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Anomaly Detection for Dummies

Unsupervised Anomaly Detection for Univariate & Multivariate Data.

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Anomaly detection is the process of identifying unexpected items or events in data sets, which differ from the norm. And anomaly detection is often applied on unlabeled data which is known as unsupervised anomaly detection. Anomaly detection has two basic assumptions:

- Anomalies only occur very rarely in the data.
- Their features differ from the normal instances significantly.

Univariate Anomaly Detection

Before we get to Multivariate anomaly detection, I think its necessary to work through a simple example of Univariate anomaly detection method in which we detect outliers from a distribution of values in a single feature space.

We are using the Super Store Sales data set that can be downloaded from here, and we are going to find patterns in Sales and Profit separately that do not conform to expected behavior. That is, spotting outliers for one variable at a time.

```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
import matplotlib
from sklearn.ensemble import IsolationForest
```

Distribution of the Sales

```
df = pd.read_excel("Superstore.xls")
df['Sales'].describe()
```

```
count     9994.000000
mean       229.858001
std        623.245101
min          0.444000
25%         17.280000
50%         54.490000
```

```
75%        209.940000
max      22638.480000
Name: Sales, dtype: float64
```

Figure 1

```
plt.scatter(range(df.shape[0]), np.sort(df['Sales'].values))
plt.xlabel('index')
plt.ylabel('Sales')
plt.title("Sales distribution")
sns.despine()
```

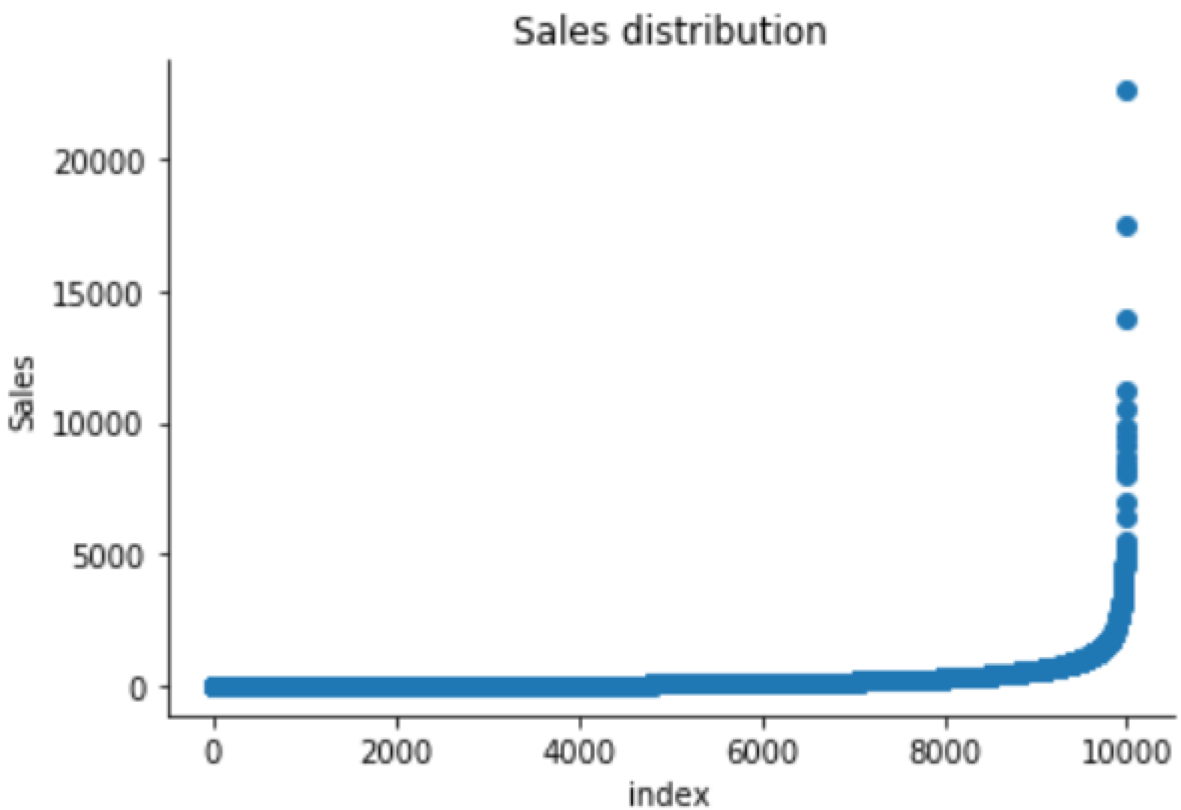


Figure 2

```
sns.distplot(df['Sales'])
plt.title("Distribution of Sales")
sns.despine()
```

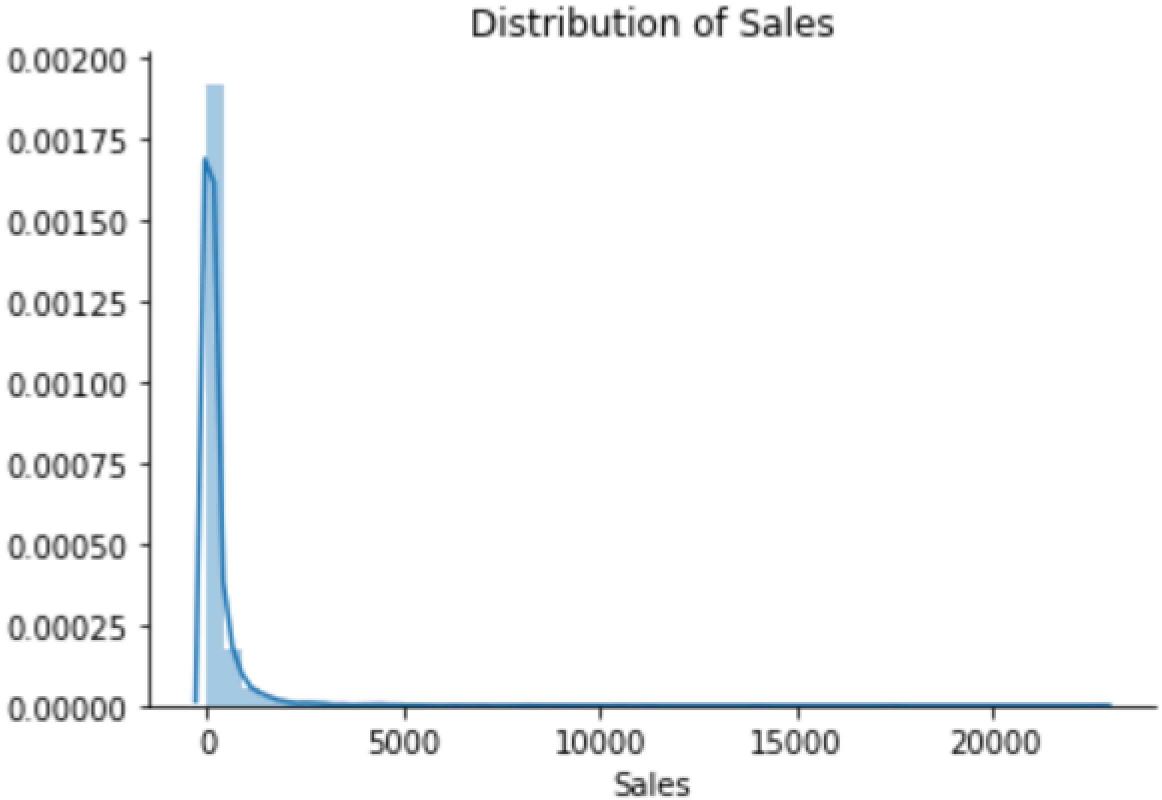


Figure 3

```
print("Skewness: %f" % df['Sales'].skew())
print("Kurtosis: %f" % df['Sales'].kurt())
```

```
Skewness: 12.972752
Kurtosis: 305.311753
```

The Superstore's sales distribution is far from a normal distribution, and it has a positive long thin tail, the mass of the distribution is concentrated on the left of the figure. And the tail sales distribution far exceeds the tails of the normal distribution.

There are one region where the data has low probability to appear which is on the right side of the distribution.

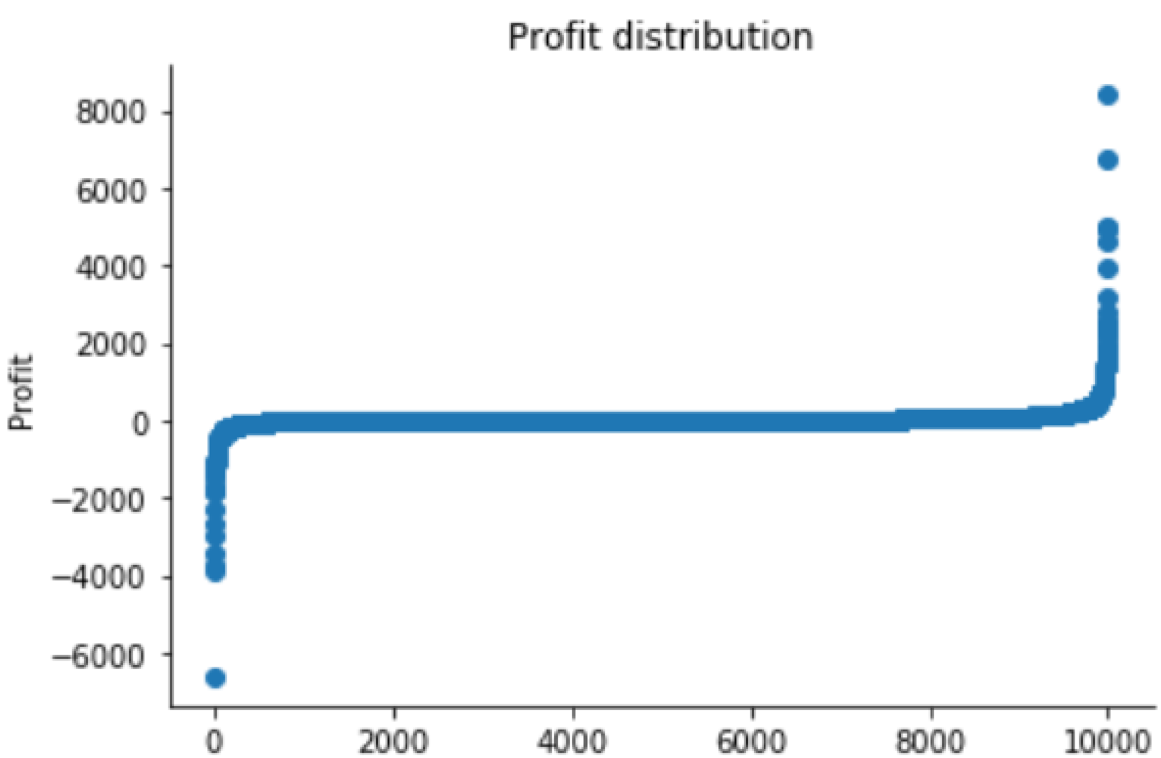
Distribution of the Profit

```
df['Profit'].describe()
```

```
count    9994.000000
mean       28.656896
std       234.260108
min     -6599.978000
25%         1.728750
50%         8.666500
75%        29.364000
max      8399.976000
Name: Profit, dtype: float64
```

Figure 4

```
plt.scatter(range(df.shape[0]), np.sort(df['Profit'].values))
plt.xlabel('index')
plt.ylabel('Profit')
plt.title("Profit distribution")
sns.despine()
```



index

Figure 5

```
sns.distplot(df['Profit'])
plt.title("Distribution of Profit")
sns.despine()
```

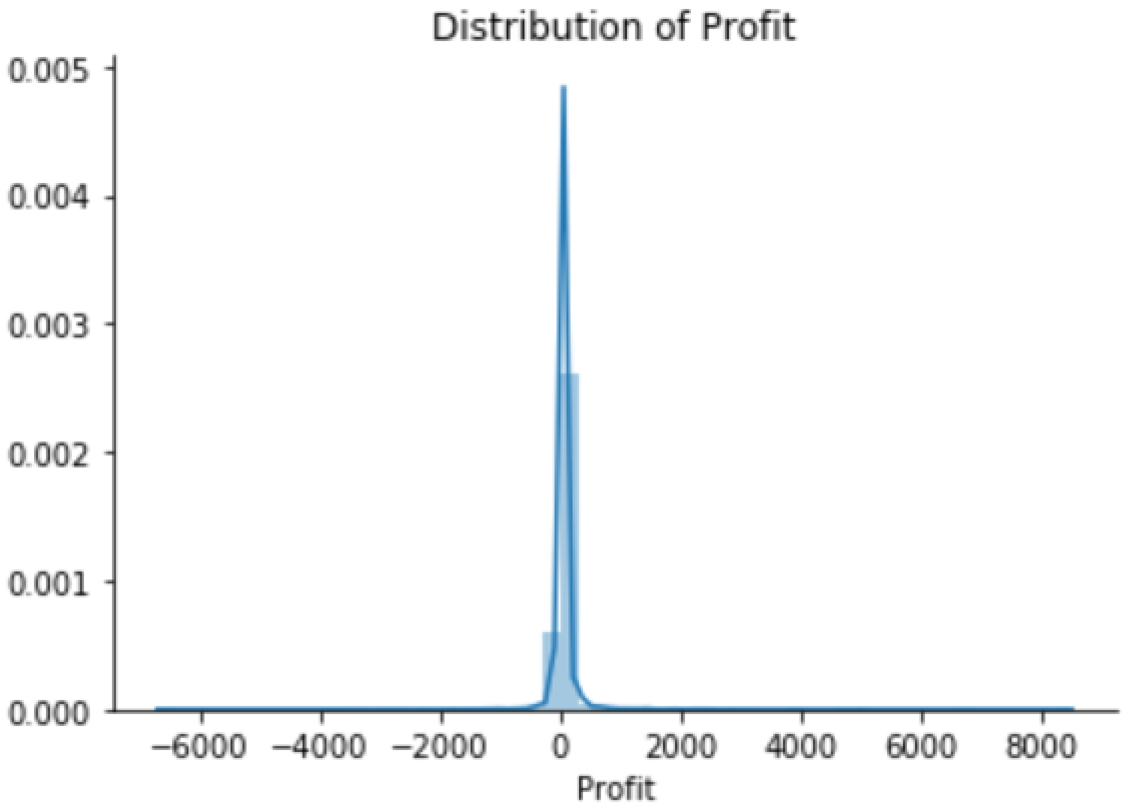


Figure 6

```
print("Skewness: %f" % df['Profit'].skew())
print("Kurtosis: %f" % df['Profit'].kurt())
```

```
Skewness: 7.561432
Kurtosis: 397.188515
```

The Superstore's Profit distribution has both a positive tail and negative tail. However, the positive tail is longer than the negative tail. So the distribution is positive skewed, and the data are heavy-tailed or profusion of outliers.

There are two regions where the data has low probability to appear: one on the right side of the distribution, another one on the left.

Univariate Anomaly Detection on Sales

Isolation Forest is an algorithm to detect outliers that returns the anomaly score of each sample using the IsolationForest algorithm which is based on the fact that anomalies are data points that are few and different. Isolation Forest is a tree-based model. In these trees, partitions are created by first randomly selecting a feature and then selecting a random split value between the minimum and maximum value of the selected feature.

The following process shows how IsolationForest behaves in the case of the Susperstore's sales, and the algorithm was implemented in Sklearn and the code was largely borrowed from this tutorial

- Trained IsolationForest using the Sales data.
- Store the Sales in the N*umPy* array for using in our models later.
- Computed the anomaly score for each observation. The anomaly score of an input sample is computed as the mean anomaly score of the trees in the forest.
- Classified each observation as an outlier or non-outlier.
- The visualization highlights the regions where the outliers fall.

```
isolation_forest = IsolationForest(n_estimators=100)
isolation_forest.fit(df['Sales'].values.reshape(-1, 1))
xx = np.linspace(df['Sales'].min(), df['Sales'].max(), len(df)).reshape(-1,1)
anomaly_score = isolation_forest.decision_function(xx)
outlier = isolation_forest.predict(xx)
plt.figure(figsize=(10,4))
plt.plot(xx, anomaly_score, label='anomaly score')
plt.fill_between(xx.T[0], np.min(anomaly_score), np.max(anomaly_score),
                 where=outlier==-1, color='r',
                 alpha=.4, label='outlier region')
plt.legend()
```

```
plt.ylabel('anomaly score')
plt.xlabel('Sales')
plt.show();
```

sales_IsolationForest.py hosted with ❤ by GitHub view raw

sales_IsolationForest.py

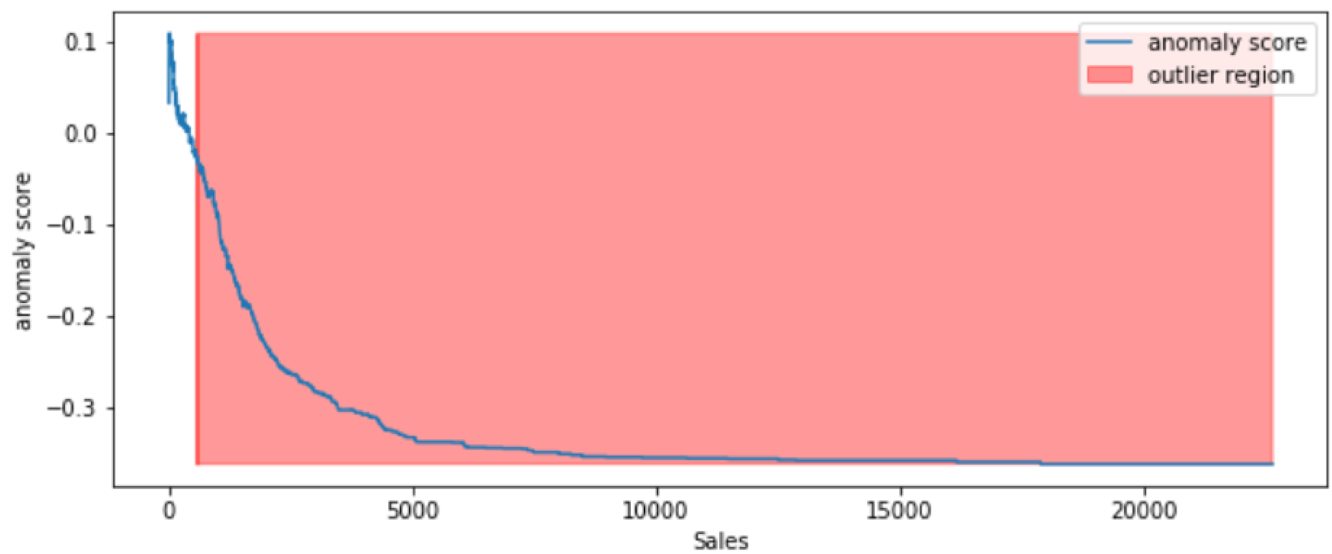


Figure 7

According to the above results and visualization, It seems that Sales that exceeds 1000 would be definitely considered as an outlier.

Visually investigate one anomaly

```
df.iloc[10]
```

```
Row ID                             11
Order ID               CA-2014-115812
Order Date        2014-06-09 00:00:00
Ship Date         2014-06-14 00:00:00
Ship Mode              Standard Class
Customer ID                  BH-11710
Customer Name         Brosina Hoffman
Segment                      Consumer
Country                 United States
```

```
City                                            Los Angeles
State                                            California
Postal Code                                           90032
Region                                                 West
Product ID                                  FUR-TA-10001539
Category                                          Furniture
Sub-Category                                         Tables
Product Name     Chromcraft Rectangular Conference Tables
Sales                                               1706.18
Quantity                                                  9
Discount                                                0.2
Profit                                              85.3092
Name: 10, dtype: object
```

Figure 8

This purchase seems normal to me expect it was a larger amount of sales compared with the other orders in the data.

Univariate Anomaly Detection on Profit

- Trained IsolationForest using the Profit variable.
- Store the Profit in the N*umPy* array for using in our models later.
- Computed the anomaly score for each observation. The anomaly score of an input sample is computed as the mean anomaly score of the trees in the forest.
- Classified each observation as an outlier or non-outlier.
- The visualization highlights the regions where the outliers fall.

```python
isolation_forest = IsolationForest(n_estimators=100)
isolation_forest.fit(df['Profit'].values.reshape(-1, 1))
xx = np.linspace(df['Profit'].min(), df['Profit'].max(), len(df)).reshape(-1,1)
anomaly_score = isolation_forest.decision_function(xx)
outlier = isolation_forest.predict(xx)
plt.figure(figsize=(10,4))
plt.plot(xx, anomaly_score, label='anomaly score')
plt.fill_between(xx.T[0], np.min(anomaly_score), np.max(anomaly_score),
                 where=outlier==-1, color='r',
                 alpha=.4, label='outlier region')
plt.legend()
```

```
plt.ylabel('anomaly score')
plt.xlabel('Profit')
plt.show();
```

profit_IsolationForest.py hosted with ❤ by GitHub view raw

profit_IsolationForest.py

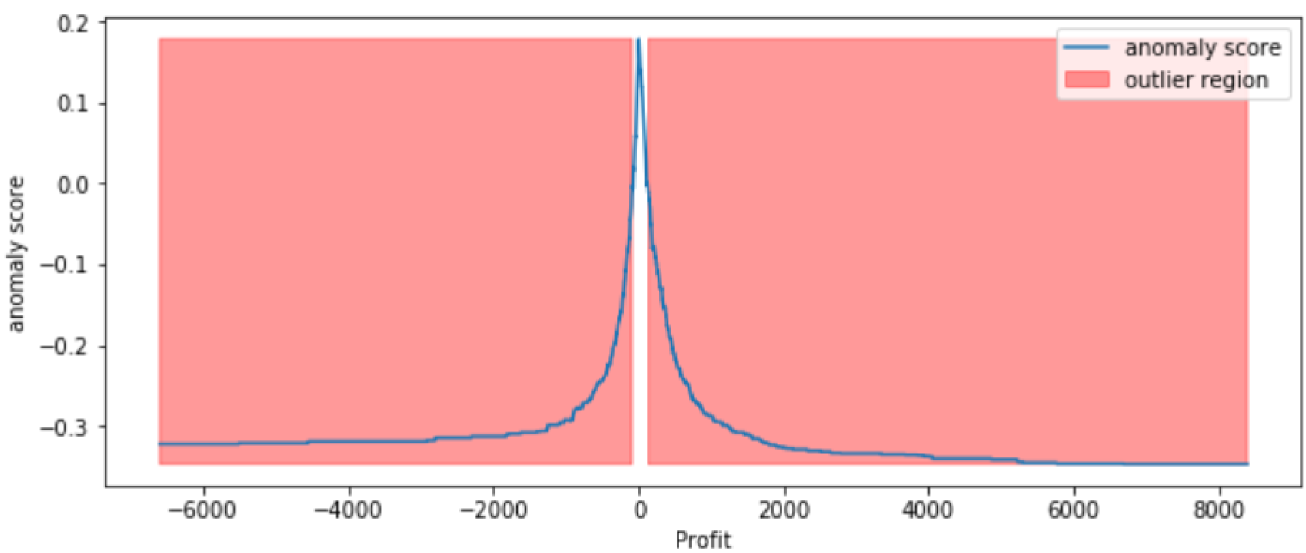


Figure 9

Visually investigate some of the anomalies

According to the above results and visualization, It seems that Profit that below -100 or exceeds 100 would be considered as an outlier, let's visually examine one example each that determined by our model and to see whether they make sense.

```
df.iloc[3]
```

```
Row ID                                    4
Order ID                     US-2015-108966
Order Date              2015-10-11 00:00:00
Ship Date               2015-10-18 00:00:00
Ship Mode                    Standard Class
Customer ID                        SO-20335
Customer Name                Sean O'Donnell
Segment                            Consumer
Country                       United States
```

```
City                                          Fort Lauderdale
State                                                 Florida
Postal Code                                             33311
Region                                                  South
Product ID                                    FUR-TA-10000577
Category                                            Furniture
Sub-Category                                           Tables
Product Name     Bretford CR4500 Series Slim Rectangular Table
Sales                                                 957.577
Quantity                                                    5
Discount                                                 0.45
Profit                                               -383.031
outlier                                                     0
Name: 3, dtype: object
```

Figure 10

Any negative profit would be an anomaly and should be further investigate, this goes without saying

```
df.iloc[1]
```

```
Row ID                                                      2
Order ID                                       CA-2016-152156
Order Date                                2016-11-08 00:00:00
Ship Date                                 2016-11-11 00:00:00
Ship Mode                                        Second Class
Customer ID                                          CG-12520
Customer Name                                     Claire Gute
Segment                                              Consumer
Country                                         United States
City                                                Henderson
State                                                Kentucky
Postal Code                                             42420
Region                                                  South
Product ID                                    FUR-CH-10000454
Category                                            Furniture
Sub-Category                                           Chairs
Product Name     Hon Deluxe Fabric Upholstered Stacking Chairs,...
```

```
Sales                                                         731.94
Quantity                                                           3
Discount                                                           0
Profit                                                       219.582
Name: 1, dtype: object
```

Figure 11

Our model determined that this order with a large profit is an anomaly. However, when we investigate this order, it could be just a product that has a relatively high margin.

The above two visualizations show the anomaly scores and highlighted the regions where the outliers are. As expected, the anomaly score reflects the shape of the underlying distribution and the outlier regions correspond to low probability areas.

However, Univariate analysis can only get us thus far. We may realize that some of these anomalies that determined by our models are not the anomalies we expected. When our data is multidimensional as opposed to **univariate**, the approaches to **anomaly detection** become more computationally intensive and more mathematically complex.

Multivariate Anomaly Detection

Most of the analysis that we end up doing are **multivariate** due to complexity of the world we are living in. In **multivariate** anomaly detection, outlier is a combined unusual score on at least two variables.

So, using the Sales and Profit variables, we are going to build an unsupervised **multivariate anomaly detection** method based on several models.

We are using **PyOD** which is a Python library for detecting anomalies in multivariate data. The library was developed by Yue Zhao.

Sales & Profit

When we are in business, we expect that Sales & Profit are positive correlated. If some of the Sales data points and Profit data points are not positive correlated, they would be considered as outliers and need to be further investigated.

```
sns.regplot(x="Sales", y="Profit", data=df)
sns.despine();
```

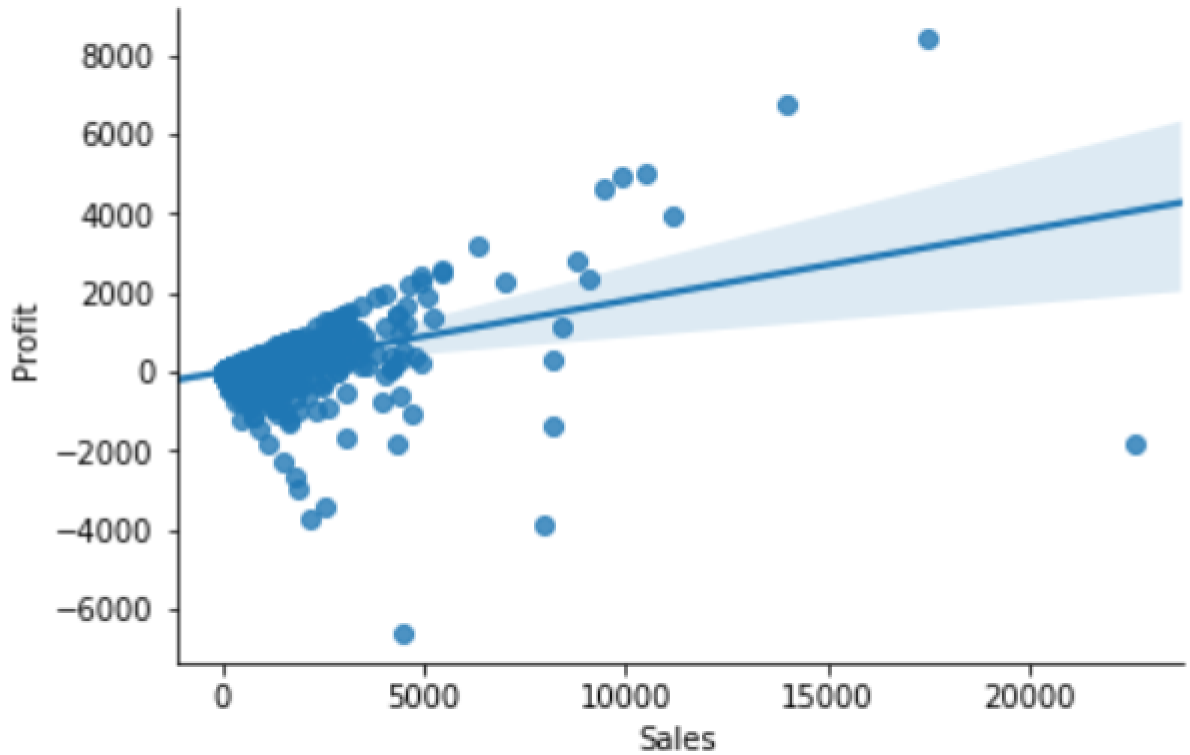


Figure 12

From the above correlation chart, we can see that some of the data points are obvious outliers such as extreme low and extreme high values.

Cluster-based Local Outlier Factor (CBLOF)

The CBLOF calculates the outlier score based on cluster-based local outlier factor. An anomaly score is computed by the distance of each instance to its cluster center multiplied by the instances belonging to its cluster. PyOD library includes the CBLOF implementation.

The following code are borrowed from PyOD tutorial combined with this article.

- Scaling Sales and Profit to between zero and one.
- Arbitrarily set outliers fraction as 1% based on trial and best guess.
- Fit the data to the CBLOF model and predict the results.
- Use threshold value to consider a data point is inlier or outlier.

- Use decision function to calculate the anomaly score for every point.

```
outliers_fraction = 0.01
xx , yy = np.meshgrid(np.linspace(0, 1, 100), np.linspace(0, 1, 100))
clf = CBLOF(contamination=outliers_fraction,check_estimator=False, random_state=0)
clf.fit(X)
scores_pred = clf.decision_function(X) * -1
y_pred = clf.predict(X)
n_inliers = len(y_pred) - np.count_nonzero(y_pred)
n_outliers = np.count_nonzero(y_pred == 1)

plt.figure(figsize=(8, 8))

df1 = df
df1['outlier'] = y_pred.tolist()

# sales - inlier feature 1,  profit - inlier feature 2
inliers_sales = np.array(df1['Sales'][df1['outlier'] == 0]).reshape(-1,1)
inliers_profit = np.array(df1['Profit'][df1['outlier'] == 0]).reshape(-1,1)

# sales - outlier feature 1, profit - outlier feature 2
outliers_sales = df1['Sales'][df1['outlier'] == 1].values.reshape(-1,1)
outliers_profit = df1['Profit'][df1['outlier'] == 1].values.reshape(-1,1)

print('OUTLIERS:',n_outliers,'INLIERS:',n_inliers)
threshold = percentile(scores_pred, 100 * outliers_fraction)
Z = clf.decision_function(np.c_[xx.ravel(), yy.ravel()]) * -1
Z = Z.reshape(xx.shape)

plt.contourf(xx, yy, Z, levels=np.linspace(Z.min(), threshold, 7),cmap=plt.cm.Blues_r)
a = plt.contour(xx, yy, Z, levels=[threshold],linewidths=2, colors='red')
plt.contourf(xx, yy, Z, levels=[threshold, Z.max()],colors='orange')
b = plt.scatter(inliers_sales, inliers_profit, c='white',s=20, edgecolor='k')

c = plt.scatter(outliers_sales, outliers_profit, c='black',s=20, edgecolor='k')

plt.axis('tight')
plt.legend([a.collections[0], b,c], ['learned decision function', 'inliers','outliers'],
           prop=matplotlib.font_manager.FontProperties(size=20),loc='lower right')
plt.xlim((0, 1))
plt.ylim((0, 1))
plt.title('Cluster-based Local Outlier Factor (CBLOF)')
plt.show();
```

CBLOF.py hosted with ❤ by GitHub view raw

CBLOF.py

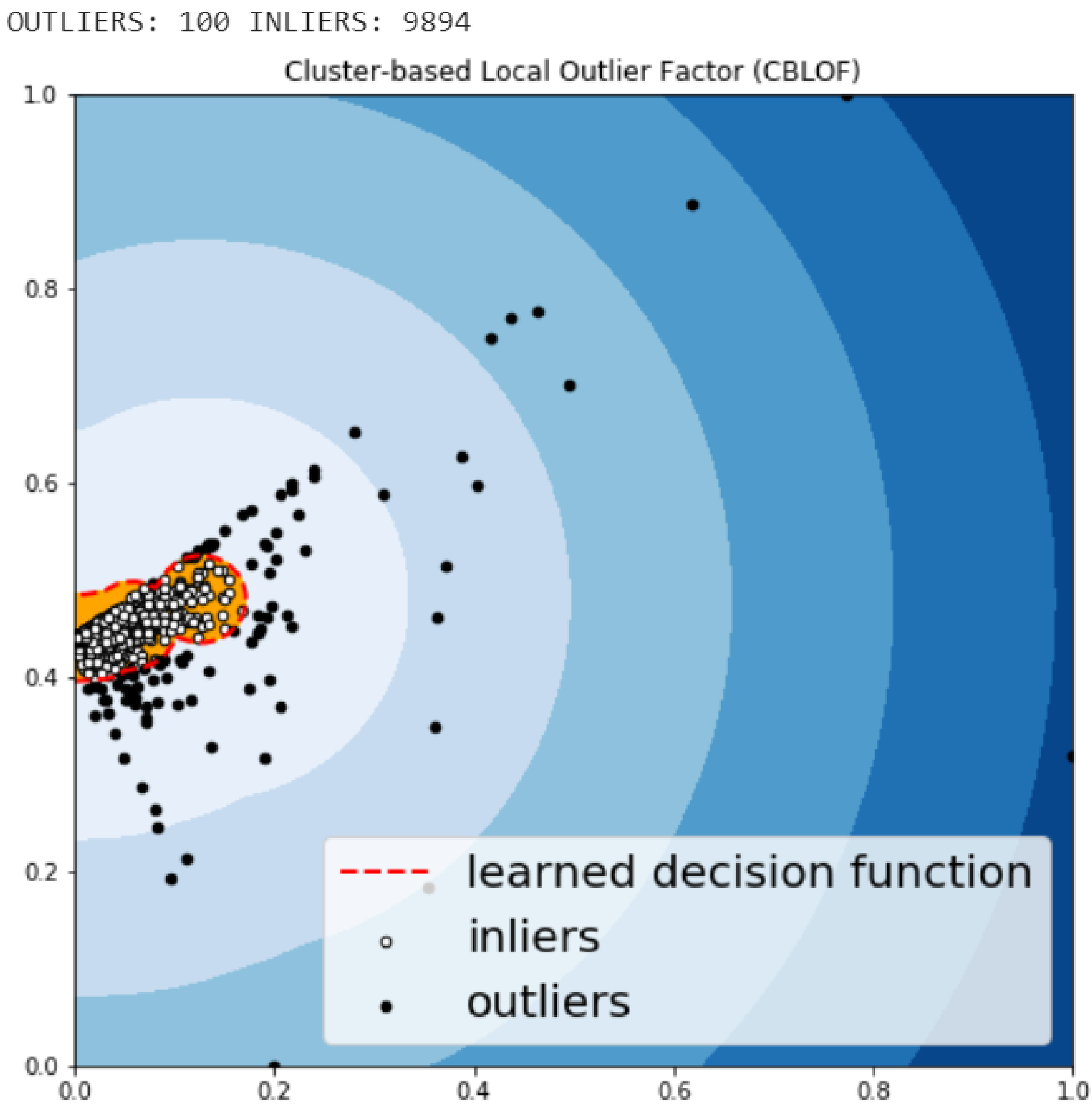


Figure 13

Histogram-based Outlier Detection (HBOS)

HBOS assumes the feature independence and calculates the degree of anomalies by building histograms. In multivariate anomaly detection, a histogram for each single feature can be computed, scored individually and combined at the end. When using PyOD library, the code are very similar with the CBLOF.

```
outliers_fraction = 0.01
xx , yy = np.meshgrid(np.linspace(0, 1, 100), np.linspace(0, 1, 100))
clf = HBOS(contamination=outliers_fraction)
clf.fit(X)
scores_pred = clf.decision_function(X) * -1
y_pred = clf.predict(X)
n_inliers = len(y_pred) - np.count_nonzero(y_pred)
n_outliers = np.count_nonzero(y_pred == 1)
plt.figure(figsize=(8, 8))
df1 = df
df1['outlier'] = y_pred.tolist()

# sales - inlier feature 1,  profit - inlier feature 2
inliers_sales = np.array(df1['Sales'][df1['outlier'] == 0]).reshape(-1,1)
inliers_profit = np.array(df1['Profit'][df1['outlier'] == 0]).reshape(-1,1)

# sales - outlier feature 1, profit - outlier feature 2
outliers_sales = df1['Sales'][df1['outlier'] == 1].values.reshape(-1,1)
outliers_profit = df1['Profit'][df1['outlier'] == 1].values.reshape(-1,1)

print('OUTLIERS:',n_outliers,'INLIERS:',n_inliers)
threshold = percentile(scores_pred, 100 * outliers_fraction)=
Z = clf.decision_function(np.c_[xx.ravel(), yy.ravel()]) * -1
Z = Z.reshape(xx.shape)

plt.contourf(xx, yy, Z, levels=np.linspace(Z.min(), threshold, 7),cmap=plt.cm.Blues_r)
a = plt.contour(xx, yy, Z, levels=[threshold],linewidths=2, colors='red')
plt.contourf(xx, yy, Z, levels=[threshold, Z.max()],colors='orange')
b = plt.scatter(inliers_sales, inliers_profit, c='white',s=20, edgecolor='k')

c = plt.scatter(outliers_sales, outliers_profit, c='black',s=20, edgecolor='k')

plt.axis('tight')
plt.legend([a.collections[0], b,c], ['learned decision function', 'inliers','outliers'],
           prop=matplotlib.font_manager.FontProperties(size=20),loc='lower right')
plt.xlim((0, 1))
plt.ylim((0, 1))
plt.title('Histogram-base Outlier Detection (HBOS)')
plt.show();
```

HBOS.py hosted with ❤ by GitHub view raw

HBOS.py

OUTLIERS: 90 INLIERS: 9904

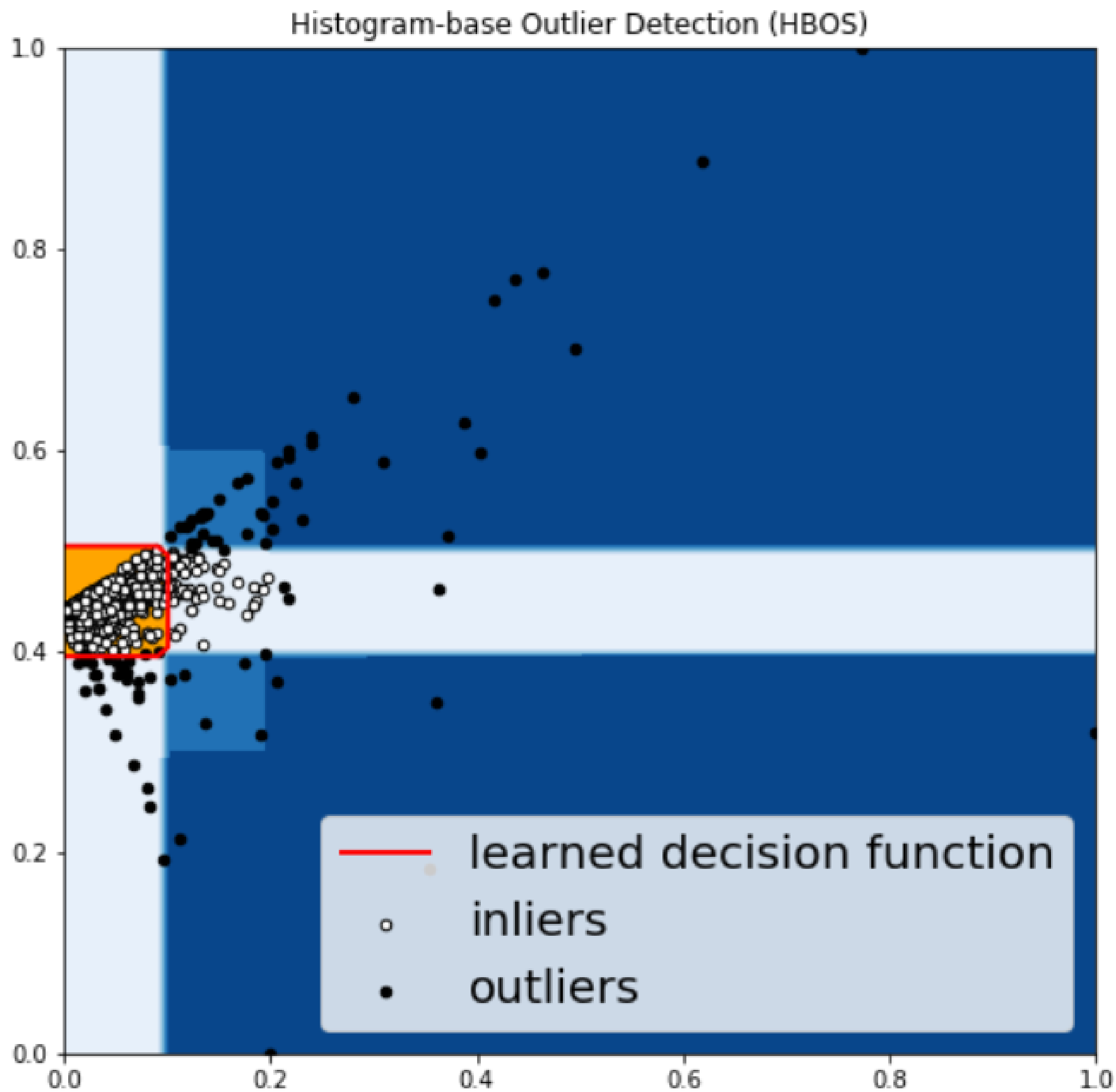


Figure 14

Isolation Forest

Isolation Forest is similar in principle to Random Forest and is built on the basis of decision trees. Isolation Forest isolates observations by randomly selecting a feature and then randomly selecting a split value between the maximum and minimum values of that selected feature.

The PyOD Isolation Forest module is a wrapper of Scikit-learn Isolation Forest with more functionalities.

```
outliers_fraction = 0.01
xx , yy = np.meshgrid(np.linspace(0, 1, 100), np.linspace(0, 1, 100))
```

```
clf = IForest(contamination=outliers_fraction,random_state=0)
clf.fit(X)
scores_pred = clf.decision_function(X) * -1

y_pred = clf.predict(X)
n_inliers = len(y_pred) - np.count_nonzero(y_pred)
n_outliers = np.count_nonzero(y_pred == 1)
plt.figure(figsize=(8, 8))

df1 = df
df1['outlier'] = y_pred.tolist()

# sales - inlier feature 1,  profit - inlier feature 2
inliers_sales = np.array(df1['Sales'][df1['outlier'] == 0]).reshape(-1,1)
inliers_profit = np.array(df1['Profit'][df1['outlier'] == 0]).reshape(-1,1)

# sales - outlier feature 1, profit - outlier feature 2
outliers_sales = df1['Sales'][df1['outlier'] == 1].values.reshape(-1,1)
outliers_profit = df1['Profit'][df1['outlier'] == 1].values.reshape(-1,1)

print('OUTLIERS: ',n_outliers,'INLIERS: ',n_inliers)

threshold = percentile(scores_pred, 100 * outliers_fraction)
Z = clf.decision_function(np.c_[xx.ravel(), yy.ravel()]) * -1
Z = Z.reshape(xx.shape)
plt.contourf(xx, yy, Z, levels=np.linspace(Z.min(), threshold, 7),cmap=plt.cm.Blues_r)
a = plt.contour(xx, yy, Z, levels=[threshold],linewidths=2, colors='red')
plt.contourf(xx, yy, Z, levels=[threshold, Z.max()],colors='orange')
b = plt.scatter(inliers_sales, inliers_profit, c='white',s=20, edgecolor='k')

c = plt.scatter(outliers_sales, outliers_profit, c='black',s=20, edgecolor='k')

plt.axis('tight')
plt.legend([a.collections[0], b,c], ['learned decision function', 'inliers','outliers'],
           prop=matplotlib.font_manager.FontProperties(size=20),loc='lower right')
plt.xlim((0, 1))
plt.ylim((0, 1))
plt.title('Isolation Forest')
plt.show();
```

IsolationForest.py hosted with ❤ by GitHub view raw

IsolationForest.Py

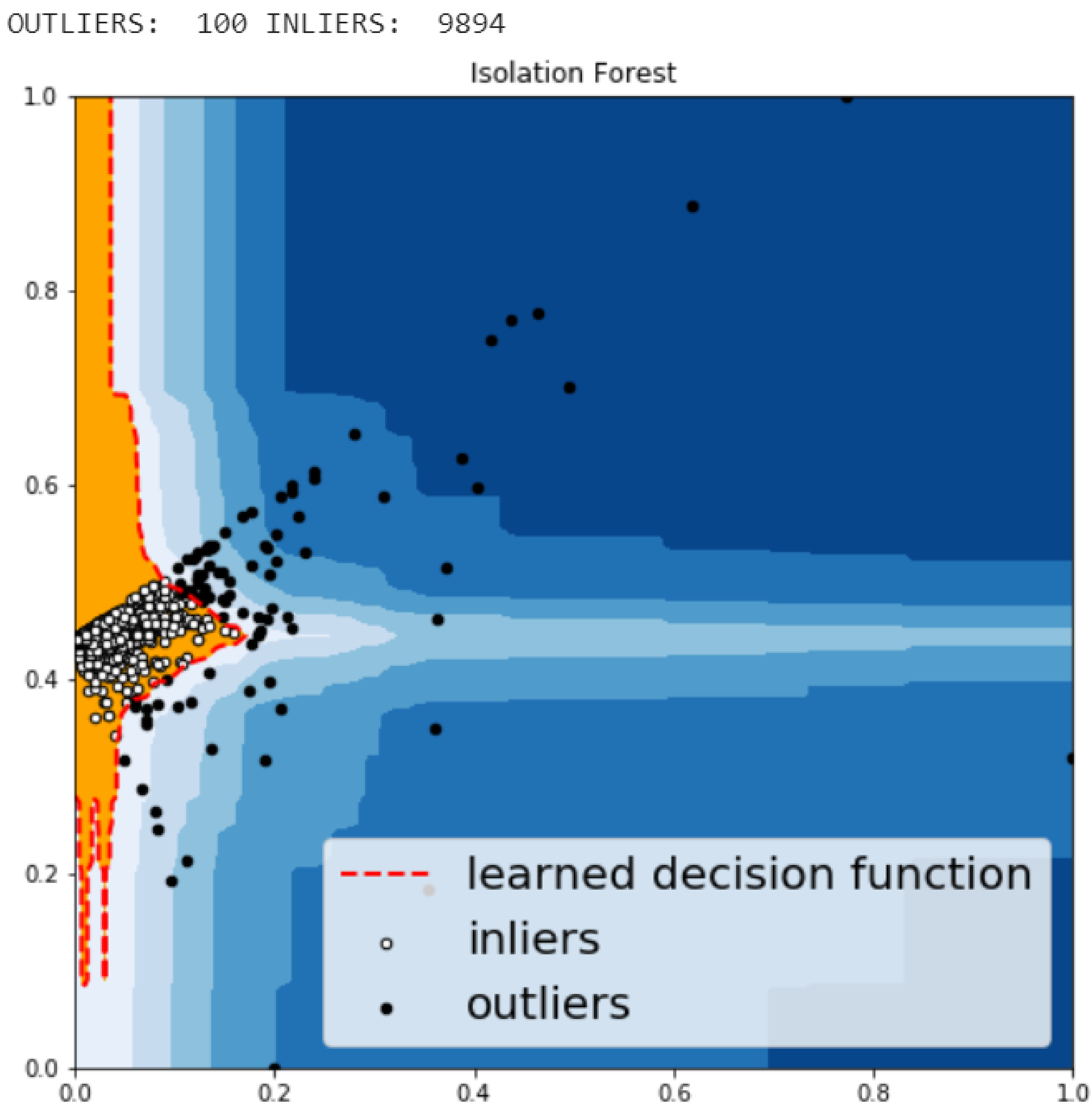


Figure 15

K - Nearest Neighbors (KNN)

KNN is one of the simplest methods in anomaly detection. For a data point, its distance to its kth nearest neighbor could be viewed as the outlier score.

```
outliers_fraction = 0.01
xx , yy = np.meshgrid(np.linspace(0, 1, 100), np.linspace(0, 1, 100))
clf = KNN(contamination=outliers_fraction)
clf.fit(X)
scores_pred = clf.decision_function(X) * -1
y_pred = clf.predict(X)
```

```python
n_inliers = len(y_pred) - np.count_nonzero(y_pred)
n_outliers = np.count_nonzero(y_pred == 1)
plt.figure(figsize=(8, 8))

df1 = df
df1['outlier'] = y_pred.tolist()

# sales - inlier feature 1,  profit - inlier feature 2
inliers_sales = np.array(df1['Sales'][df1['outlier'] == 0]).reshape(-1,1)
inliers_profit = np.array(df1['Profit'][df1['outlier'] == 0]).reshape(-1,1)

# sales - outlier feature 1, profit - outlier feature 2
outliers_sales = df1['Sales'][df1['outlier'] == 1].values.reshape(-1,1)
outliers_profit = df1['Profit'][df1['outlier'] == 1].values.reshape(-1,1)

print('OUTLIERS: ',n_outliers,'INLIERS: ',n_inliers)

threshold = percentile(scores_pred, 100 * outliers_fraction)

Z = clf.decision_function(np.c_[xx.ravel(), yy.ravel()]) * -1
Z = Z.reshape(xx.shape)

plt.contourf(xx, yy, Z, levels=np.linspace(Z.min(), threshold, 7),cmap=plt.cm.Blues_r)
a = plt.contour(xx, yy, Z, levels=[threshold],linewidths=2, colors='red')
plt.contourf(xx, yy, Z, levels=[threshold, Z.max()],colors='orange')
b = plt.scatter(inliers_sales, inliers_profit, c='white',s=20, edgecolor='k')
c = plt.scatter(outliers_sales, outliers_profit, c='black',s=20, edgecolor='k')
plt.axis('tight')
plt.legend([a.collections[0], b,c], ['learned decision function', 'inliers','outliers'],
           prop=matplotlib.font_manager.FontProperties(size=20),loc='lower right')
plt.xlim((0, 1))
plt.ylim((0, 1))
plt.title('K Nearest Neighbors (KNN)')
plt.show();
```

KNN.py hosted with ❤ by GitHub view raw

KNN.py

OUTLIERS: 91 INLIERS: 9903

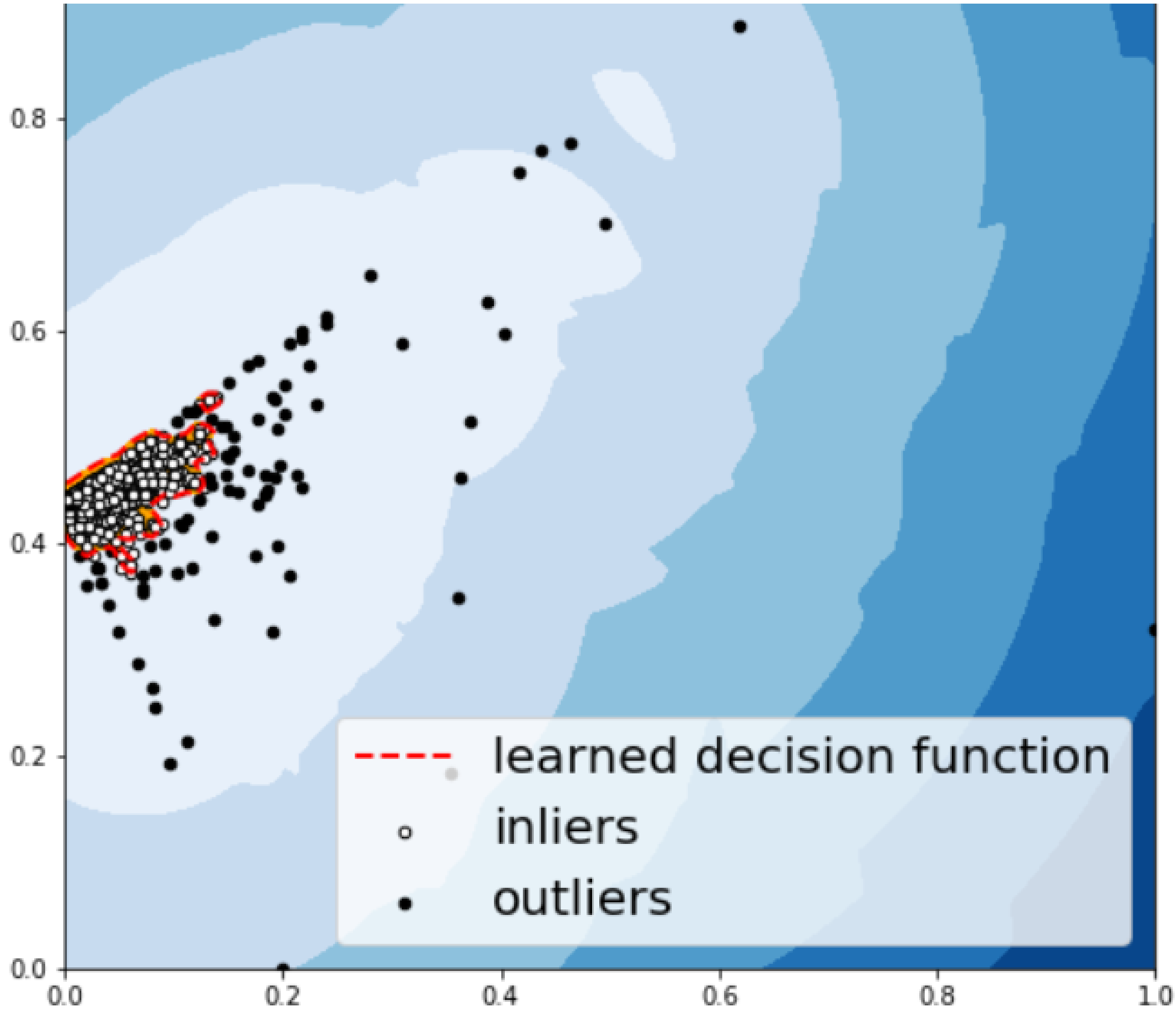


Figure 16

The anomalies predicted by the above four algorithms were not very different.

Visually investigate some of the anomalies

We may want to investigate each of the outliers that determined by our model, for example, let's look in details for a couple of outliers that determined by KNN, and try to understand what make them anomalies.

```
df.iloc[1995]
```

```
Row ID                                    1996
Order ID                        US-2017-147221
Order Date                 2017-12-02 00:00:00
```

```
Ship Date                                       2017-12-04 00:00:00
Ship Mode                                              Second Class
Customer ID                                                JS-16030
Customer Name                                            Joy Smith
Segment                                                   Consumer
Country                                              United States
City                                                       Houston
State                                                        Texas
Postal Code                                                  77036
Region                                                     Central
Product ID                                         OFF-AP-10002534
Category                                           Office Supplies
Sub-Category                                            Appliances
Product Name     3.6 Cubic Foot Counter Height Office Refrigerator
Sales                                                       294.62
Quantity                                                         5
Discount                                                       0.8
Profit                                                    -766.012
Name: 1995, dtype: object
```

Figure 17

For this particular order, a customer purchased 5 products with total price at 294.62 and profit at lower than -766, with 80% discount. It seems like a clearance. We should be aware of the loss for each product we sell.

```
df.iloc[9649]
```

```
Row ID                                   9650
Order ID                       CA-2016-107104
Order Date                2016-11-26 00:00:00
Ship Date                 2016-11-30 00:00:00
Ship Mode                      Standard Class
Customer ID                          MS-17365
Customer Name             Maribeth Schnelling
Segment                              Consumer
Country                         United States
City                              Los Angeles
State                              California
```

```
State                                          California
Postal Code                                         90045
Region                                               West
Product ID                                FUR-BO-10002213
Category                                        Furniture
Sub-Category                                    Bookcases
Product Name     DMI Eclipse Executive Suite Bookcases
Sales                                             3406.66
Quantity                                                8
Discount                                             0.15
Profit                                            160.314
Name: 9649, dtype: object
```

Figure 18

For this purchase, it seems to me that the profit at around 4.7% is too small and the model determined that this order is an anomaly.

```
df.iloc[9270]
```

```
Row ID                                               9271
Order ID                                   US-2017-102183
Order Date                            2017-08-21 00:00:00
Ship Date                             2017-08-28 00:00:00
Ship Mode                                  Standard Class
Customer ID                                      PK-19075
Customer Name                                  Pete Kriz
Segment                                          Consumer
Country                                     United States
City                                        New York City
State                                            New York
Postal Code                                         10035
Region                                               East
Product ID                                OFF-BI-10001359
Category                                  Office Supplies
Sub-Category                                      Binders
Product Name     GBC DocuBind TL300 Electric Binding System
```

```
Sales                                   4305.55
Quantity                                      6
Discount                                    0.2
Profit                                  1453.12
Name: 9270, dtype: object
```

Figure 19

For the above order, a customer purchased 6 product at 4305 in total price, after 20% discount, we still get over 33% of the profit. We would love to have more of these kind of anomalies.

Jupyter notebook for the above analysis can be found on Github. Enjoy the rest of the week.

Data Science Machine Learning Anomaly Detection Machine Learning Tutorial

Unsupervised Learning