Anomaly Detection Density Based Methods

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- clustering, distance and density
- k-Nearest Neighbors
- Local Outlier Factor
- Local Correlation Integral

The course references are Aggarwal 2017, Ch.4 with initial papers for K-NN by Cover and Hart 1967 and LOF by Breunig et al. 2000.



Algorithm Types

Given a data point, discriminate based on

- Clustering
 - non-membership to any data cluster of the data point
 - distance to other clusters
 - size of the closest cluster
 - binary: either belongs to cluster else is an anomaly
- Distance
 - proximity: distance to its k-nearest neighbor (KNN)
 - variants change distance type or average the distance score
 - Iarge KNN distances define the anomalies
 - high granularity results
 - ▶ high algorithmic complexity (e.g. $O(N^2)$)

Density

- split data space into regions
- compute the local density of each region
- data density is turned into anomaly score for each point
- clustering partitions data-points, density partitions data-space



Data Points vs Data Space



Figure: Data points and data space (Aggarwal 2017)



k-Nearest Neigbors



Exact KNN. The anomaly score of a point x is given by its distance to its k-th nearest neighbor.

Assumption: anomalous data points are further away than normal data points.

Example

We can identify small isolated clusters of k_0 anomalous data-points by selecting a value $k \ge k_0$ in the KNN algorithm.



KNN: the choice of k_0

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Figure: The choice of $k \ge k_0$ (Aggarwal 2017)





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- 2. Choose a distance function: $||x y||_2$ where $y \neq x$ and $y \in X$.
- 3. Compute the distances:



1. Choose a data-point: Let x be an *m*-dimensional point from the dataset $X \in \mathbb{R}^{m \times N}$.

2. Choose a distance function: $||x - y||_2$ where $y \neq x$ and $y \in X$.

3. Compute the distances: $dist(x) = \{ s \mid s = ||x - y||_2, \forall y \in X, y \neq X \}.$

4. Set the anomaly score:



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3. Compute the distances: $dist(x) = \{ s \mid s = ||x - y||_2, \forall y \in X, y \neq X \}.$

4. Set the anomaly score: $knn(x) = min_k(dist(x))$ where $min_k(\cdot)$ is the function computing the k-th smallest number in a set.

5. Repeat steps 1–4 for all points in X.



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Mitigations:

- pre-select a sample of data points $\tilde{N} \ll N$
- ▶ all N points are scored based on these \tilde{N} scores
- smoothing or averaging techniques can be applied post-processing to reduce sensibility to choice of \$\tilde{N}\$
- converges to a sort of clustering method





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Particular approach. Smoothen the anomaly score so that it is less sensible to a particular choice of k.



Average KNN score. The anomaly score of $x \in X$ is its average distance to its *k*-nearest neighbors.

Average KNN is:

- better suited for unsupervised grid-search where a range of k's are used
- \blacktriangleright it is less sensitive to the particular choices for k
- averages Exact-KNN over a range of k
- provides worse results than the true k value in the Exact-KNN variant

Formally, $avgknn(x) = \mu_k(dist(X))$, where $\mu_k(\cdot)$ is the average of the smallest k numbers in the set.



KNN Variants: Harmonic KNN Scores

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Local Outlier Factor



Problems: Density and Cluster Orientation



Figure: Data Locality (Aggarwal 2017)

- impacts data density and cluster orientation
- varying density across data space
- distance-based limitations when density variation is high



Example: Distance versus Locality



Figure: Distance versus Locality (Aggarwal 2017)

- two cluster with different sparsity
- A requires small distance threshold
- ▶ if k is small, then lots of false-positives in the sparse cluster
- need multiple distance thresholds in heterogeneous data distributions



Local Outlier Factor (LOF)

Let $L_k(\cdot)$ be the set of points that are the knn of a given point:

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- reachability is not symmetric!



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Proof in class



We now define the average reachability of a point in regards to its KNN's:

$$AR_k(x) = \mu_{y \in L_k(x)}R_k(x,y)$$

where μ is the average of each pair $R_k(x, y)$ with $y \in L_k(x)$. The inverse of AR_k is defined as the reachability density.



$$LOF_k(x) = \mu_{y \in L_k(x)} \frac{AR_k(x)}{AR_k(y)} = AR_k(x)\mu_{y \in L_k(x)} \frac{1}{AR_k(y)}$$



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- anomalous points have $LOF \gg 1$



Example: LOF Scoring

LOF normalization factor is the harmonic mean

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Source: https://en.wikipedia.org/wiki/Local_outlier_factor



A few remarks about LOF:

we can use other means of smoothing for normalization



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- can be seen as relative distance-based approach with smoothing



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- tightly coupled data within a single data distribution will impact the scores
- small values of k increases false-positive risks




Let the counting neighborhood of data point *x* be:

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where $\delta > \varepsilon$ is the sampling neighborhood of x.

In practice we choose $\varepsilon = c\delta$ where $c = \frac{1}{2}$ is a popular choice.



Let us now define the equivalent neighborhood-aware averaging score of a point

$$MDEF(x, \varepsilon, \delta) = 1 - \frac{M(x, \varepsilon)}{AM(X, \varepsilon, \delta)}$$

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where STD computes the standard deviation of the sampling neighborhood.

In practice $MDEF \ge k\sigma$ is used with k = 3 being a popular choice inspired from statistics.





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- \blacktriangleright anomaly if MDEF is large within any of the δ settings
- \blacktriangleright sub-sample considered neighborhoods based on invariance to δ choice



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