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*** *which introduces the algorithm DBSCAN. 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 the algorithm is very sensitive to this and can be difficult to tune in high dimensional space. DBSCAN is compared against other common cluster implementations using a machine learning toolkit for Python before more recent extensions are considered.*

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 naturally occurring geometric and geographical data or engineering 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 where first principles are introduced, 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 therefore favouring large datasets (Krause, 1986). Only two input patterns are compared 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 possibly 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. Equation (2) takes the sum of connected data points attributed to a single point which used for the comparison in Equation (3). The parameter, λ, if successfully applied to Equation (3) decides when to build a cluster around the point.

$$C(\mathbf{x}_i, \mathbf{x}, \epsilon) = \sum_{\substack{j=1 \\ j \neq i}}^{n} N(\mathbf{x}_i, \mathbf{x}_j, \epsilon) \tag{2}$$

$$1 \leq \lambda \leq C(\mathbf{p}, \epsilon) \;\; where \;\; \lambda \in \mathbb{N} \tag{3}$$

A low dimensional representation of the constraints held by DBSCAN is shown in Figure 1. Six points, **C** to **G**, are density connected in the centre of the diagram, **A** and **B** form another connection while **H** is unconnected. The locus of each point is set by ϵ and must engulf another point for the algorithm to consider them connected. Equation (4) describes how possible values of λ, while keeping ϵ fixed, can change the clustering of Figure 1.

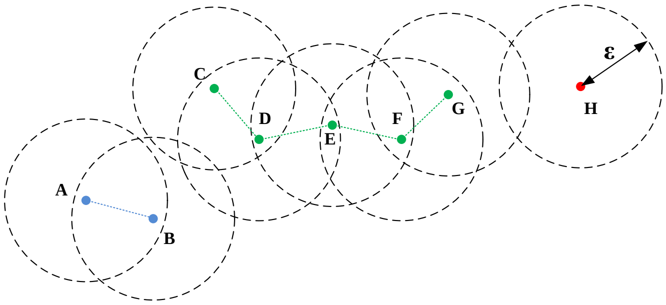


Figure 1: 2D application of DBSCAN.

$$\#Clusters = \begin{cases} 0 \, if \;\; \lambda \geq 6 \\ 1 \, if \;\; \lambda = 5 \\ 2 \, if \;\; 2 \leq \lambda \leq 5 \\ 3 \, if \;\; \lambda = 1 \end{cases} \tag{4}$$

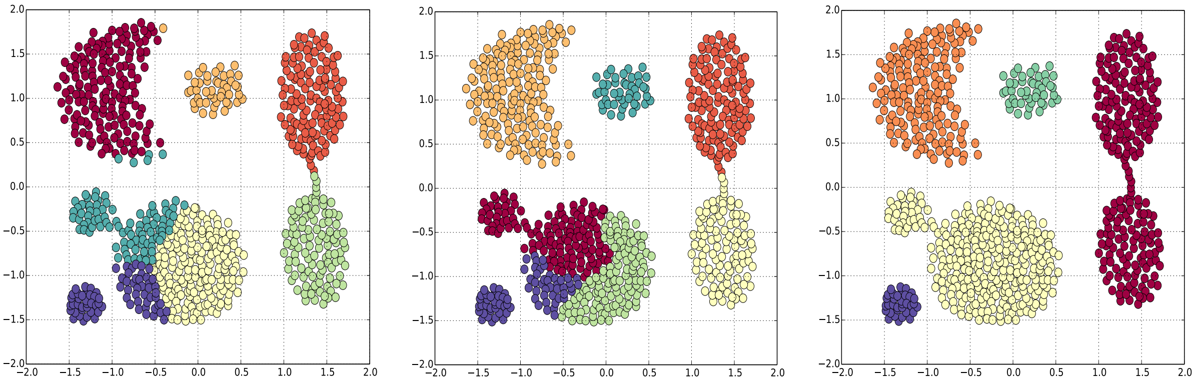
It is clear there is a lot of scope for optimisation in practice. A list containing all data points at the start of the algorithm can be used to check off points which have been found to belong to a cluster. This means for an input space containing α clusters that can be perfectly segmented by DBSCAN requires only α calls of Equation (2). Formally a set of unclassified vectors, $\mathbf{b} \in \mathbf{x}$, can be defined and passed to Equation (2) requiring much fewer evaluations.

3 Performance

The worst case performance of the basic algorithm is determined by the number of end cluster found by DBSCAN compared to the number of input patterns. If all the input patterns combined with a massive value of ϵ produce single cluster classification it is possible that $O(n)$ holds; this is based on the number of times Equation (1) has to be computed. Equation (5) shows how that as the number of clusters increase the algorithm tends towards $O(n^2)$. The first input pattern requires $n-1$ calls of Equation (1) regardless but in the worst case is has no reachable neighbours. The second requires $n-2$ as one pattern has already been identified as solitary yet again has no reachable neighbours. If this continues so that the last pattern is known to be solitary then Equation (5) shows how this geometric progression places an lower bound on performances. Low order polynomial time complexity is expected for an algorithm designed for large datasets.

$$\sum_{i=1}^{n-1} i = \frac{n}{2}(n-1) \approx O(n^2) \tag{5}$$

DBSCAN suffers from sensitivity to input parameters and also clustering in high dimensional space (Han et al., 2001). When attempting to cluster regions of different density it is clear that this is a major problem for the algorithm in certain applications. The graphs in Figure 2 are different clustering algorithms applied to a shape dataset taken from Gionis et al. (2005) which is chosen to empathise some less obvious shortcomings. 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[1] 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 of the space 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 ability to negate relatively tight clusters. These sorts of issues are the reason for ϵ sensitivity.



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

FIGURE 2: A comparison against DBSCAN.

[1] Code using the toolkit in Appendix A

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 a crafted cornerstone case intended to trap algorithms and is not particularly sparse. The two algorithms used for comparison both perform worse than DBSCAN.

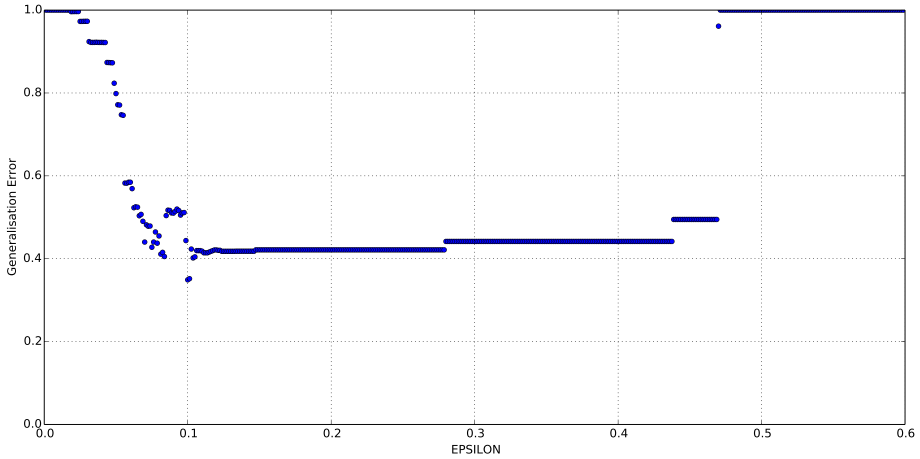


FIGURE 3: Generalisation error while varying the ϵ input parameter.

4 Extensions

The algorithm was revisited by its creators when they devised Generalzed-DBSCAN (Ester et al., 1998). GDBSCAN attempts to reduce sensitivity to input parameters by comparing prospective additions to a cluster against the sparsity of the rest of the cluster. There's also HDBSCAN (Hierarchical) which focuses on parallel optimisation (Li and Xi, 2011). A subset of the original authors went on the create OPTICS (Ordering Points to Identify the Clustering Structure) which is also a density based algorithm (Ankerst et al., 1999). This proved to become very popular as it performs well on datasets containing clusters of varying density. Duan et al. (2007) developed LDBSCAN (Local-DBSCAN) which draw on both DBSCAN and OPTICS to produce an easily tunable algorithm that adapts to local cluster density.

5 Conclusions

DBSCAN performs well on spatial databases and can be optimised to be extremely efficient. Datasets which are both large and spatial are common for which this algorithm is designed to classifiy. As per most unsupervised clustering algorithms this is particularly appealing for good results whilst using simple methods. There are downsides to algorithm such as sensitivity to input parameters and poor performance on mixed density clustering. As described in Section 3 there are also cornerstone cases which can trap the density process but are easily handled by standard centroid approaches.

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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('EPSILON')
pl.ylabel('Generalisation Error')
raw_input("Press Enter to continue...")
```

Listing 4: Tuning DBSCAN.