In [ ]:

```

```

In [ ]:

```

```

Fit kNN in Python Using scikit-learn

```
While coding an algorithm from scratch is great for learning purposes, it’s usually not very practical when working on a machine learning task.
In this section, you’ll explore the implementation of the kNN algorithm used in scikit-learn, one of the most comprehensive machine learning packages in Python.
```

Splitting Data Into Training and Test Sets for Model Evaluation

```
In this section, you’ll evaluate the quality of your abalone kNN model. In the previous sections, you had a technical focus, but you’re now going to have a more pragmatic and results-oriented point of view.
```

```
There are multiple ways of evaluating models, but the most common one is the train-test split. When using a train-test split for model evaluation, you split the dataset into two parts:

1- Training data is used to fit the model. For kNN, this means that the training data will be used as neighbors.
2- Test data is used to evaluate the model. It means that you’ll make predictions for the number of rings of each of the abalones in the test data and compare those results to the known true number of rings.
```

In [20]:

```python
# You can split the data into training and test sets in Python using scikit-learn’s bui
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=0.2, random_state=12345
)
```

```
The test_size refers to the number of observations that you want to put in the training data and the test data.
If you specify a test_size of 0.2, your test_size will be 20 percent of the original data, therefore leaving the other 80 percent as training data.

The random_state is a parameter that allows you to obtain the same results every time the code is run.
train_test_split() makes a random split in the data, which is problematic for reproducing the results.
Therefore, it’s common to use random_state. The choice of value in random_state is arbitrary.

In the above code, you separate the data into training and test data.
This is needed for objective model evaluation.
You can now proceed to fit a kNN model on the training data using scikit-learn.
```

Fitting a kNN Regression in scikit-learn to the Abalone Dataset

```
To fit a model from scikit-learn, you start by creating a model of the correct class.
At this point, you also need to choose the values for your hyperparameters.
For the kNN algorithm, you need to choose the value for k, which is called n_neighbors in the scikit-learn implementation. Here’s how you can do this in Python:
```

In [21]:

```python
from sklearn.neighbors import KNeighborsRegressor
knn_model = KNeighborsRegressor(n_neighbors=3)
```

```
You create an unfitted model with knn_model.
This model will use the three nearest neighbors to predict the value of a future data point.
To get the data into the model, you can then fit the model on the training dataset:
```

In [22]:

```python
knn_model.fit(X_train, y_train)
```

Out[22]:

```
KNeighborsRegressor(n_neighbors=3)
```

```
Using .fit(), you let the model learn from the data.
At this point, knn_model contains everything that’s needed to make predictions on new abalone data points.
That’s all the code you need for fitting a kNN regression using Python!
```

Using scikit-learn to Inspect Model Fit

Fitting a model, however, isn’t enough.

In this section, you’ll look at some functions that you can use to evaluate the fit.

There are many evaluation metrics available for regression, but you’ll use one of the most common ones, the root-mean-square error (RMSE). The RMSE of a prediction is computed as follows:

1- Compute the difference between each data point’s actual value and predicted value.

2- For each difference, take the square of this difference.

3- Sum all the squared differences.

4- Take the square root of the summed value.

```
To start, you can evaluate the prediction error on the training data.
This means that you use the training data for prediction, so you know that the result should be relatively good.
You can use the following code to obtain the RMSE:
```

In [23]:

```
from sklearn.metrics import mean_squared_error
from math import sqrt
train_preds = knn_model.predict(X_train)
mse = mean_squared_error(y_train, train_preds)
rmse = sqrt(mse)
print(rmse)
```

```
1.653705966446084
```

In this code, you compute the RMSE using the knn_model that you fitted in the previous code block.

You compute the RMSE on the training data for now. For a more realistic result, you should evaluate the performances on data that aren’t included in the model.

This is why you kept the test set separate for now.

You can evaluate the predictive performances on the test set with the same function as before:

In [24]:

```
test_preds = knn_model.predict(X_test)
mse = mean_squared_error(y_test, test_preds)
rmse = sqrt(mse)
print(rmse)
```

```
2.375417924000521
```

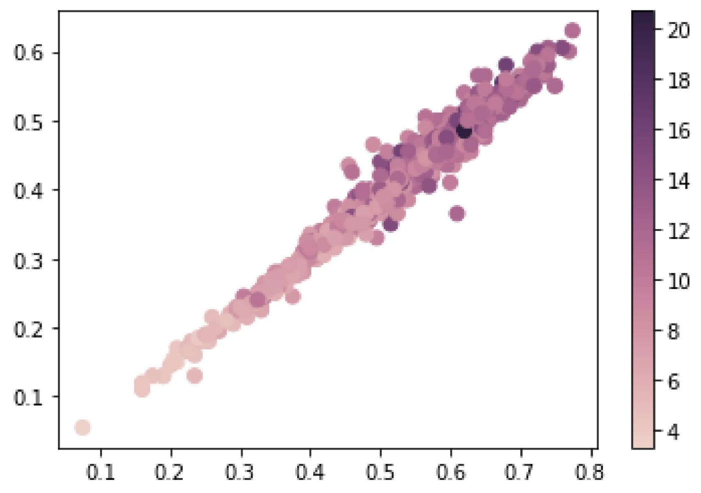
```
In this code block, you evaluate the error on data that wasn’t yet known by the model. This more-realistic RMSE is slightly higher than before. The RMSE measures the average error of the predicted age, so you can interpret this as having, on average, an error of 1.65 years. Whether an improvement from 2.37 years to 1.65 years is good is case specific. At least you’re getting closer to correctly estimating the age.

Until now, you’ve only used the scikit-learn kNN algorithm out of the box. You haven’t yet done any tuning of hyperparameters and a random choice for k. You can observe a relatively large difference between the RMSE on the training data and the RMSE on the test data. This means that the model suffers from overfitting on the training data: It does not generalize well.

This is nothing to worry about at this point. In the next part, you’ll see how to optimize the prediction error or test error using various tuning methods.
```

Plotting the Fit of Your Model

```
A last thing to look at before starting to improve the model is the actual fit of your model.
To understand what the model has learned, you can visualize how your predictions have been made using Matplotlib:
```

In [25]:

```python
import seaborn as sns
cmap = sns.cubehelix_palette(as_cmap=True)
f, ax = plt.subplots()
points = ax.scatter(
    X_test[:, 0], X_test[:, 1], c=test_preds, s=50, cmap=cmap
)
f.colorbar(points)
plt.show()
```



In this code block, you use Seaborn to create a scatter plot of the first and second columns of X_test by subsetting the arrays X_test[:,0] and X_test[:,1].

Remember from before that the first two columns are Length and Diameter.

They are strongly correlated, as you've seen in the correlations table.

You use c to specify that the predicted values (test_preds) should be used as a colorbar.

The argument s is used to specify the size of the points in the scatter plot.

You use cmap to specify the cubehelix_palette color map.

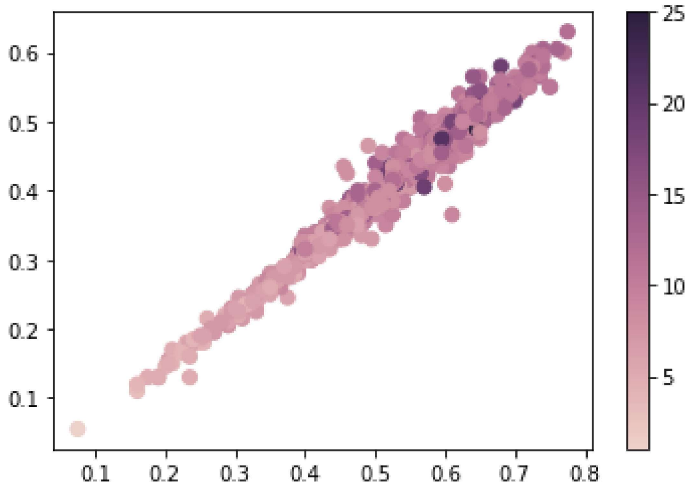
To learn more about plotting with Matplotlib, check out Python Plotting With Matplotlib.

```
On this graph, each point is an abalone from the test set, with its actual length and
actual diameter on the X- and Y-axis, respectively. The color of the point reflects
the predicted age.
You can see that the longer and larger an abalone is, the higher its predicted age.
This is logical, and it's a positive sign.
It means that your model is learning something that seems correct.
```

To confirm whether this trend exists in actual abalone data, you can do the same for the actual values by simply replacing the variable that is used for c:

In [26]:

```python
cmap = sns.cubehelix_palette(as_cmap=True)
f, ax = plt.subplots()
points = ax.scatter(
    X_test[:, 0], X_test[:, 1], c=y_test, s=50, cmap=cmap
)
f.colorbar(points)
plt.show()

# This code uses Seaborn to create a scatterplot with a colorbar. It produces the follo
```



```
This confirms that the trend your model is learning does indeed make sense.

You could extract a visualization for each combination of the seven independent variables.
For this tutorial, that would be too long, but don’t hesitate to try it out.
The only thing to change is the columns that are specified in the scatter.

These visualizations are two-dimensional views of a seven-dimensional dataset.
If you play around with them, it will give you a great understanding of what the model is learning and, maybe, what it’s not learning or is learning wrong.
```

Tune and Optimize kNN in Python Using scikit-learn

```
There are numerous ways you can improve your predictive score.
Some improvements could be made by working on the input data using data wrangling, but in this tutorial, the focus is on the kNN algorithm.
Next, you’ll look at ways to improve the algorithm part of the modeling pipeline.
```

Improving kNN Performances in scikit-learn Using GridSearchCV

Until now, you’ve always worked with k=3 in the kNN algorithm, but the best value for k is something that you need to find empirically for each dataset.

```
When you use few neighbors, you have a prediction that will be much more variable than when you use more neighbors:

```

```
* If you use one neighbor only, the prediction can strongly change from one point to the other.
When you think about your own neighbors, one may be quite different from the others.
If you lived next to an outlier, your 1-NN prediction would be wrong.

* If you have multiple data points, the impact of one extremely different neighbor will be much less.

* If you use too many neighbors, the prediction of each point risks being very close.
Let’s say that you use all neighbors for a prediction.
In that case, every prediction would be the same.
```

```
To find the best value for k, you’re going to use a tool called GridSearchCV.
This is a tool that is often used for tuning hyperparameters of machine learning models.
In your case, it will help by automatically finding the best value of k for your dataset.
```

GridSearchCV is available in scikit-learn, and it has the benefit of being used in almost the exact same way as the scikit-learn models:

In [27]:

```python
from sklearn.model_selection import GridSearchCV
parameters = {"n_neighbors": range(1, 50)}
gridsearch = GridSearchCV(KNeighborsRegressor(), parameters)
gridsearch.fit(X_train, y_train)
```

Out[27]:

```
GridSearchCV(estimator=KNeighborsRegressor(),
             param_grid={'n_neighbors': range(1, 50)})
```

```
Here, you use GridSearchCV to fit the model.
In short, GridSearchCV repeatedly fits kNN regressors on a part of the data and tests the performances on the remaining part of the data.
Doing this repeatedly will yield a reliable estimate of the predictive performance of each of the values for k.
In this example, you test the values from 1 to 50.
```

In the end, it will retain the best performing value of k, which you can access with .best_params_:

In [28]:

```python
gridsearch.best_params_
```

Out[28]:

```
{'n_neighbors': 25}
```

In this code, you print the parameters that have the lowest error score.

With .best_params_, you can see that choosing 25 as value for k will yield the best predictive performance

```
Now that you know what the best value of k is, you can see how it affects your train and test performances:
```

In [29]:

```
train_preds_grid = gridsearch.predict(X_train)
train_mse = mean_squared_error(y_train, train_preds_grid)
train_rmse = sqrt(train_mse)
test_preds_grid = gridsearch.predict(X_test)
test_mse = mean_squared_error(y_test, test_preds_grid)
test_rmse = sqrt(test_mse)
print(train_rmse)

print(test_rmse)
```

```
2.0731180327543384
2.1700197339962175
```

```
With this code, you fit the model on the training data and evaluate the test data.
You can see that the training error is worse than before, but the test error is better than before.
This means that your model fits less closely to the training data.
Using GridSearchCV to find a value for k has reduced the problem of overfitting on the training data.
```

Adding Weighted Average of Neighbors Based on Distance

```
Using GridSearchCV, you reduced the test RMSE from 2.37 to 2.17.
In this section, you’ll see how to improve the performances even more.

Below, you’ll test whether the performance of your model will be any better when predicting using a weighted average instead of a regular average.
This means that neighbors that are further away will less strongly influence the prediction.
```

You can do this by setting the weights hyperparameter to the value of "distance".

However, setting this weighted average could have an impact on the optimal value of k.

Therefore, you’ll again use GridSearchCV to tell you which type of averaging you should use:

In [30]:

```
parameters = {
    "n_neighbors": range(1, 50),
    "weights": ["uniform", "distance"],
}
gridsearch = GridSearchCV(KNeighborsRegressor(), parameters)
gridsearch.fit(X_train, y_train)



gridsearch.best_params_

test_preds_grid = gridsearch.predict(X_test)
test_mse = mean_squared_error(y_test, test_preds_grid)
test_rmse = sqrt(test_mse)
print(test_rmse)
```

```
2.1634265584947485
```

Here, you test whether it makes sense to use a different weighing using your GridSearchCV.

Applying a weighted average rather than a regular average has reduced the prediction error from 2.17 to 2.1634.

Although this isn't a huge improvement, it's still better, which makes it worth it.

Further Improving on kNN in scikit-learn With Bagging

```
As a third step for kNN tuning, you can use bagging. Bagging is an ensemble method, or a method that takes a relatively straightforward machine learning model and fits a large number of those models with slight variations in each fit.
Bagging often uses decision trees, but kNN works perfectly as well.

Ensemble methods are often more performant than single models. One model can be wrong from time to time, but the average of a hundred models should be wrong less often. The errors of different individual models are likely to average each other out, and the resulting prediction will be less variable.
```

You can use scikit-learn to apply bagging to your kNN regression using the following steps.

First, create the KNeighborsRegressor with the best choices for k and weights that you got from GridSearchCV:

In [41]:

```
best_k = gridsearch.best_params_["n_neighbors"]
best_weights = gridsearch.best_params_["weights"]
bagged_knn = KNeighborsRegressor(n_neighbors=best_k, weights=best_weights)
```

Then import the BaggingRegressor class from scikit-learn and create a new instance with 100 estimators using the bagged_knn model:

In [54]:

```
from sklearn.ensemble import BaggingRegressor
bagging_model = BaggingRegressor(bagged_knn, n_estimators=100)
bagging_model.fit(X_train, y_train)
```

Out[54]:

```
BaggingRegressor(base_estimator=KNeighborsRegressor(n_neighbors=25,
                                                    weights='distance'),
                 n_estimators=100)
```

In [55]:

```
# Now you can make a prediction and calculate the RMSE to see if it improved:
test_preds_grid = bagging_model.predict(X_test)
test_mse = mean_squared_error(y_test, test_preds_grid)
test_rmse = sqrt(test_mse)
test_rmse
```

Out[55]:

```
2.164753415586377
```

The prediction error on the bagged kNN is 2.1616, which is slightly smaller than the previous error that you obtained. It does take a little more time to execute, but for this example, that’s not problematic.

In [ ]:

```

```