demo-generic-pipeline

February 19, 2018

1 Demo: Generic Supervised Machine Learning Pipeline

This Jupyter notebook implements and explains the end-to-end machine learning pipeline discussed in Chapter 2 of the following the book:

Hands-On Machine Learning with Scikit-Learn and TensorFlow, Aurélien Géron, O'Reilly, 2017 (http://shop.oreilly.com/product/0636920052289.do)

For more information on the book above, or the Python code provided by the author, see: https://github.com/ageron/handson-ml

This pipeline contains an embedded (publicly downloadable) data set of California housing data. The embedded data set contains 1990 median house values of California census block groups, and other information about these census block groups. This pipeline performs the following:

(1) some basic diagnostics on the embedded data set,

(2) randomly split the data set into training and testing sets,

(3) perform some basic visualization on the training set,

(4) train four regression models based on the training set so as to predict the median house value based on the rest of the variables.

The first three regression models are linear regression, regression trees and random forests as implemented in the Python library Scikit-Learn with default (hyper)parameters (hence no hyperparameter tuning). The last regression model is random forests with hyperparameters specified in a certain "grid" of prescribed hyperparameter configurations, where the hyperparameter tuning is carried out using 10-fold cross validation.

1.1 Set up the pipeline environment

More specifically:

(1) Load required Python modules and classes.

(2) Define paths to the code and data directories.

```
In [28]: # import required modules and classes

         import os, sys, shutil, getpass
```

```
import pprint, logging, datetime
import stat

import numpy   as np
import pandas  as pd
import seaborn as sns
```

In [29]:
```
# Define path of the parent folder of this jupyter notebook, and the code and data dire
# The code directory contains Python source code for custom-built Python modules, which
# The data directory contains the data we will use to demonstrate this supervised machi

dir_MASTER = ".."
dir_code   = os.path.join(dir_MASTER, "code")
dir_data   = os.path.join(dir_MASTER, "data")
```

In [30]:
```
# check dir_code has been set correctly, by displaying the Python source code files it

print(os.listdir(dir_code))
```

```
['__init__.py', '__pycache__', 'examineData.py', 'PipelinePreprocessHousingData.py', 'splitTrain
```

1.2 The embedded data set: California 1990 "census block group" housing data

The data set we use is downloadable from the Internet:
https://github.com/ageron/handson-ml/tree/master/datasets/housing
https://www.kaggle.com/camnugent/california-housing-prices

It is a table with 10 columns and 20640 rows. Each row corresponds to a 1990 California census block group. One of the variables is median_house_value, which we will use as the response variable for the regression exercise below. The rest of the variables contain information about the census block groups, for example, geo-coordinates (longitude, latitude), population size, median income, etc. These will be used as predictor variables (features) in the regression exercise below. For more information about the embedded data set, refer to the two web pages cited above.

Basic diagnostics on the full data set

In [31]:
```
# Load California housing data into the data frame housingDF.

housingFILE = os.path.join(dir_data,'housing.csv')
housingDF   = pd.read_csv(housingFILE);
```

In [32]:
```
# Basic info on housingDF: number of rows and name and data type of each column.

housingDF.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 20640 entries, 0 to 20639
Data columns (total 10 columns):
longitude             20640 non-null float64
```

```
latitude              20640 non-null float64
housing_median_age    20640 non-null float64
total_rooms           20640 non-null float64
total_bedrooms        20433 non-null float64
population            20640 non-null float64
households            20640 non-null float64
median_income         20640 non-null float64
median_house_value    20640 non-null float64
ocean_proximity       20640 non-null object
dtypes: float64(9), object(1)
memory usage: 1.6+ MB
```

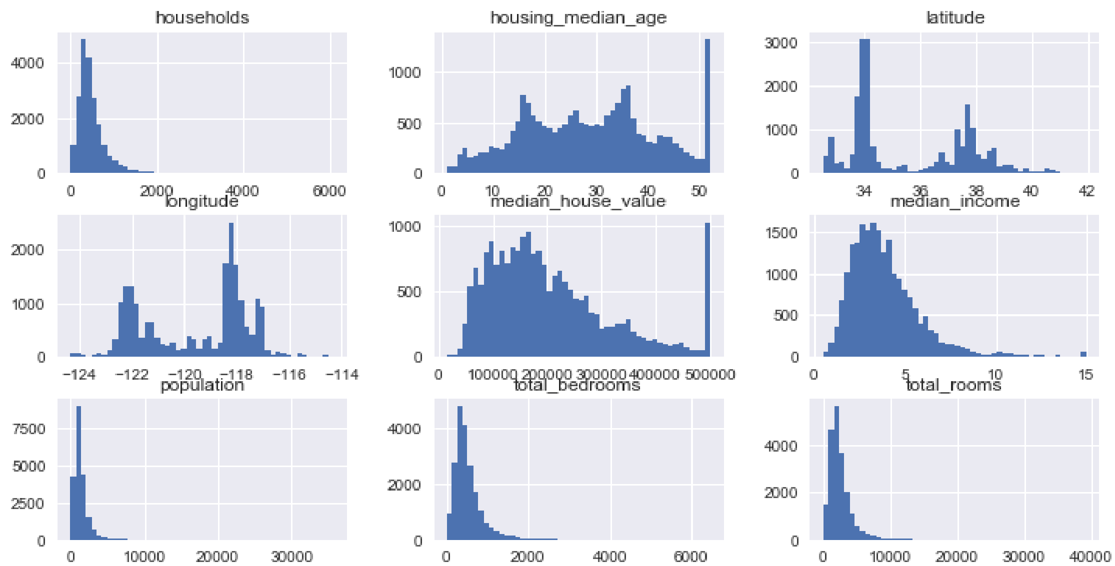
In [33]:
```python
# View the first several rows of housingDF.

housingDF.head()
```

Out[33]:

	longitude	latitude	housing_median_age	total_rooms	total_bedrooms	\
0	-122.23	37.88	41.0	880.0	129.0	
1	-122.22	37.86	21.0	7099.0	1106.0	
2	-122.24	37.85	52.0	1467.0	190.0	
3	-122.25	37.85	52.0	1274.0	235.0	
4	-122.25	37.85	52.0	1627.0	280.0	

	population	households	median_income	median_house_value	ocean_proximity
0	322.0	126.0	8.3252	452600.0	NEAR BAY
1	2401.0	1138.0	8.3014	358500.0	NEAR BAY
2	496.0	177.0	7.2574	352100.0	NEAR BAY
3	558.0	219.0	5.6431	341300.0	NEAR BAY
4	565.0	259.0	3.8462	342200.0	NEAR BAY

In [34]:
```python
# histograms on the nine continuous variables

import matplotlib.pyplot as plt
myHistogram = housingDF.hist(bins = 50, figsize = (12,6))
plt.show()
```



1.3 Split the full data set into training and testing sets.

In [35]:
```
# First, we add the code directory to the Python system path.
# (so that Python knows where to look for the source code of the custom built Python mo

sys.path.append(dir_code)
```

In [36]:
```
# Next, we import the function splitTrainTest() from the custom built Python module spl
# We then split the full data set, housingDF, into training and testing sets using spli
# Note that the splitting is done in a stratified manner.
# The stratification is based income category (a derived variable from median_income).
# The splitting is required to preserve the distribution of income category.

from splitTrainTest import splitTrainTest
trainSet, testSet = splitTrainTest(inputDF = housingDF, random_state = 19)
```

```
income category relative sizes (whole data set)
3.0    0.350581
2.0    0.318847
4.0    0.176308
5.0    0.114438
1.0    0.039826
Name: income_category, dtype: float64
```

In [37]:
```
# Check the shapes of the training and testing data sets, and compare those with the or
# Note that the number of variables of housingDF is now 11 (instead of 10 as above)
# because, during the splitting process, we added the derived variable of income catego
```

```python
print(housingDF.shape)
print(trainSet.shape)
print(testSet.shape)
```

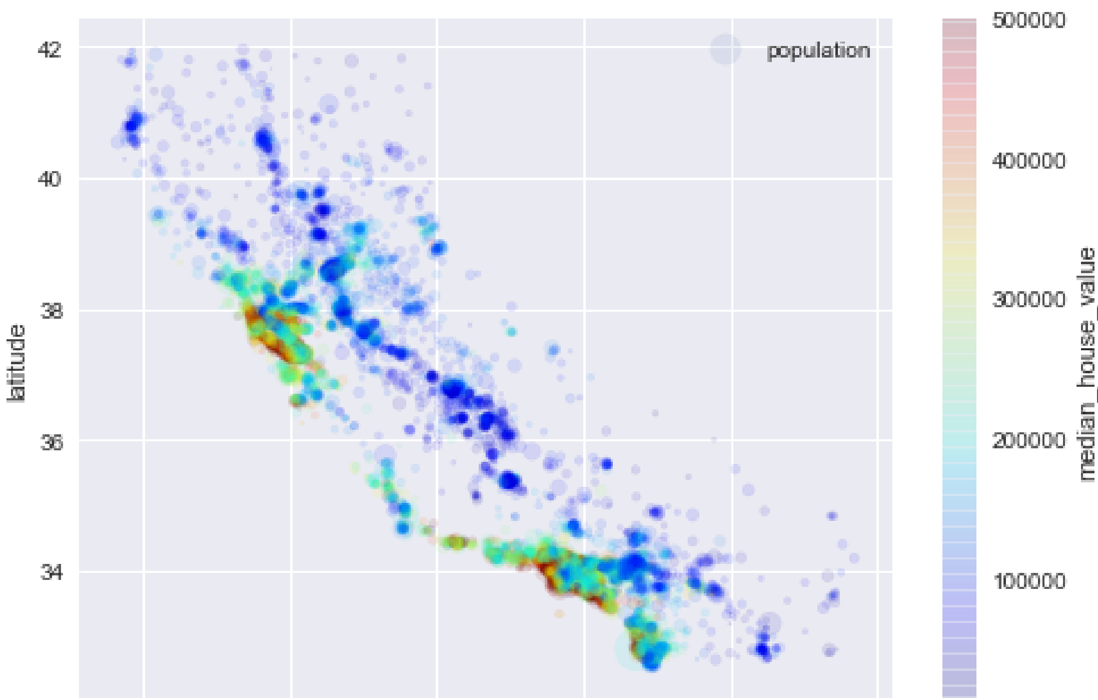
```
(20640, 11)
(16512, 10)
(4128, 10)
```

In [38]:
```python
# We check that housingDF now indeed has a new variable called income_category,
# which was added by splitTrainTest().

housingDF.info()
trainSet.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 20640 entries, 0 to 20639
Data columns (total 11 columns):
longitude             20640 non-null float64
latitude              20640 non-null float64
housing_median_age    20640 non-null float64
total_rooms           20640 non-null float64
total_bedrooms        20433 non-null float64
population            20640 non-null float64
households            20640 non-null float64
median_income         20640 non-null float64
median_house_value    20640 non-null float64
ocean_proximity       20640 non-null object
income_category       20640 non-null float64
dtypes: float64(10), object(1)
memory usage: 1.7+ MB
<class 'pandas.core.frame.DataFrame'>
Int64Index: 16512 entries, 8663 to 7054
Data columns (total 10 columns):
longitude             16512 non-null float64
latitude              16512 non-null float64
housing_median_age    16512 non-null float64
total_rooms           16512 non-null float64
total_bedrooms        16336 non-null float64
population            16512 non-null float64
households            16512 non-null float64
median_income         16512 non-null float64
median_house_value    16512 non-null float64
ocean_proximity       16512 non-null object
dtypes: float64(9), object(1)
memory usage: 1.4+ MB
```

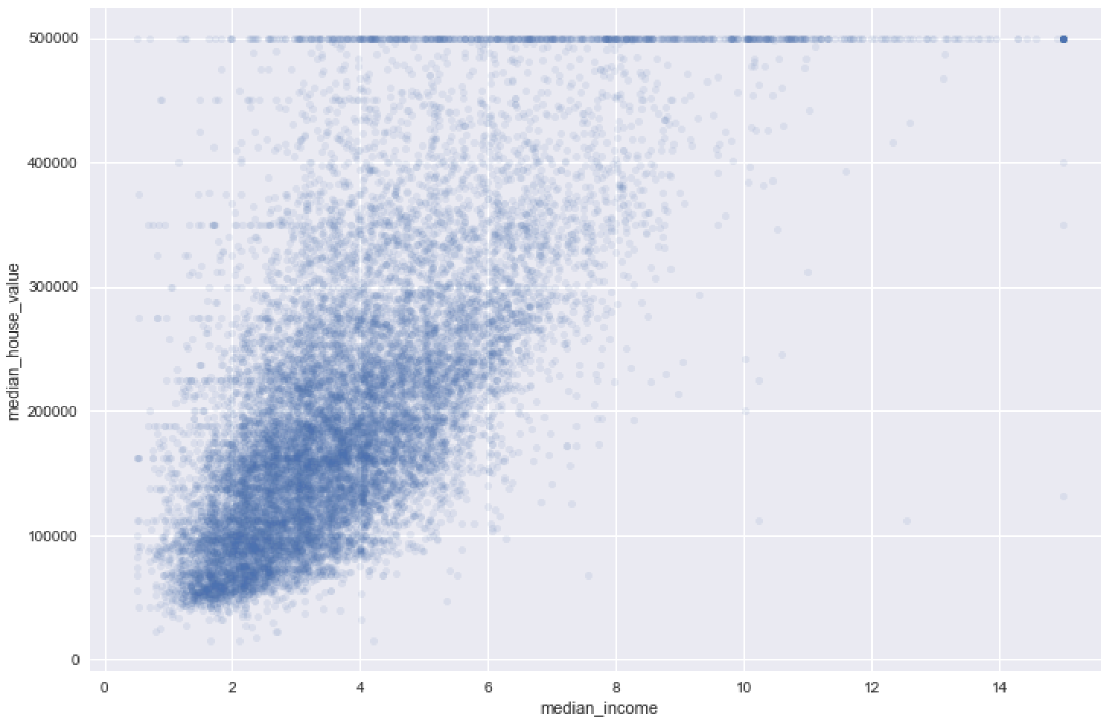
1.4 Visualization of training set (we emphasize: we exclude the testing set in the visualization)

```
In [39]: # Bubble Heat Map:
         # (*)  Each bubble represents a California census block group.
         # (*)  Horizontal and vertical coordinates are longitude and latitude, respectively.
         # (*)  Bubble size indicates population size.
         # (*)  Bubble colour indicates median house value.

         myPlot = trainSet.plot(
             label    = 'population',
             kind     = 'scatter',
             x        = 'longitude',
             y        = 'latitude',
             s        = housingDF["population"] / 100,
             c        = 'median_house_value',
             cmap     = plt.get_cmap("jet"),
             colorbar = True,
             alpha    = 0.1
             )
         plt.show()
```

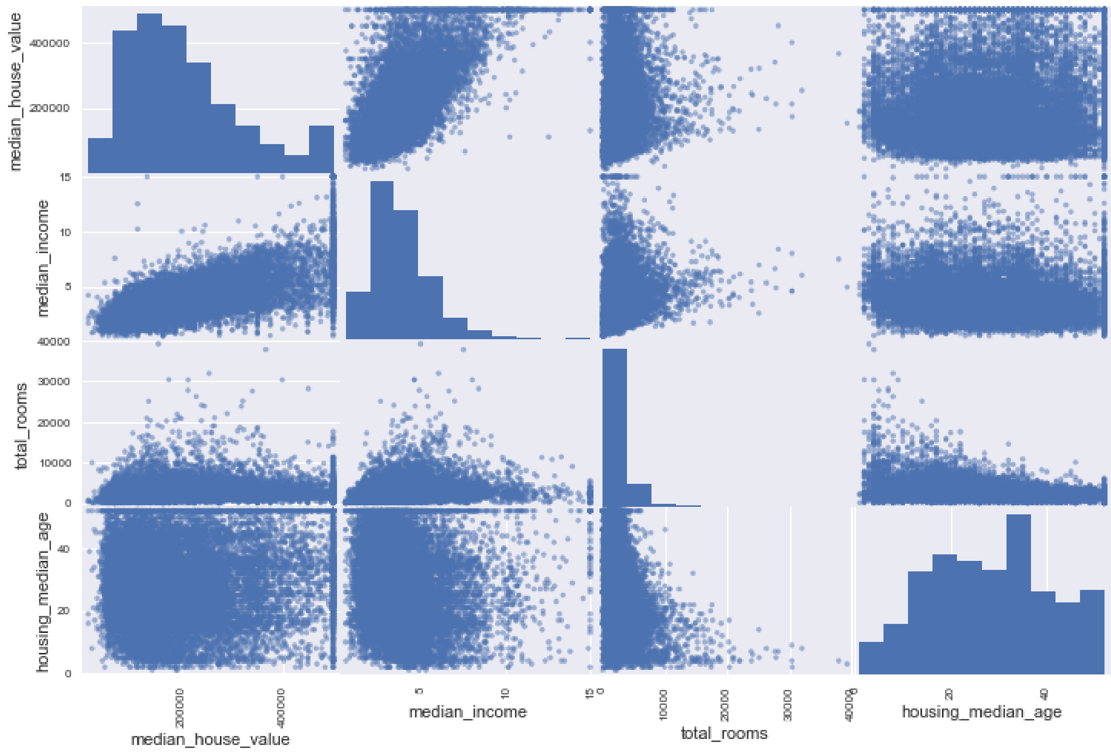



```
In [40]: # Scatter plot of median house value (response variable) against median income.
         # Note the rather strong correlation between these two variables.
```

```
myPlot = trainSet.plot(
    kind    = 'scatter',
    x       = "median_income",
    y       = "median_house_value",
    alpha   = 0.1,
    figsize = (12,8)
    )
plt.show()
```



In [41]:
```
# Scatter plots and histograms for four of the continuous variables.

from pandas.plotting import scatter_matrix
corrMatrix = trainSet.corr()
attributes = ["median_house_value","median_income","total_rooms","housing_median_age"]
myPlot = scatter_matrix(frame=trainSet[attributes], figsize=(12,8))
plt.show()
```



1.5 Preprocessing

```
In [42]: # The preprocessing includes the following tasks:
         #  (1)  median imputation for continuous variables
         #  (2)  add two derived variables: number of rooms per household, population per househ
         #  (3)  binarize the categorical variable: ocean_proximity (replace it with a collectio

         # Note that the preprocessing here is done by fitting a data preprocessing sub-pipeline
         # PipelinePreprocessHousingData. Note that the fitting is done only to the training sub
         # This fitted preprocessing sub-pipeline will be used as an input to the trainEvaluate(

         from PipelinePreprocessHousingData import PipelinePreprocessHousingData
         preprocessedTrainSet = PipelinePreprocessHousingData.fit_transform(
             trainSet.drop(["median_house_value"],axis=1)
             )

In [43]: # Take a look at the top three rows of the preprocessed training data.

         print(type(preprocessedTrainSet))
         preprocessedTrainSet[0:3,]

<class 'numpy.ndarray'>
```

Out[43]: array([[0.59311284, -0.84368509, 0.91777934, 0.19522684, 0.07694854,
               -0.14480532, 0.01372209, 0.68219324, 0.27712397, -0.09712907,
               -0.42595431, 1.   , 0.   , 0.   , 0.   ,
                0.   ],
              [1.09212684, -1.13781385, -0.91562623, -0.35121612, 0.10330353,
               -0.12355599, -0.19581394, -1.01636674, -0.44156162, 0.00596612,
                1.46978359, 0.   , 0.   , 0.   , 0.   ,
                1.   ],
              [1.29173244, -1.35257454, -0.91562623, 0.59509667, 0.73103156,
                0.5024137 , 0.6947142 , -0.61817454, -0.12078124, -0.0762501 ,
                0.0045411 , 1.   , 0.   , 0.   , 0.   ,
                0.   ]])

1.6 Custom-built module: trainEvaluate.py

We now fit the three hyperparameter-free regression models: linear regression, regression trees, and random forest regression.

For each of these three models, we go through the same sequence of steps, namely:

(1) preprocess the training data,

(2) fit the model to the training data,

(3) compute the training error,

(4) compute the 10-fold cross validation error,

(5) compute the testing error.

Due to this repetition, we implemented the trainEvaluate( ) function, which accepts the choice of regression model as an input, and executes the preceding steps for the given model.

In [44]:
```
########################################################
#
# source code for the Python module: trainEvaluate.py
#
########################################################

# import numpy as np
# from sklearn.metrics import mean_squared_error

# import importlib
# from importlib.util import find_spec
# ms_spec = importlib.util.find_spec(name="sklearn.model_selection")
# if ms_spec is not None:
#     from sklearn.model_selection import cross_val_score
# else:
#     from sklearn.cross_validation import cross_val_score
#
# def trainEvaluate(trainData, testData, trainedPreprocessor, myModel, modelName):
```

```
#
#     preprocessedTrainData = trainedPreprocessor.transform(
#         trainData.drop(["median_house_value"],axis=1)
#         )
#
#     myModel.fit(X = preprocessedTrainData, y = trainData["median_house_value"])
#     myPredictions = myModel.predict(X = preprocessedTrainData)
#
#     myTrainMSE  = mean_squared_error(myPredictions,trainData["median_house_value"])
#     myTrainRMSE = np.sqrt(myTrainMSE)
#
#     ### ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~ ###
#     nFold =10
#
#     CVScores = cross_val_score(
#         estimator = myModel,
#         X         = preprocessedTrainData,
#         y         = trainData["median_house_value"],
#         scoring   = "neg_mean_squared_error",
#         cv        = nFold
#         )
#     CVRMSE = np.sqrt( - CVScores )
#
#     ### ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~ ###
#     preprocessedTestData = trainedPreprocessor.transform(
#         testData.drop(["median_house_value"],axis=1)
#         )
#
#     myPredictions = myModel.predict(X = preprocessedTestData)
#
#     myTestMSE  = mean_squared_error(myPredictions,testData["median_house_value"])
#     myTestRMSE = np.sqrt(myTestMSE)
#
#     ### ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~ ###
#     print("\n### ~~~~~~~~~~~~~~~~~~~~ ###")
#     print("###  " + modelName)
#
#     print("\nTrain RMSE: " + str(myTrainRMSE))
#
#     print("\nCV RMSE (" + str(nFold) + "-fold):")
#     print(CVRMSE)
#     print("\nCV RMSE (mean): " + str(CVRMSE.mean()) )
#     print("\nCV RMSE (std): "  + str(CVRMSE.std())  )
#
#     print("\nTest RMSE: " + str(myTestRMSE))
#
#     ### ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~ ###
#     return( None )
```

```
#
```

1.7 trainEvaluate(LinearRegression)

```
In [45]: # import the trainEvaluate() function from the custom-built trainEvaluate module

         from trainEvaluate import trainEvaluate
```

```
In [46]: # import Scikit-learn's LinearRegression classs
         from sklearn.linear_model import LinearRegression

         # instantiate a LinearRegression object
         myLinearModel = LinearRegression()

         # train and evaluate a linear model (this underfits the data)
         trainEvaluate(
             trainData            = trainSet,
             testData             = testSet,
             trainedPreprocessor = PipelinePreprocessHousingData,
             myModel              = myLinearModel,
             modelName            = "Linear Model"
             )
```

```
### ~~~~~~~~~~~~~~~~~~~~ ###
###  Linear Model

Train RMSE: 68205.5245154

CV RMSE (10-fold):
[ 71216.30938995  69374.24757249  69744.15111082  67634.72605826
  67556.95118003  70447.0948898   66602.78109188  67053.6825131
  69152.900413    68090.74548673]

CV RMSE (mean): 68687.3589706

CV RMSE (std): 1450.99222303

Test RMSE: 68763.2267712
```

1.8 trainEvaluate(RegressionTree)

```
In [47]: # regression tree (this overfits the data: zero MSE on training data)

         from sklearn.tree import DecisionTreeRegressor
         myRegressionTreeModel = DecisionTreeRegressor()
         trainEvaluate(
```

```
            trainData            = trainSet,
            testData             = testSet,
            trainedPreprocessor  = PipelinePreprocessHousingData,
            myModel              = myRegressionTreeModel,
            modelName            = "Regression Tree"
            )
```

```
### ~~~~~~~~~~~~~~~~~~~~ ###
###  Regression Tree

Train RMSE: 0.0

CV RMSE (10-fold):
[ 70680.39359097  70406.12919439  69287.61261197  70497.44115995
  67852.84062332  70839.05162866  72207.53313939  74738.69091041
  64739.06561172  66226.60828442]

CV RMSE (mean): 69747.5366755

CV RMSE (std): 2744.15840222

Test RMSE: 71701.587735
```

1.9 trainEvaluate(RandomForest)

In [48]:
```
# random forest

from sklearn.ensemble import RandomForestRegressor
myRandomForestModel = RandomForestRegressor()
trainEvaluate(
    trainData            = trainSet,
    testData             = testSet,
    trainedPreprocessor  = PipelinePreprocessHousingData,
    myModel              = myRandomForestModel,
    modelName            = "Random Forest"
    )
```

```
### ~~~~~~~~~~~~~~~~~~~~ ###
###  Random Forest

Train RMSE: 22194.0536877

CV RMSE (10-fold):
[ 52784.12775102  55188.47657689  54127.86072866  50922.16479478
  50401.97860418  55204.61465749  52058.34069663  53040.55051752
```

```
 49682.10243744  53386.14360542]

CV RMSE (mean): 52679.636037

CV RMSE (std): 1818.10691379

Test RMSE: 52660.4331948
```

1.10 trainEvaluateGrid(RandomForest)

We now fit the fourth and last regression model: random forests regression model with hyperparameters.

The trainEvaluateGrid( ) function from the custom-built module trainEvaluateGrid is an extension of the eariler trainEvaluate( ) function, where trainEvaluateGrid() accepts a GridSearchCV object as an additional input that specifies the "grid" of hyperparameter configurations on which to search for an optimal (in the sense of minimizing the cross validation error) hyperparameter configuration via cross validation.

```
In [49]: # import the trainEvaluateGrid() function from the custom-built module trainEvaluateGri
         from trainEvaluateGrid import trainEvaluateGrid

         # random forest with hyperparameter tuning via grid search
         import importlib
         from importlib.util import find_spec

         ms_spec = importlib.util.find_spec(name="sklearn.model_selection")
         if ms_spec is not None:
             from sklearn.model_selection import GridSearchCV
         else:
             from sklearn.grid_search import GridSearchCV

         # instantiate random forest regressor
         from sklearn.ensemble import RandomForestRegressor
         newRandomForestModel = RandomForestRegressor()

         # define the hyperparameter grid (on which to search for the optimal hyperparameter con
         parameterGrid = [
             { 'n_estimators':[3,10,30], 'max_features':[2,4,6,8]                      },
             { 'n_estimators':[3,10],    'max_features':[2,3,4],  'bootstrap':[False] }
             ]

         # instantiate a GridSearchCV object
         gridSearch = GridSearchCV(
             estimator  = newRandomForestModel,
             param_grid = parameterGrid,
             scoring    = "neg_mean_squared_error",
             cv         = 5
```

```
        )

    trainEvaluateGrid(
        trainData           = trainSet,
        testData            = testSet,
        trainedPreprocessor = PipelinePreprocessHousingData,
        myModel             = gridSearch,
        modelName           = "Random Forest, Cross Validation, Grid Search"
        )
```

```
### ~~~~~~~~~~~~~~~~~~~~ ###
###  Random Forest, Cross Validation, Grid Search

Train RMSE: 19016.9313616

(Cross Validation, Grid Search) RSME:
64181.9126509 {'max_features': 2, 'n_estimators': 3}
55290.1115007 {'max_features': 2, 'n_estimators': 10}
52672.3576805 {'max_features': 2, 'n_estimators': 30}
59934.1255197 {'max_features': 4, 'n_estimators': 3}
53666.9706172 {'max_features': 4, 'n_estimators': 10}
50332.8956649 {'max_features': 4, 'n_estimators': 30}
59010.8610364 {'max_features': 6, 'n_estimators': 3}
52155.4992653 {'max_features': 6, 'n_estimators': 10}
50077.536463 {'max_features': 6, 'n_estimators': 30}
58760.5954571 {'max_features': 8, 'n_estimators': 3}
52307.4196577 {'max_features': 8, 'n_estimators': 10}
50172.3753172 {'max_features': 8, 'n_estimators': 30}
62421.0302876 {'bootstrap': False, 'max_features': 2, 'n_estimators': 3}
54534.1510086 {'bootstrap': False, 'max_features': 2, 'n_estimators': 10}
59557.6283102 {'bootstrap': False, 'max_features': 3, 'n_estimators': 3}
52479.4621839 {'bootstrap': False, 'max_features': 3, 'n_estimators': 10}
58780.0802231 {'bootstrap': False, 'max_features': 4, 'n_estimators': 3}
51748.923956 {'bootstrap': False, 'max_features': 4, 'n_estimators': 10}

best_params_:
{'max_features': 6, 'n_estimators': 30}

gridSearch.best_estimator_
RandomForestRegressor(bootstrap=True, criterion='mse', max_depth=None,
           max_features=6, max_leaf_nodes=None, min_impurity_split=1e-07,
           min_samples_leaf=1, min_samples_split=2,
           min_weight_fraction_leaf=0.0, n_estimators=30, n_jobs=1,
           oob_score=False, random_state=None, verbose=0, warm_start=False)

Test RMSE: 49147.8221853
```

```
featureImportances
(0.33447308756630334, 'median_income')
(0.15755789829455008, '<1H OCEAN')
(0.09754615725500658, 'roomsPerHhold')
(0.078448870819000274, 'longitude')
(0.076045355198927259, 'popPerHhold')
(0.071528193022828701, 'latitude')
(0.057036841777294241, 'median_house_value')
(0.041858480125080172, 'housing_median_age')
(0.018665860086358833, 'population')
(0.017815926565703962, 'total_rooms')
(0.016918692849366479, 'total_bedrooms')
(0.015943173131565767, 'households')
(0.009108354420097893, 'bedroomsPerRoom')
(0.0041442425117166719, 'NEAR BAY')
(0.0028539641174511331, 'ISLAND')
(5.4902258748667759e-05, 'INLAND')
```