COMP6036: Advanced Machine Learning
An investigation into DBSCAN

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Abstract

The paper chosen for the research report is entitled ***A density-based algorithm for discovering clusters in large spatial databases with noise*** *where the algorithm DBSCAN is introduced. DBSCAN is used for clustering sparse spatial databases using data point density. The algorithm performs well at this but has some shortcomings when applied to tasks which hold clusters of different densities. Only one priori, cluster density, is required but this can be difficult to tune in high dimensional space. The algorithm is compared against other common cluster implementations using a machine learning toolkit for Python.*

1 Motivation for Algorithm

DBSCAN (Density-Based Spatial Clustering of Applications with Noise) is an unsupervised application of machine learning introduced by Ester et al. (1996). Intended to address Spatial Database Systems (SDBS) which can be produced from natural geometric and geographical datasets or applications such a layout for integrated circuit design (Güting, 1994). It has three main objectives. To minimise the required domain knowledge needed to set input parameters, have the capability to discover clusters of arbitrary shapes and to perform well on large spatial databases.

At the time of creation the algorithms was compared to a recent development called CALARANS (Raymond and Jiawei, 1994) which is an extension of CLARA (Clustering LARge Applications) (Kaufman and Rousseeuw, 1990). Both algorithms are intended for use on large databases but CLARANS uses random noise to improve performance. Apart from traditional clustering algorithms, such a K-means, DBSCAN was a breakthrough in terms of a density approach to datasets.

2 Technical Explanation

DBSCAN uses cluster density to classify data. It is intuitive to build a community of data points by attempting to draw a path of connectivity between points. This leads to the first input parameter to the algorithm, ϵ, which is a threshold for the distance that DBSCAN is permitted to move yet

remain in the same cluster. Equation (1), adapted from Ester et al. (1996), is the basic function used to determine membership by thresholding; euclidean distance is used in this case but the measure of distance can be replaced with a Manhattan norm to scale down computational overheads (Krause, 1986). Only two input patterens are compare at once and all belong to the set of training data, $\mathbf{x}$, containing n input patterns.

$$N(\mathbf{p}, \mathbf{q}, \epsilon) = \begin{cases} 1, \ ||\mathbf{p} - \mathbf{q}|| \leq \epsilon \\ 0, \ ||\mathbf{p} - \mathbf{q}|| > \epsilon \end{cases} \quad where \ \mathbf{q}, \mathbf{p} \in \mathbf{x} \tag{1}$$

This approach is simple for compact clusters but when noise is introduced the algorithm will identify a few points as a whole cluster. This is down to a badly tuned value for ϵ but can be negated by introducing a second threshold to set the minimum number of members a cluster can have however this is unnecessary to perform basic DBSCAN clustering. This parameter, λ, if successfully applied to Equation (2) decides when to build a cluster around the point. Equation (3) takes the sum of connected datapoints attributed to a single point which used for the comparison in Equation (2). A low dimensional representation of the constraints used in DBSCAN is held in Figure 1. A string of points are density connected in the centre of the diagram but the two points on the left and right are both outside the set range. Increasing ϵ will introduce the right point to the growing cluster first then the left point. In this case λ set to 1 would produce 3 clusters, no clusters if above 5 and one cluster otherwise.

$$\lambda \leq C(\mathbf{p}, \epsilon) \tag{2}$$

$$C(\mathbf{x}_i, \epsilon) = \sum_{\substack{j=1 \\ j \neq i}}^{n} N(\mathbf{x}_i, \mathbf{x}_j, \epsilon) \tag{3}$$

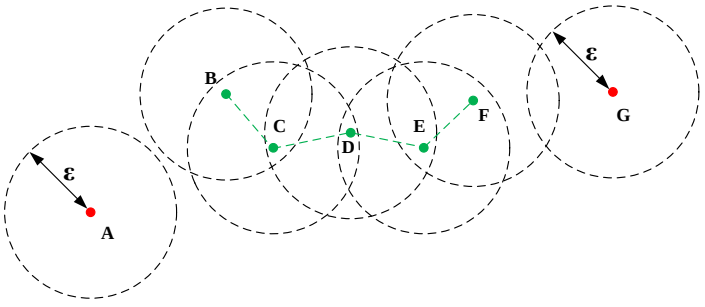
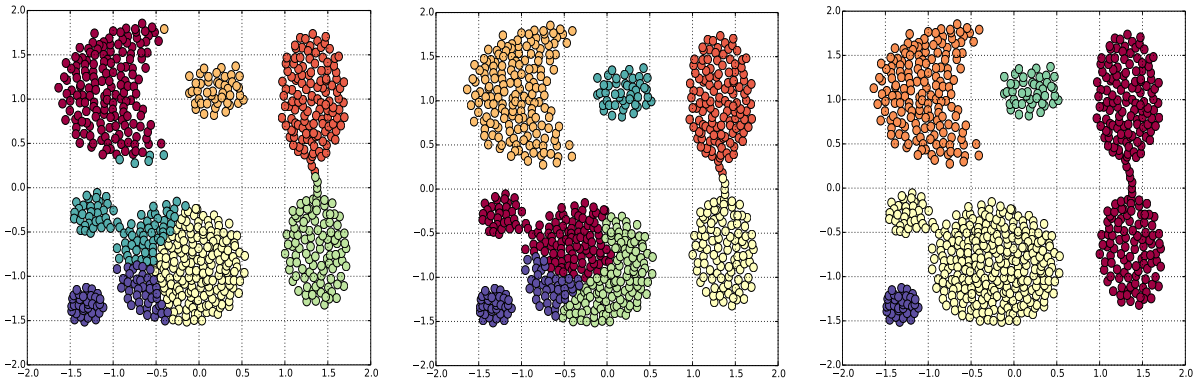


FIGURE 1: 2D application of DBSCAN.

It is clear there is a lot of scope for optimisation in practice. A list containing all datapoints at the start of the algorithm can be used to check off points which have been found to belong to a cluster. This means for an input space containing α clusters that can be perfectly segmented by DBSCAN requires only α calls of Equation (3). Formally a set of unclassified vectors, $\mathbf{b} \in \mathbf{x}$, can be defined and passed to Equation (3) requiring much fewer evaluations.

3 Performance

The graphs in Figure 2 are different clustering algorithms applied to a shape dataset taken from Gionis et al. (2005). Chosen for comparison is K-Means because it is arguably the most well-known clustering algorithm and WARD because of its performance on this dataset when compared against other available algorithms. Implementations were taken from a machine learning toolbox for Python (scikit learn, 2013). The dataset contains seven clusters but in two cases there are *bridges* between the clusters. On the far right K-Means and WARD correctly divides the data where DBSCAN incorrectly groups both clusters together; shown in Figures 2(a), 2(b) and 2(c) respectively. DBSCAN deals well with the remaining data where the other two algorithms fail due to its ability to negate relatively tight clusters.



(a) K-Means (b) WARD (c) DBSCAN

FIGURE 2: A comparison against DBSCAN.

The algorithm exhibits variation in performance as per the standard bias-variance dilemma. Figure 3 shows how the error varies for with ϵ when applied to data used in Figure 2. Objectively DBSCAN doesn't perform well on this dataset missing two clusters completely however this is crafted cornerstone case intended to trap algorithms.

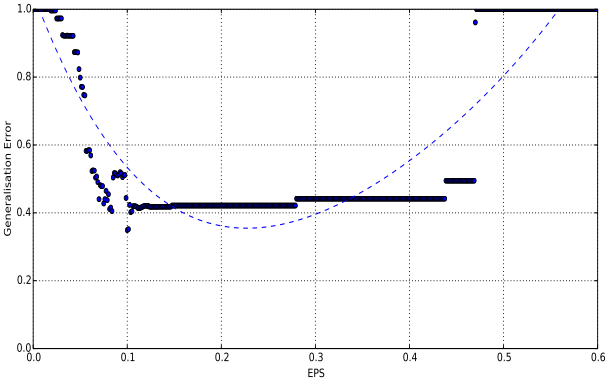


FIGURE 3: Generalisation error while varying the ϵ input parameter.

4 Extensions

Since the creation of this algorithm extension have been trialed .

Duan et al. (2007) considered the difficulty to select a value for ϵ and adapted the algorithm to LDBSCAN (Local-DBSCAN).

5 Conclusions

DBSCAN performs well on spatial database and can be optimised to be extremely efficient. As per most unsupervised clustering algorithms this is particularly appealing for good results with using simple methods. There are downsides to algorithm

References

Lian Duan, Lida Xu, Feng Guo, Jun Lee, and Baopin Yan. A local-density based spatial clustering algorithm with noise. In *Informations Systems Journal*, volume 32, pages 978–986, Now 2007.

Martin Ester, Hans peter Kriegel, Jrg S, and Xiaowei Xu. A density-based algorithm for discovering clusters in large spatial databases with noise. In *2nd International Conference on Knowledge Discovery and Data Mining (KDD-96)*, pages 226–231. AAAI Press, 1996.

Aristides Gionis, Heikki Mannila, and Panayiotis Tsaparas. Clustering aggregation. In *In Proceedings of the 21st International Conference on Data Engineering (ICDE)*, pages 341–352, 2005. Hosted by Speech and Image Processing Unit, University of Eastern Finland, `http://cs.joensuu.fi/sipu/datasets/` (Visited on 27/02/2014).

Ralf Hartmut Güting. An introduction to spatial database systems. *Very Large Database Journal (VLDB J.)*, 3(4):357–399, 1994.

Leonard Kaufman and Peter J. Rousseeuw. *Finding groups in data: an introduction to cluster analysis.* John Wiley and Sons, New York, 1990.

E.F. Krause. *Taxicab Geometry: An Adventure in Non-Euclidean Geometry.* Dover Books on Mathematics Series. Dover Publications, 1986. ISBN 9780486252025.

Ng T. Raymond and Han Jiawei. Efficient and effective clustering methods for spatial data mining. In *20th Very Large Database Conference, Santiago, Chile, 1994*, pages 144–155, 1994.

scikit learn. machine learning in python. `http://scikit-learn.org/stable/index.html`, 2013. (Visited on 02/27/2014).

A Code Listings

```
import numpy as np
from sklearn.cluster import KMeans
from sklearn import metrics
from sklearn.datasets.samples_generator import make_blobs
from sklearn.preprocessing import StandardScaler
import pylab as pl
pl.ion()

##############################################################################
# Load data
f = open('Datasets/Aggregation.txt','r')
X = []
labels_true = []
for line in f:
  x = line.split('\t')[0]
  y = line.split('\t')[1]
  label = line.split('\t')[0]
  label = label.replace('\n','')
  X.append([x,y])
  labels_true.append(label)
X = StandardScaler().fit_transform(X)

##############################################################################
# K-means Parameters
num = 7

##############################################################################
# Compute DBSCAN
db = KMeans(init='random',n_clusters=num).fit(X)
labels = db.labels_
# Number of clusters in labels, ignoring noise if present.
n_clusters_ = len(set(labels)) - (1 if -1 in labels else 0)

##############################################################################
# Plot result
# Black removed and is used for noise instead.
#fig = fig + 1
pl.figure(1)
unique_labels = set(labels)
colors = pl.cm.Spectral(np.linspace(0, 1, len(unique_labels)))
for k, col in zip(unique_labels, colors):
    if k == -1:
        # Black used for noise.
        col = 'k'
        markersize = 6
    class_members = [index[0] for index in np.argwhere(labels == k)]
    for index in class_members:
        x = X[index]
        pl.plot(x[0], x[1], 'o', markerfacecolor=col,
                markeredgecolor='k',markersize=10)
pl.grid()
pl.show()
raw_input("Press Enter to continue...")
```

LISTING 1: K-Means clustering.

```
import numpy as np
from sklearn.cluster import Ward
from sklearn import metrics
from sklearn.datasets.samples_generator import make_blobs
from sklearn.preprocessing import StandardScaler
import pylab as pl
pl.ion()

##############################################################################
# Load data
f = open('Datasets/Aggregation.txt','r')
X = []
labels_true = []
for line in f:
  x = line.split('\t')[0]
  y = line.split('\t')[1]
  label = line.split('\t')[0]
  label = label.replace('\n','')
  X.append([x,y])
  labels_true.append(label)
X = StandardScaler().fit_transform(X)

##############################################################################
# K-means Parameters
num = 7

##############################################################################
# Compute WARD
db = Ward(n_clusters=num,connectivity=None).fit(X)
labels = db.labels_
# Number of clusters in labels, ignoring noise if present.
n_clusters_ = len(set(labels)) - (1 if -1 in labels else 0)

##############################################################################
# Plot result
# Black removed and is used for noise instead.
#fig = fig + 1
pl.figure(1)
unique_labels = set(labels)
colors = pl.cm.Spectral(np.linspace(0, 1, len(unique_labels)))
for k, col in zip(unique_labels, colors):
    if k == -1:
        # Black used for noise.
        col = 'k'
        markersize = 6
    class_members = [index[0] for index in np.argwhere(labels == k)]
    for index in class_members:
        x = X[index]
        pl.plot(x[0], x[1], 'o', markerfacecolor=col,
                markeredgecolor='k',markersize=10)
pl.grid()
pl.show()
raw_input("Press Enter to continue...")
```

Listing 2: WARD Clustering.

```
import numpy as np
from sklearn.cluster import DBSCAN
from sklearn import metrics
from sklearn.datasets.samples_generator import make_blobs
from sklearn.preprocessing import StandardScaler
import pylab as pl
pl.ion()

##############################################################################
# Load data
f = open('Datasets/Aggregation.txt','r')
X = []
labels_true = []
for line in f:
  x = line.split('\t')[0]
  y = line.split('\t')[1]
  label = line.split('\t')[0]
  label = label.replace('\n','')
  X.append([x,y])
  labels_true.append(label)
X = StandardScaler().fit_transform(X)

##############################################################################
# DBSCAN Parameters
eps = 0.2
min_samples = 1
##############################################################################
# Compute DBSCAN
db = DBSCAN(eps, min_samples).fit(X)
core_samples = db.core_sample_indices_
labels = db.labels_
# Number of clusters in labels, ignoring noise if present.
n_clusters_ = len(set(labels)) - (1 if -1 in labels else 0)

##############################################################################
# Plot result
pl.figure(1)
unique_labels = set(labels)
colors = pl.cm.Spectral(np.linspace(0, 1, len(unique_labels)))
for k, col in zip(unique_labels, colors):
    if k == -1:
        # Black used for noise.
        col = 'k'
        markersize = 6
    class_members = [index[0] for index in np.argwhere(labels == k)]
    cluster_core_samples = [index for index in core_samples
                            if labels[index] == k]
    for index in class_members:
        x = X[index]
        if index in core_samples and k != -1:
            markersize = 14
        else:
            markersize = 6
        pl.plot(x[0], x[1], 'o', markerfacecolor=col,
                markeredgecolor='k', markersize=10)
#pl.title('DBSCAN - %d Clusters' % n_clusters_)
pl.grid()
pl.show()
raw_input("Press Enter to continue...")
```

LISTING 3: DBSCAN Clustering.

```
import numpy as np
from sklearn.cluster import DBSCAN
from sklearn import metrics
from sklearn.datasets.samples_generator import make_blobs
from sklearn.preprocessing import StandardScaler
import pylab as pl
pl.ion()

##############################################################################
# Load data
f = open('Datasets/Aggregation.txt','r')
X = []
labels_true = []
for line in f:
  x = line.split('\t')[0]
  y = line.split('\t')[1]
  label = line.split('\t')[0]
  label = label.replace('\n','')
  X.append([x,y])
  labels_true.append(label)
X = StandardScaler().fit_transform(X)
##############################################################################
# DBSCAN Parameters
eps = 0.47
min_samples = 1
score = []
para = []
for test in range(1,480):
  eps = float(test)/float(800)
  ##############################################################################
  # Compute DBSCAN
  db = DBSCAN(eps, min_samples).fit(X)
  core_samples = db.core_sample_indices_
  labels = db.labels_
  # Number of clusters in labels, ignoring noise if present.
  n_clusters_ = len(set(labels)) - (1 if -1 in labels else 0)
  score.append(metrics.adjusted_mutual_info_score(labels_true, labels))
  para.append(eps)
  if(score[test-1] < 0):
    score[test-1] = 0;
  score[test-1] = 1 - (score[test-1]*10)
  print("%0.3f: Score: %0.3f" % (eps, score[test-1]))
pl.plot(para,score, '.', markeredgecolor='k', markersize=10)
coefs = np.lib.polyfit(para, score, 4) #4
fit_y = np.lib.polyval(coefs, para) #5
pl.plot(para, fit_y, 'b—') #6
pl.ylim([0,1])
pl.grid()
pl.xlabel('EPS')
pl.ylabel('Generalisation Error')
raw_input("Press Enter to continue...")
```

Listing 4: Tuning DBSCAN.