Mean-shift outlier detection

Jiawei YANG[a], Susanto RAHARDJA[b] and Pasi FRÄNTI[a,1]
[a] School of Computing, University of Eastern Finland
[b] Northwestern Polytechnical University, Xi'an, China

Abstract. We propose mean-shift to detect outlier points. The method processed every point by calculating its *k-nearest neighbors* (k-NN), and then shifting the point to the mean of its neighborhood. This is repeated three times. The bigger the movement, the more likely the point is an outlier. Boundary points are expected to move more than inner points; outliers more than inliers. The outlier detection is then a simple thresholding based on standard deviation of all movements. Points that move more than that are detected as outliers. The method outperforms all compared outlier detection methods.

Keywords. Boundary point, noise removal, outlier removal, mean-shift

Introduction

Outliers are points that deviate from the typical data. They can represent significant information that are wanted to be detected such as fraud detection, public health, and network intrusion [1], and they can affect statistical conclusions based on significance tests [2]. Outliers can also be noise points who might harm the data analysis process. In any case, it is desired that the outliers can be detected.

Outlier detection approaches fall roughly into *global* and *local* outlier models [3]. The global methods make a binary decision whether an observation is outlier while local methods assign a score to each point. This score indicates how likely a point is an outlier. The method then retrieves the top-n rankings as outliers, which gives more flexibility how to interpret the data.

However, even the local outlier models need to select the top-n parameter; how many points are chosen as outliers. In this paper, we propose a new local outlier detection method in which such parameter is not needed. We first calculate *outlier score* for all data points, and then calculate the standard deviation from the distribution of all outlier scores to serve as a global threshold. This can be automatically determined.

The way how we calculate the outlier scores is based on the idea presented in [4]. The effect of the noise is reduced by applying few iterations of medoid-shifting as follows. First we find *k-nearest neighbors* (k-NN) for every data point. Then we

[1] Corresponding Author.

replace the original points by the mean (or medoid) value of its neighbors. This process is iterated few times. This iterative process is demonstrated in Figure 1. However, instead of replacing the original point by its shifted version as in [4], we merely calculate how much it was moved, i.e. the distance between the original point and its shifted location. This distance defines the outlier score. Example of the outlier scores is shown in Figure 2.

The accuracy of the proposed method is far better than any other we tested. The method is robust as it provides the same result with the same global threshold parameter whereas all comparative methods use the a priori knowledge of the amount of noise. Unlike the other methods, it has only one parameter to set (the size of neighborhood k). The proposed method is also easy to understand and simple to implement.

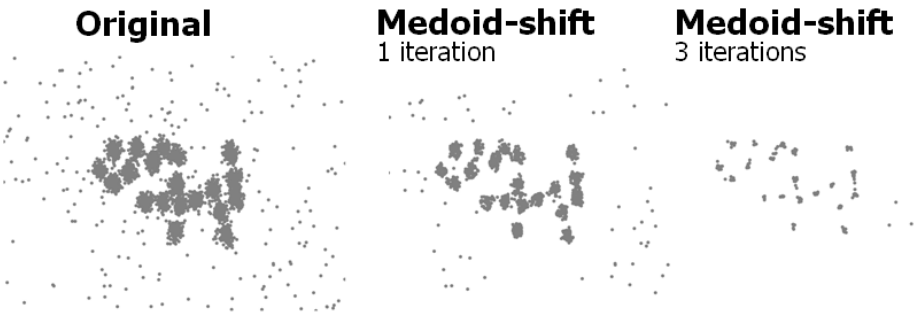

Figure 1. Example of the iterative process of the medoid-shift [4].

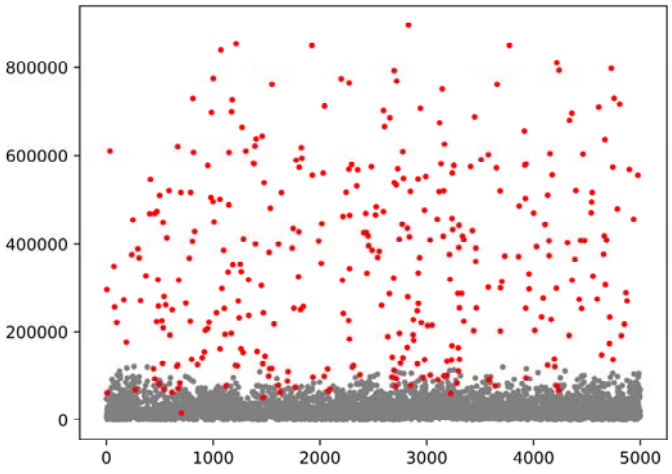

Figure 2. Outlier scores (y-axis) for S1 dataset: true data points (gray) and noise points (red). The results are for the proposed DOD method (using medoid).

1 Existing work and their limitations

Minimum covariance determinant (MCD) [5] is based on statistical test with the assumption that the true data objects follow a (known) distribution and occur in a high probability region of this model. Outliers are expected to deviate strongly from this distribution.

Distance-based approaches [6, 7, 8] are based on the assumption that true data objects have a dense neighborhood whereas outliers lie far apart from their neighbors. For example, in [9] a data point is marked as an outlier if there are at most k points within a given distance. The method in [6] calculates the k-nearest neighbors (k-NN), and use the distance to the k^{th} neighbor. A slightly modified variant in [7] uses the average distance to all the k neighbors. Points with largest distances are considered as outliers.

However, distance-based outlier detection models have problems if the data has areas of varying densities. Instead of using the distance values directly, a method called ODIN [7] analyzes the relationship of the point. For a given point, it calculates how many other points consider it as their k-nearest neighbor. The smaller the value, the more likely the point is an outlier.

Density-based approaches are based on analyzing the neighborhood of the points. *Local outlier factor* (LOF) [10] calculates the local density of the neighborhood. Points that have lower density than their neighbors are more likely outliers. LOF is the best method among those compared in [11], which comprises a very systematic set of experiments.

Topology of the neighborhood has also been considered in recent methods. In [12], a point is represented by convex combination of its k-nearest neighbors. For each point, the negative components in its representation correspond to the boundary points among its affine combination of points.

2 Mean-shift outlier detection

In this work, we proposed a simple and effective method, which has fewer parameters than the existing methods. We analyze data points locally based on their k-neighborhoods. We propose a method called *mean-shift outlier detection* (MOD).

2.1 Mean-shift process

The idea of mean-shift is to calculate k-nearest neighbors, and then replace the point by the mean of its k neighbors. This forces points to move towards denser areas. Hence the distance of movement can be an evidence of being outlier; points with greater movement are more likely to be outliers. The mean-shift process is summarized in Algorithm 1.

The idea is closely related to mean-shift filtering used in image processing [13], and mean-shift clustering algorithm [14]. The first one takes pixel value and its coordinates as the feature vector, and transforms each feature towards the mean of its neighbors. It has been used for detecting fingerprint and contamination defects in

multicrystalline solar wafers [15]. The idea resembles also low-pass and median filtering used for image denoising.

2.2 Mean-shift for outlier detection

Mean-shift clustering [14] iterates the process until convergence. However, since we are not clustering the data but aim at finding outliers, we use the processing result merely for analysis purpose. In specific, we calculate the location of the points before and after the shifting. This difference is used as the outlier score, called *mean-shift score*.

The final step is to detect the outliers. The key idea is to analyze the distribution of the obtained mean-shift scores. In specific, we calculate the standard deviation (SD) of all the scores in the dataset. This value is then used as global threshold; any point with bigger outlier score than SD is marked as an outlier. The pseudo code of the algorithm is summarized in Algorithm 2.

Both *mean* and *median* have been used in the mean-shift clustering concept [14, 16]. The benefit of using mean is that it is trivial to calculate for numeric data. However, it can cause blurring because a very noisy point can bias the calculation of the mean of clean points as well. *Medoid* can be more robust in this sense. It is calculated as the point that has minimal total distance to all other points in the same k-NN neighborhood. We call the two variants as *mean-shift outlier detection* (MOD) and *medoid-shift outlier detection* (DOD).

The method in [6] can be considered as a special case of our method with the following differences: (a) we iterate the process three times, (b) we calculate the threshold automatically, and (c) we use medoid instead of the mean. If we iterated only once, used mean, and did not calculate the SD then the method would equal to the variant of [6] except using the average distance to neighborhood [7]. The parameter three was chosen based on the experiments in [4].

Algorithm 1: Mean-shift process

Input: $\mathbf{X} \in R^{d \times n}$, k

Output: $\mathbf{Y} \in R^{d \times n}$

For every point $x \in \mathbf{X}$:

Step 1: Find its k-nearest neighbors $kNN(x)$
Step 2: Calculate the mean M of the neighbors $kNN(x)$
Step 3: Replace the point x by the mean M and save it to $\mathbf{Y}$

Algorithm 2: Mean-shift outlier detection (MOD)

Input: $\mathbf{X} \in R^{d \times n}$, k

Output: $\mathbf{N} \in R^{d \times n}$

Step 1: Repeat **Algorithm 1** three times to get $\mathbf{Y}$

Step 2: For every point $x_i \in \mathbf{X}$ and its shifted version $y_i \in \mathbf{Y}$ calculate distance $D_i = |x_i - y_i|$

Step 3:	Calculate the standard deviation (*SD*) of all D_i
Step 4:	For a point $x_i \in \mathbf{X}$ if $D_i > SD$, then x_i is detected as an outlier; save it to **N**.

3 Experiments

We test the proposed method based on Algorithm 2 with four existing outlier detection algorithms summarized in Table 1. We use the 9 benchmark datasets in Table 2 and visualized in Figure 4. The S sets have varying level of cluster overlap. A sets have varying number of clusters; unbalance and XOR datasets [17] have clusters with different densities. We evaluate the methods by F1-measure, which is basically the average of precision and recall. *Precision* is the ability of the classifier not to label as positive a sample that is negative, and *recall* is the ability of the classifier to find all the positive samples.

Table 1: Compared outlier detection algorithms; k=15 has been used in all tests.

Algorithms	Ref	Type	Parameters	Year	Publication
LOF	[9]	Density-based	k, top-N	2000	ACM SIGMOD
ODIN	[7]	Distance-based	k, top-N	2004	Int. Conf. on Pattern Recognition
MCD	[5]	Statistical testing	top-N	1984	J. Am. Stat. Assoc.
NC	[12]	Math. optimization	k, top-N	2018	IEEE-TNNLS
MOD	new	Shifting-based	k	2018	Int. Conf. Fuzzy Syst. Data Mining

Table 2: Datasets used in the experiments. (http://cs.uef.fi/sipu/datasets/)

Dataset:	Size:	Clusters:
S1-S4	5000	15
A1-A3	3000, 5250, 7500	20, 35, 50
Unbalance	6500	8
XOR	2000	4

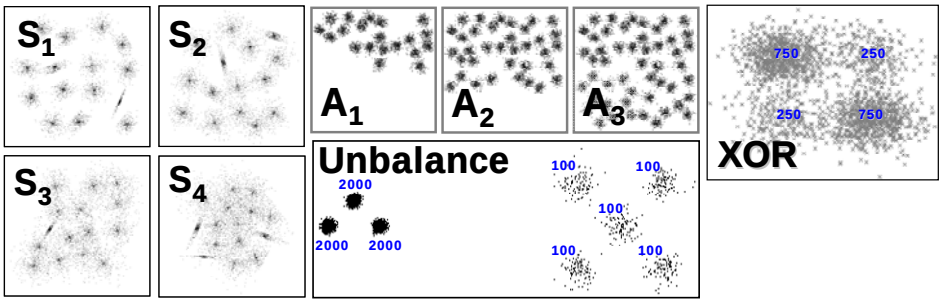

Figure 4. Datasets used in the experiments.

3.1 Noise models

We consider two types of noise:

1. Random noise
2. Data-dependent noise

In the first case, uniformly distributed random noise is added to the data. Random values are generated in each dimension between [x_{mean}-2·*range*, x_{mean}+2·*range*], where x_{mean} is the mean of all data points, and *range* is the maximum distance of any point from the mean: *range* = max(|x_{max}- x_{mean}|, |x_{mean}- x_{min}|). The amount of noise is 7% of data size. In the second case, 7% of the original points are copied and moved to random direction. Noisy datasets are shown in Figure 5.

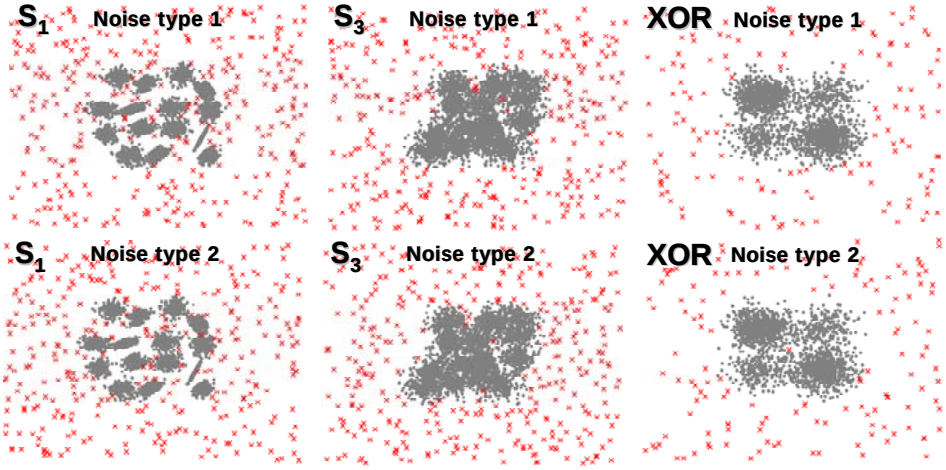

Figure 5. Noisy datasets S1, S3 and XOR with noise type 1 (up) and noise type 2 (down).

3.2 Results

The detection results are summarized in Fig. 6. The first results (gray) are obtained using a priori knowledge of the amount of noise (7%). Each method selects exactly the same amount of outliers. The second results (red) are when no a priori parameter is allowed but the algorithm is forced to solve the thresholding by its own.

Both proposed methods are better clearly better than the other methods tested (gap more than 4%). We can also see that the proposed method perform almost equally well when no threshold parameter (red results). No automatic thresholding were developed for the other methods, so comparative results are missing.

All methods based on k-NN require O(N^2) calculations. With our data this was not a problem but with bigger data it might become a bottleneck. For example, the running time for a dataset of size N=100,000 would be about 5 minutes. In this case, faster approximate like *NNDES* [18] or the *Random pair divisive* (RP-div) [19] can reduce the running time down to just a few seconds with only 1% gap in the accuracy.

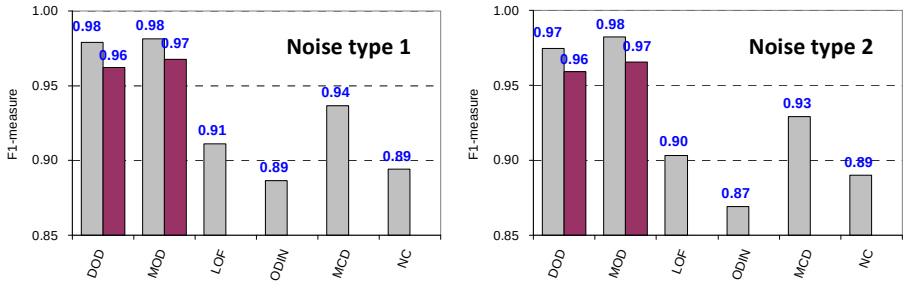

Figure 6. Average detection results for the 9 datasets in Table 2 and Figure 4. The gray results are obtained using a priori (7%) number of outliers, and the red results using the number of outliers automatically determined by the method.

4 Conclusions

Mean-shift outlier detection (MOD) was proposed. The results show that mean-shift variant (DOD) is slightly more effective than the medoid-shift. For the studied noise patterns, the proposed approach clearly outperforms existing outlier detection methods: LOF, ODIN, MCD and NC. The most important property of the proposed method is that it does not require any threshold parameter to tune.

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