K Means++

Measuring Cluster Quality

Supervised method

Homogeneity: Each cluster contains only members of a single class.

Completeness: All members of a given class are assigned to the same cluster.

Unsupervised method

Sihouette Coefficient: Evaluate how well the **compactness** and the **separation** of the clusters are. (Note that the notation below is consistent with the above content.) Using Sihouette Coefficient, we can choose an optimal value for number of clusters.

 $a(x_i)$ denotes the **mean intra-cluster distance**. Evaluate the compactness of the cluster to which x_i belongs. (The smaller the more compact)

$$a(x_i) = rac{\sum_{x_k \in C_j, \, k
eq i} D(x_i, x_k)}{|C_i| - 1}$$

For the data point x_i , caculate its average distance to all the other data points in its cluster. (Minusing one in denominator part is to leave out the current data point x_i)

 $b(x_i)$ denotes the **mean nearest-cluster distance**. Evaluate how x_i is separated from other clusters. (The larger the more separated)

$$b(x_i) = \min_{C_j:\, 1 \leq j \leq k, \, x_i
otin C_j} \left\{ rac{\sum_{x_k \in C_j} D(x_i, x_k)}{|C_j|}
ight\}$$

For the data point x_i and all the other clusters not containing x_i , caculate its average distance to all the other data points in the given clusters. Find the minimum distance value with respect to the given clusters.

Finally, Silhouette Coefficient: $s(x_i) = \frac{b(x_i) - a(x_i)}{\max\{a(x_i), b(x_i)\}}, \quad -1 \leq s(x_i) \leq 1.$ Want $a(x_i) < b(x_i)$ and $a(x_i) \to 0$ so as to $s(x_i) \to 1$.

KMeans groups all data points to each one of the 'K' clusters. These clusters have similar variance and they are derived by minimizing a specific cost function: sum of squares distance (Euclidean) within the cluster. K-Means can be seen as a special case of Gaussian mixture model (discussed later) with equal covariance per component.

- 1. Number of clusters are chosen
- 2. Randomly guess K cluster center locations
- 3. Each data point finds out which center it is closest to
- 4. Each center finds the centroid of the points in owns
- 5. K cluster center jumps to the new centroid and repeats steps 3 and 4
- 6. Step 5 is repeated until it is terminated

The k-means algorithm makes all-or-nothing assignments of data points to clusters, and these hard decisions can often lead to poor solutions corresponding to local minima. Also it is very sensitive to initialization therefore prone to local minima. It responds poorly to elongated clusters, or manifolds with irregular shapes. In very high-dimensional spaces, Euclidean distances tend to become inflated (this is an instance of the so-called "curse of dimensionality"). Running a dimensionality reduction algorithm such as PCA (discussed later) prior to K-means clustering can alleviate this problem and speed up the computations.

K-Means++ is the default setting. It is a variant of K-means, where the algorithm randomly chooses one centroid from data points using weighted probability distribution proportional to the distance square. This initializes the centroids to be (generally) distant from each other, leading to provably better results than random initialization Speeds up convergence.

The Algorithm

- 1. Randomly choose k centroids $C=\{c_1,c_2,\dots,c_k\}$ from the data points $X=\{x_1,x_2,\dots,x_n\}\in\mathbb{R}^D.$
- 2. For each data point x_i , find the nearest centroid c_j as its corresponding cluster using sum of squared distance $D(x_i,c_j)=\sum_{i=1}^n\|x_i-c_j\|^2$.
- 3. For each cluster, update its centroid by computing means value along the dimension of data points in the cluster.
- 4. Compute the displacement between the old and the new centroids and repeat steps 2 and 3 if the displacement is less than a threshold (converged).

```
In [1]: | from sklearn import datasets
        from sklearn import preprocessing
        from sklearn.model selection import train test split
        from sklearn.cluster import KMeans
        from sklearn.ensemble import IsolationForest
        from sklearn.neighbors import LocalOutlierFactor
        from sklearn import svm, neighbors
        from sklearn.neighbors import NearestNeighbors
        from sklearn.metrics import classification report
        from sklearn.metrics import confusion_matrix
        from sklearn.metrics import recall score
        from sklearn.metrics import roc auc score
        from sklearn.model selection import GridSearchCV
        from sklearn.metrics import make scorer
        from sklearn.metrics import accuracy score
        import pandas as pd
        import numpy as np
        import itertools
        import matplotlib.pyplot as plt
        import datetime
        %matplotlib inline
```

```
Out[2]: (237024, 58)
```

```
In [3]: column_list=df.columns.tolist()
```

In [4]: df.head()

Out[4]: _____

	originalloanamount	originalloanterm	originalinterestratepercentage	graceperiodnuml
0	66711.84	60	3.29	1
1	16258.45	60	0.90	0
2	31930.41	72	2.90	1
3	26065.02	65	0.90	0
4	42091.00	72	3.90	0

5 rows × 58 columns

```
In [5]: # prepare label for scikit-learn
Y=df.label.values
Y.shape
```

Out[5]: (237024,)

```
In [6]: # prepare input data for scikit-learn
input=df.values
input.shape
```

Out[6]: (237024, 58)

```
In [7]: # calculate train/test split
    len_train = int(len(input)*train_split)
    print(len_train)
```

189619

```
In [8]: # apply train/test split to labels
    y_train = Y[0:len_train]
    y_test = Y[len_train:]
    x_train = input[0:len_train]
    x_test = input[len_train:]
    x_train.shape
```

Out[8]: (189619, 58)

```
In [9]: export_x_test = pd.DataFrame(data=x_test)
```

```
In [10]: export_x_test.columns=column_list
    export_x_test.rename(columns={'label':'True Label'}, inplace=True)
    export_x_test.head()
```

Out[10]:

	originalloanamount	originalloanterm	originalinterestratepercentage	graceperiodnuml
0	36863.24	72.0	1.00	1.0
1	23811.32	60.0	1.90	0.0
2	30669.00	48.0	1.00	1.0
3	54083.21	72.0	1.00	0.0
4	31557.75	72.0	3.89	1.0

5 rows × 58 columns

```
In [11]: #from sklearn.preprocessing import MinMaxScaler
    # from sklearn.preprocessing import minmax_scale
    # from sklearn.preprocessing import MaxAbsScaler
    from sklearn.preprocessing import StandardScaler
    # from sklearn.preprocessing import RobustScaler
    # from sklearn.preprocessing import Normalizer
    # from sklearn.preprocessing import QuantileTransformer
    # from sklearn.preprocessing import PowerTransformer
```

```
In [12]: x_scaler=StandardScaler()
x_train = x_scaler.fit_transform(x_train)
x_test = x_scaler.fit_transform(x_test)
```

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http://localhost:8888/nbconvert/html/31.%20loan_K_Means%2B%2B%20-Unsupervised.ipynb?download=false

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done sorting end inner loop Iteration 4, inertia 9207731.28326 start iteration done sorting end inner loop Iteration 5, inertia 9200325.73697 start iteration done sorting end inner loop Iteration 6, inertia 9195591.1339 start iteration done sorting end inner loop Iteration 7, inertia 9192574.90395 start iteration done sorting end inner loop Iteration 8, inertia 9190517.56316 start iteration done sorting end inner loop Iteration 9, inertia 9188959.97424 start iteration done sorting end inner loop Iteration 10, inertia 9187554.944 start iteration done sorting end inner loop Iteration 11, inertia 9186226.77247 start iteration done sorting end inner loop Iteration 12, inertia 9184945.07166 start iteration done sorting end inner loop Iteration 13, inertia 9183525.72792 start iteration done sorting end inner loop Iteration 14, inertia 9181905.20171 start iteration done sorting end inner loop Iteration 15, inertia 9179921.12828 start iteration done sorting end inner loop Iteration 16, inertia 9177114.05967 start iteration done sorting end inner loop Iteration 17, inertia 9173118.54183 start iteration done sorting

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Initialization complete

start iteration

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```
start iteration

done sorting

end inner loop

Iteration 28, inertia 8971527.64063

start iteration

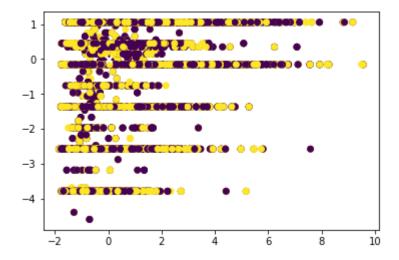
done sorting

end inner loop

Iteration 29, inertia 8971527.64063

center shift 0.000000e+00 within tolerance 8.965517e-05
```

Out[15]: <matplotlib.collections.PathCollection at 0x27507e84320>



```
In [16]: x_pred = x_test
```

```
In [17]: prediction_kmeans = kmeans_plus_plus.predict(x_pred)
```

```
In [18]: # We can get distances from data point to every centroid

""" The below code is equivalent to:
    from sklearn.metrics.pairwise import euclidean_distances
    euclidean_distances(X_new, kmeans.cluster_centers_)
    """

kmeans_plus_plus.transform(x_pred)
```

In [19]: export_x_test['Predicted Label']=prediction_kmeans

In [20]: export_x_test.head()

Out[20]:

	originalloanamount	originalloanterm	originalinterestratepercentage	graceperiodnuml
0	36863.24	72.0	1.00	1.0
1	23811.32	60.0	1.90	0.0
2	30669.00	48.0	1.00	1.0
3	54083.21	72.0	1.00	0.0
4	31557.75	72.0	3.89	1.0

5 rows × 59 columns

In [21]: export_x_test.shape

Out[21]: (47405, 59)

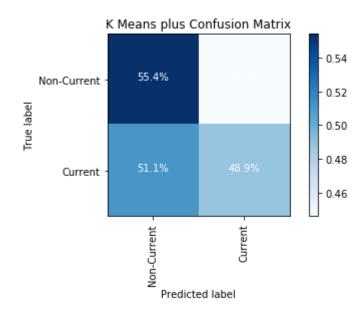
In [22]: export_x_test.to_csv(path+"prediction/kmeans/predicated_kmeans_plus_unsupervis
ed_abs_loans_"+str(nrows)+".csv", chunksize=10000)

```
In [23]: def plot confusion matrix(cm, title, classes=['Non-Current', 'Current'],
                                    cmap=plt.cm.Blues, save=False, saveas="MyFigure.pn"
         g"):
             # print Confusion matrix with blue gradient colours
             cm = cm.astype('float') / cm.sum(axis=1)[:, np.newaxis]
             plt.imshow(cm, interpolation='nearest', cmap=cmap)
             plt.title(title)
             plt.colorbar()
             tick_marks = np.arange(len(classes))
             plt.xticks(tick_marks, classes, rotation=90)
             plt.yticks(tick marks, classes)
             fmt = '.1%'
             thresh = cm.max() / 2.
             for i, j in itertools.product(range(cm.shape[0]), range(cm.shape[1])):
                  plt.text(j, i, format(cm[i, j], fmt),
                           horizontalalignment="center",
                           color="white" if cm[i, j] > thresh else "black")
             plt.tight layout()
             plt.ylabel('True label')
             plt.xlabel('Predicted label')
             if save:
                 plt.savefig(saveas, dpi=100)
```

```
In [24]:
         def plot gridsearch cv(results, estimator, x min, x max, y min, y max,save=Fal
         se, saveas="MyFigure.png"):
             # print GridSearch cross-validation for parameters
             plt.figure(figsize=(10,8))
             plt.title("GridSearchCV for "+estimator, fontsize=24)
             plt.xlabel(estimator)
             plt.ylabel("Score")
             plt.grid()
             ax = plt.axes()
             ax.set xlim(x min, x max)
             ax.set ylim(y min, y max)
             pad = 0.005
             X axis = np.array(results["param "+estimator].data, dtype=float)
             for scorer, color in zip(sorted(scoring), ['b', 'k']):
                 for sample, style in (('train', '--'), ('test', '-')):
                     sample_score_mean = results['mean_%s_%s' % (sample, scorer)]
                     sample score std = results['std %s %s' % (sample, scorer)]
                     ax.fill between(X axis, sample score mean - sample score std,
                                  sample score mean + sample score std,
                                  alpha=0.1 if sample == 'test' else 0, color=color)
                     ax.plot(X axis, sample score mean, style, color=color,
                         alpha=1 if sample == 'test' else 0.7,
                         label="%s (%s)" % (scorer, sample))
                 best_index = np.nonzero(results['rank_test_%s' % scorer] == 1)[0][0]
                 best_score = results['mean_test_%s' % scorer][best_index]
                 # Plot a dotted vertical line at the best score for that scorer marked
          by x
                 ax.plot([X_axis[best_index], ] * 2, [0, best_score],
                     linestyle='-.', color=color, marker='x', markeredgewidth=3, ms=8)
                 # Annotate the best score for that scorer
                 ax.annotate("%0.2f" % best score,
                         (X_axis[best_index], best_score+pad))
             plt.legend(loc="best")
             plt.grid('off')
             plt.tight layout()
             if save:
                 plt.savefig(saveas, dpi=100)
             plt.show()
```

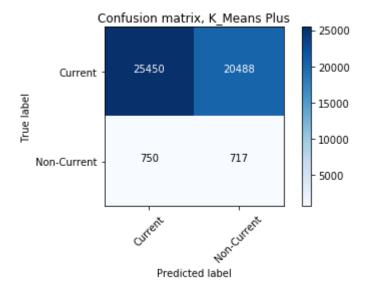
	precision	recall	f1-score	support
Non-Current	0.97	0.55	0.71	45938
Current	0.03	0.49	0.06	1467
avg / total	0.94	0.55	0.69	47405

AUC: 52.1%



```
In [26]: class names = ['Current', 'Non-Current']
         def plot confusion matrix(cm, classes,
                                    normalize=False,
                                    title='Confusion matrix',
                                    cmap=plt.cm.Blues):
              .. .. ..
             This function prints and plots the confusion matrix.
             Normalization can be applied by setting `normalize=True`.
             if normalize:
                  cm = cm.astype('float') / cm.sum(axis=1)[:, np.newaxis]
                 print("Normalized confusion matrix")
             else:
                  print('Confusion matrix, without normalization')
             print(cm)
             plt.imshow(cm, interpolation='nearest', cmap=cmap)
             plt.title(title)
             plt.colorbar()
             tick_marks = np.arange(len(classes))
             plt.xticks(tick marks, classes, rotation=45)
             plt.yticks(tick_marks, classes)
             fmt = '.2f' if normalize else 'd'
             thresh = cm.max() / 2.
             for i, j in itertools.product(range(cm.shape[0]), range(cm.shape[1])):
                  plt.text(j, i, format(cm[i, j], fmt),
                           horizontalalignment="center",
                           color="white" if cm[i, j] > thresh else "black")
             plt.ylabel('True label')
             plt.xlabel('Predicted label')
             plt.tight_layout()
         print('ROC_AUC_SCORE ; ', roc_auc_score(y_test, prediction_kmeans))
         # Compute confusion matrix
         cnf matrix = confusion matrix(y test, prediction kmeans)
         np.set_printoptions(precision=2)
         # Plot non-normalized confusion matrix
         plt.figure()
         plot confusion matrix(cnf matrix, classes=class names, title= 'Confusion matri
         x, K Means Plus')
         plt.savefig('prediction/kmeans/cm'+str(' K_Means plus Prediction-')+str(nrows)
         +'.jpg')
         plt.show()
```

ROC_AUC_SCORE; 0.521380065832 Confusion matrix, without normalization [[25450 20488] [750 717]]

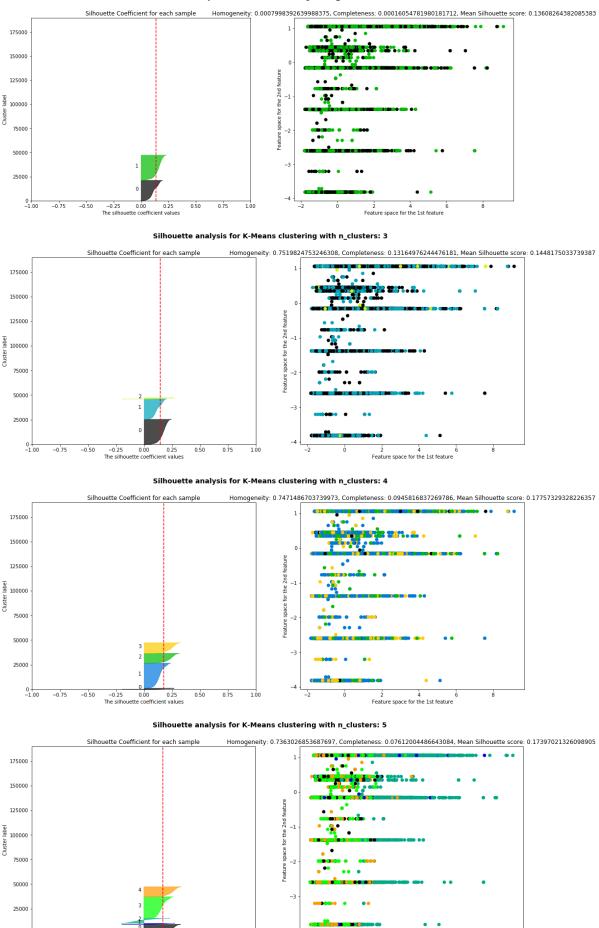


Silhoutte Analysis Various cluster Sizes

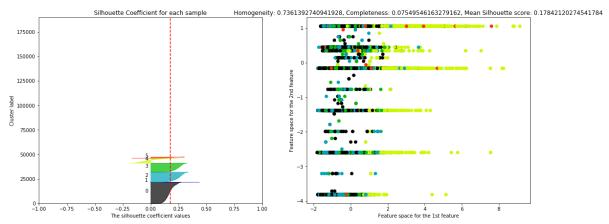
```
In [30]: from sklearn import metrics
         import matplotlib.cm as cm
         # List of number of clusters
         range_n_clusters = [2, 3, 4, 5, 6]
         # For each number of clusters, perform Silhouette analysis and visualize the
         results.
         for n_clusters in range_n_clusters:
            # Perform k-means.
            kmeans = KMeans(n_clusters=n_clusters, random_state=10)
            y_pred = kmeans.fit_predict(x_test)
            # Compute the cluster homogeneity and completeness.
            homogeneity = metrics.homogeneity_score(y_test, y_pred)
            completeness = metrics.completeness_score(y_test, y_pred)
            # Compute the Silhouette Coefficient for each sample.
            s = metrics.silhouette samples(x test, y pred)
            # Compute the mean Silhouette Coefficient of all data points.
            s mean = metrics.silhouette score(x test, y pred)
            # For plot configuration -------
                 -----
            fig, (ax1, ax2) = plt.subplots(1, 2)
            fig.set_size_inches(18, 7)
            # Configure plot.
            plt.suptitle('Silhouette analysis for K-Means clustering with n_cluster
         s: {}'.format(n_clusters),
                         fontsize=14, fontweight='bold')
            # Configure 1st subplot.
            ax1.set_title('Silhouette Coefficient for each sample')
            ax1.set_xlabel("The silhouette coefficient values")
            ax1.set_ylabel("Cluster label")
            ax1.set xlim([-1, 1])
            ax1.set_ylim([0, len(x_train) + (n_clusters + 1) * 10])
            # Configure 2st subplot.
            ax2.set_title('Homogeneity: {}, Completeness: {}, Mean Silhouette score:
          {}'.format(homogeneity,
                    completeness,
                    s_mean))
            ax2.set xlabel("Feature space for the 1st feature")
            ax2.set ylabel("Feature space for the 2nd feature")
            # For 1st subplot ------
            # Plot Silhouette Coefficient for each sample
            y_lower = 10
```

```
for i in range(n_clusters):
   ith_s = s[y_pred == i]
   ith_s.sort()
   size_cluster_i = ith_s.shape[0]
   y_upper = y_lower + size_cluster_i
   color = cm.nipy_spectral(float(i) / n_clusters)
   ax1.fill_betweenx(np.arange(y_lower, y_upper), 0, ith_s,
                    facecolor=color, edgecolor=color, alpha=0.7)
   ax1.text(-0.05, y_lower + 0.5 * size_cluster_i, str(i))
   y lower = y upper + 10
# Plot the mean Silhouette Coefficient using red vertical dash line.
ax1.axvline(x=s mean, color="red", linestyle="--")
# For 2st subplot ------
# Plot the predictions
colors = cm.nipy_spectral(y_pred.astype(float) / n_clusters)
ax2.scatter(x_test[:,0], x_test[:,1], c=colors)
```

Silhouette analysis for K-Means clustering with n_clusters: 2



Silhouette analysis for K-Means clustering with n_clusters: 6



In []: