([0.00707507, 0.00852728, 0.01298165, 0.01271415, 0.00511885,
        0.01690269, 0.01000237, 0.00870967, 0.00879359, 0.00915956]),
 'test_score': array([-0.50009976, -0.52183352, -0.55931218, -0.52110499,
-0.56059203,
        -0.50510767, -0.52386194, -0.54775518, -0.5007161 , -0.54713448]),
 'train_score': array([-0.52578695, -0.52035137, -0.51095597, -0.52049611,
-0.51060835,
        -0.52453922, -0.51994311, -0.5144039 , -0.52578473, -0.51397105])}
```

There are 10 values in each dictionary key. That is because of `cv=10` or 10-fold cross validation that we used.

We compare training and test errors to assess generalization performance of our model. However we have training and test scores in the `cv_results` dictionary.

> Multiply these scores by -1 and convert them to errors.

```
train_error = -1 * lin_reg_cv_results['train_score']
test_error = -1 * lin_reg_cv_results['test_score']

print(f"Mean squared error of linear regression model on the train set:\n"
      f"{train_error.mean():.3f} +/- {train_error.std():.3f}")
print(f"Mean squared error of linear regression model on the test set:\n"
      f"{test_error.mean():.3f} +/- {test_error.std():.3f}")
```

```
Mean squared error of linear regression model on the train set:
0.519 +/- 0.006
Mean squared error of linear regression model on the test set:
0.529 +/- 0.022
```

- The training and test errors are high, which is an indication of underfitting, which we will confirm by plotting the learning curves.
- Test error has higher variability across different folds compared to the train error.

Effect of training set size on error

Let's understand how the training set size or #samples affect the error. We can use `learning_curve` API that calculates cross validation scores for different #samples as specified in its argument `train_sizes`.

[Plot learning curves]

```
#@title [Plot learning curves]
def plot_learning_curve(train_sizes, train_scores, test_scores):


  train_scores_mean = np.mean(-train_scores, axis=1)
  train_scores_std = np.std(-train_scores, axis=1)
  test_scores_mean = np.mean(-test_scores, axis=1)
  test_scores_std = np.std(-test_scores, axis=1)
  fit_times_mean = np.mean(fit_times, axis=1)
  fit_times_std = np.std(fit_times, axis=1)

  plt.fill_between(
      train_sizes,
      train_scores_mean - train_scores_std,
      train_scores_mean + train_scores_std,
      alpha=0.1,
      color="r",)
  plt.fill_between(
      train_sizes,
```

```
      train_sizes,
      test_scores_mean - test_scores_std,
      test_scores_mean + test_scores_std,
      alpha=0.1,
      color="g",)
  plt.plot(train_sizes, train_scores_mean, "o-", color="r", label="T
  plt.plot(train_sizes, test_scores_mean, "o-", color="g", label="Cr
  plt.xlabel("Training examples")
  plt.ylabel("MSE")
  plt.legend(loc="best")

def plot_scalability_curve(train_sizes, fit_times):
  fit_times_mean = np.mean(fit_times, axis=1)
  fit_times_std = np.std(fit_times, axis=1)

  plt.fill_between(
      train_sizes,
      fit_times_mean - fit_times_std,
      fit_times_mean + fit_times_std,
      alpha=0.1,)
  plt.plot(train_sizes, fit_times_mean, "o-")
  plt.xlabel("Training examples")
  plt.ylabel("Fit time")
  plt.title("Scalability of the model")
```

Based on the scores calculated by `learning_curve` API, we plot the error and its standard deviation for different #samples.

```
  (train_sizes, train_scores, test_scores, fit_times, score_times) = \
    learning_curve(
      lin_reg_pipeline, train_features, train_labels, cv=shuffle_split_cv,
      scoring='neg_mean_squared_error', n_jobs=-1,
      return_times=True, train_sizes=np.linspace(0.2, 1.0, 10))

plot_learning_curve(train_sizes, train_scores, test_scores)
```

Observe that

- Both curves have reached a plateau; they are close and fairly high.
- Few instances in the training set means the model can fit them perfectly. But as more instances are added to the training set, it becomes impossible for the model to fit the training data perfectly.
- When the model is trained on very few training instances, it is not able of generalizing properly, which is why the validation error is initially quite high. Then as the model learns on more training examples, the training and validation error reduce slowly.

These learning curves are typical of an underfitting model.

We can also study how model training scales as the function of number of training samples.

```
plot_scalability_curve(train_sizes, fit_times)
```

As the number of training examples grows, the time to fit also increases.

Model examination

Let's examine the weight vectors and how much variability exists between them across different cross-validated models.

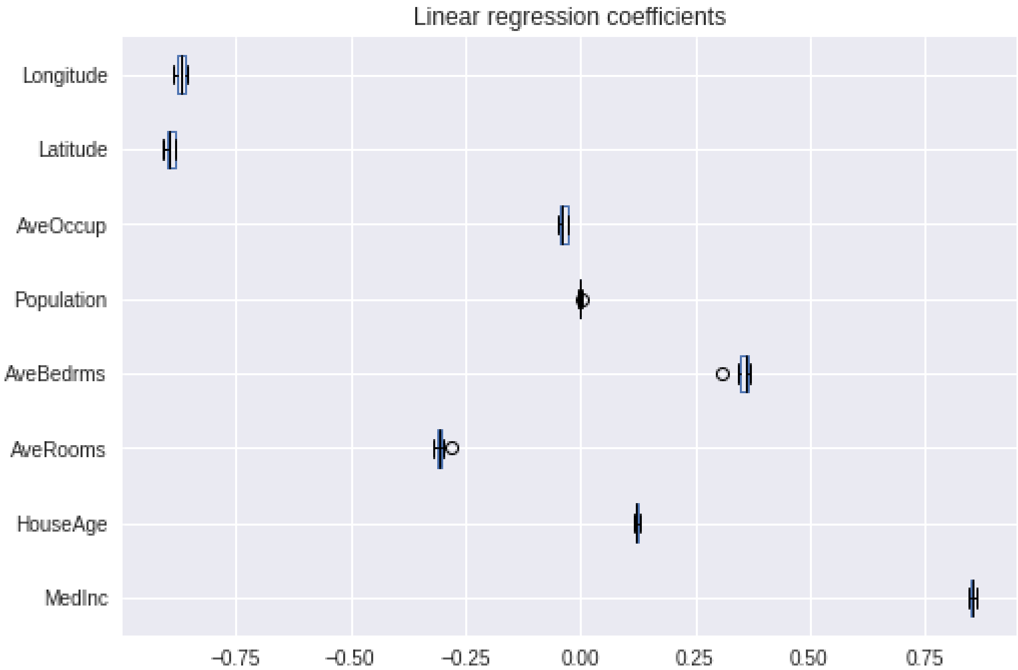
```
feature_names = train_features.columns
feature_names
```

```
Index(['MedInc', 'HouseAge', 'AveRooms', 'AveBedrms', 'Population', 'AveOccup',
       'Latitude', 'Longitude'],
      dtype='object')
```

For this, we will first construct a dataframe of weight vectors and then plot them with `box` plot.

```
coefs = [est[-1].coef_ for est in lin_reg_cv_results["estimator"]]
weights_df = pd.DataFrame(coefs, columns=feature_names)

color = {"whiskers": "black", "medians": "black", "caps": "black"}
weights_df.plot.box(color=color, vert=False) #, figsize=(6, 16))
_ = plt.title("Linear regression coefficients")
```



There is not much variability in weights learned by different models. It can also by standard deviation of weights as seen in `std` row below:

```
weights_df.describe()
```

	MedInc	HouseAge	AveRooms	AveBedrms	Population	AveOccup	Latitude	L
std	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	
50%	0.852711	0.121592	-0.305795	0.360139	-0.002063	-0.042325	-0.895370	-
max	0.861659	0.130560	-0.278426	0.367952	0.005297	-0.026331	-0.881884	-

Selecting best model

Let's select the model with the lowest cross validated test error as the best performing model.

```
# Let's find out the best model that resulted in the least test error.
best_model_index = np.argmin(test_error)
selected_model = lin_reg_cv_results['estimator'][best_model_index]
```

Let's examine the model coefficients.

```
print ("Intercept (w_0): ", selected_model['lin_reg'].intercept_)
print ("Coefficients (w_1, ..., w_m): ", selected_model['lin_reg'].coef_)
```

```
Intercept (w_0):  2.0779898917958657
Coefficients (w_1, ..., w_m):  [ 8.44324888e-01  1.18463901e-01 -3.04619574e-01  3.56
  1.74458509e-04 -4.23964612e-02 -8.96045642e-01 -8.68906479e-01]
```

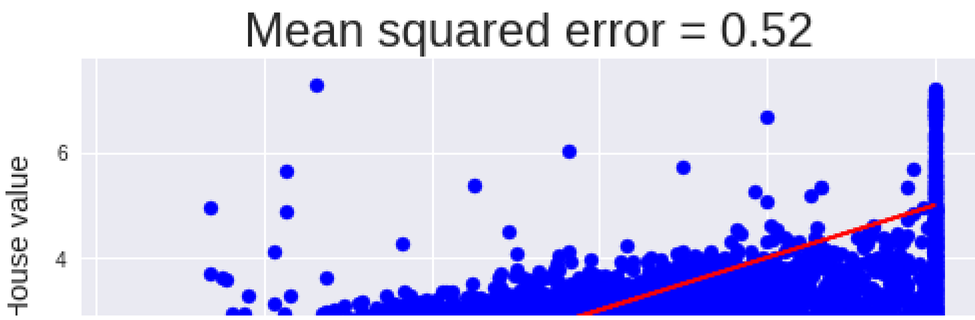
Model performance

Towards this, let's first obtain the predictions for test points in cross validation.

```
from sklearn.model_selection import cross_val_predict
cv_predictions = cross_val_predict(lin_reg_pipeline, train_features, train_labels)
```

```
mse_cv = mean_squared_error(train_labels, cv_predictions)

plt.scatter(train_labels, cv_predictions, color='blue')
plt.plot(train_labels, train_labels, 'r-')
plt.title(f"Mean squared error = {mse_cv:.2f}", size=24)
plt.xlabel('Actual Median House value', size=15)
plt.ylabel('Predicted Median House value',size=15)
plt.show()
```



- The model seems to all over the place in its predictions for examples with label 5.
- There are some negative predictions. We can fix this by adding a constraints on the weights to be positive.

At this stage, we should perform error analysis and check where the predictions are going wrong. We can revisit feature construction, preprocessing or model stages and make the necessary course corrections to get better performance.

Step #5: Predictions

We can use the best performing model from cross validation for getting predictions on the test set.

```
test_predictions_cv = selected_model.predict(test_features)
test_predictions_cv[:5]
```

```
array([0.73548515, 1.7725621 , 2.70011199, 2.83716602, 2.60743151])
```

We can also obtain predictions using the initial model that we built without cross validation.

```
test_predictions = lin_reg_pipeline.predict(test_features)
test_predictions[:5]
```

```
array([0.72412832, 1.76677807, 2.71151581, 2.83601179, 2.603755  ])
```

Step 6: Report model performance

We report model performance on the test set.

```
score_cv = selected_model.score(test_features, test_labels)
score = lin_reg_pipeline.score(test_features, test_labels)

print ("R2 score for the best model obtained via cross validation: ", score_cv)
print ("R2 score for model without cv: ", score)
```

```
R2 score for the best model obtained via cross validation:  0.5923577635319088
R2 score for model without cv:  0.5910509795491352
```

Alternatively we can use any other metric of interest and report performance based on that. For example, the mean squared error is as follows:

```
mse = mean_squared_error(test_labels, test_predictions)
mse_cv = mean_squared_error(test_labels, test_predictions_cv)

print ("MSE for the best model obtained via cross validation: ", mse_cv)
print ("MSE for model without cv: ", mse)
```

```
MSE for the best model obtained via cross validation:  0.5393995876218523
MSE for model without cv:  0.5411287478470688
```

The cross validation based model has slightly lower MSE than the other model and hence better performance.

Exercise:

1. Change the scoring scheme to other scoring metrics provided in `sklearn` metrics and compare results across different metrics.
2. Repeat the modeling steps with `SGDRegressor`.