Anomaly Detection

Density Based Methods

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Outline

- 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
  - large 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

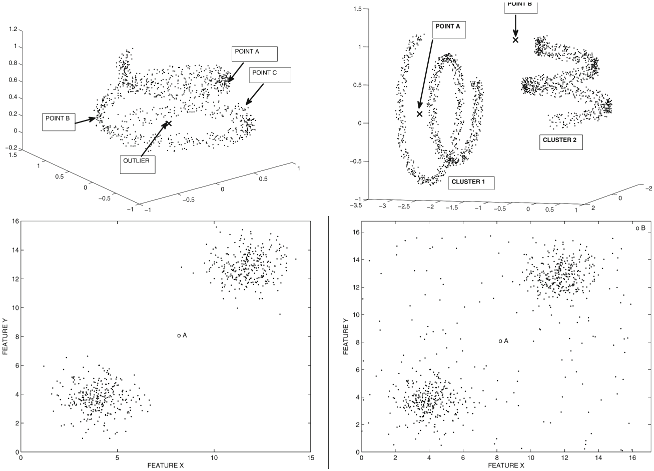

Figure: Data points and data space (Aggarwal 2017)

k-Nearest Neigbors

Nearest Neighbors

Definition

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 $k \geq k_0$ in the KNN algorithm.

KNN: the choice of k_0

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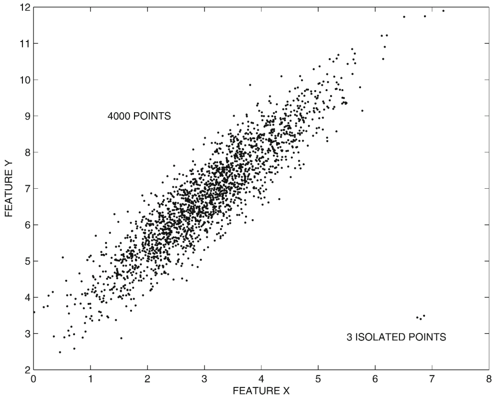

Figure: The choice of $k \geq k_0$ (Aggarwal 2017)

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2. Choose a distance function:

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

4. Set the anomaly score:

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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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General approach. Naturally we train multiple KNN models where we vary k and create an ensemble where voting methods are employed in order to decide which data is anomalous.

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

KNN Variants: Average KNN Scores

Definition

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
- 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.

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- worse results than the true k value in the Exact-KNN

Local Outlier Factor

Problems: Density and Cluster Orientation

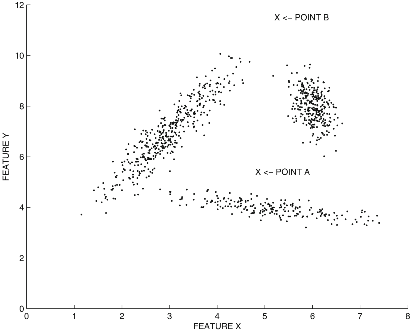
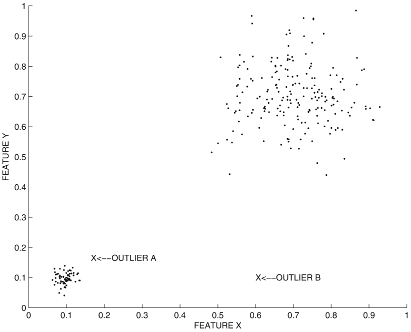


Figure: Data Locality (Aggarwal 2017)

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

Example: Distance versus Locality



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- 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:

$$L_k(x) = \{y \mid \|x - y\| \leq knn(x),\ \forall y \in X\}$$

this can contain more than k points, but not less!

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- reachability is not symmetric!

LOF: Reachability

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Proof in class

LOF: Average Reachability Distance

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: Scoring

The local outlier factor is the mean average reachability of x compared to its neighbors average:

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

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- anomalous points have $LOF \gg 1$

Example: LOF Scoring

LOF normalization factor is the harmonic mean

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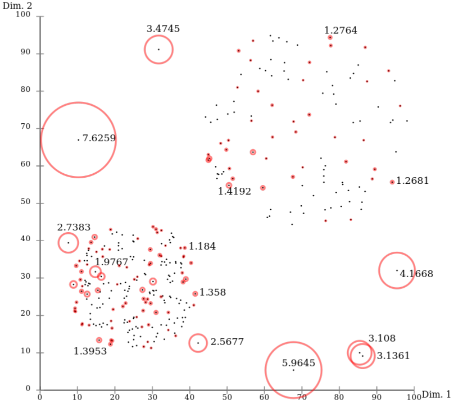

Source: https://en.wikipedia.org/wiki/Local_outlier_factor

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- raw distances instead of reachability distances
- arithmetic mean instead of harmonic mean
- local distance-based outlier factor (LDOF) by Zhang, Hutter, and Jin 2009 uses averaged pairwise distances from L_k

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- small values of k increases false-positive risks

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

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where STD computes the standard deviation of the sampling neighborhood.

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

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- sub-sample considered neighborhoods based on invariance to δ choice

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