

# Visualizing Big Data Outliers through Distributed Aggregation

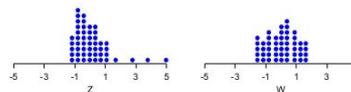
Leland Wilkinson, Proc VAST 2017, TVCG to appear.

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## Outliers

- General definition
  - Observations which appear to be inconsistent with the remainder of a set of data (Barrett and Lewis)
- Principles of detection
  - Each observation represents a point in vector space of a random variable
  - Likelihood that a point outlies the distribution of a sample is proportional to the probability that the point is a member of the distribution

## Example



## The Gaps Rule

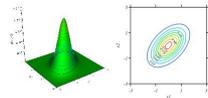
- Looks for gaps in data that do not match assumed generating distribution
- Can detect aberrations in the middle of a distribution, not just at its extremes

$$Q = \frac{x_n - x_{n-1}}{x_n - x_1} \quad \text{Dixon}$$

$$f(x; \theta, \psi) = \exp \left[ \frac{x\theta - a(\theta)}{b(\theta)} + c(x, \theta) \right] \quad \text{Burridge and Taylor}$$

## Higher-Dimensional Outlier Detection

- Mahalanobis Distance**
  - Detects outliers based on Euclidean distance of multidimensional point from centroid of multivariate Normal distribution
    - Only valid if assumption of normality is satisfied
  - Squared Mahalanobis distance = chi-square variate with  $p$  degrees of freedom



## Higher-Dimensional Outlier Detection

- Clustering**
  - Process:
    - Pre-cluster data
    - Target points with large distance from nearest cluster
  - Effective for samples of moderate size with limited singleton frequency
  - Does not typically scale well for larger data sets
    - Outlier aggregation
    - Convergence in Euclidean space
    - Efficiency
  - Generally not based on probability model
    - Susceptible to error

## hdoutliers

- Purpose**
  - Statistical method for identifying subsets of data which do not match underlying distribution of sample
  - Generate highlighted points representing outliers in visualization of data
- Design Criteria**
  - Identify outliers in mixed data sets containing both ordinal and categorical variables
  - Exploit random projection for a large number of dimensions
  - Handle large sets through single-pass aggregation
  - Overcome masking effects resulting from interaction of outlying points
  - Function for both univariate and multivariate data

## hdoutliers

- Algorithm**
  - Convert all categorical variables to continuous variables
    - Correspondence Analysis
  - If > 10,000 columns, reduce via random projections using error bound to squared distances
  - Normalize resultant columns
  - Initialize *exemplars*
    - Initializes with row 1 as sole member of set
    - Rows added to *exemplar set* if row distance from existing exemplars exceeds threshold
  - Initialize *members*
    - List of lists with initial entry defined by rows in *exemplars*.
    - Each *exemplar* has list of affiliated members

## hdoutliers

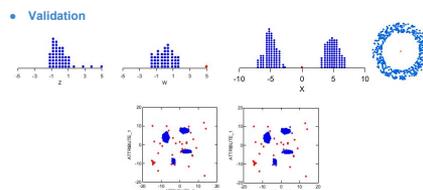
- Algorithm**
  - Single pass
 

```

                    forall the row(i), j = 1, ..., n do
                    if d(i, j) < delta then
                    add i to members list associated with closest exemplar
                    else
                    add row(i) to exemplars
                    add row(i) to members, initialized with {}
                    end
                    
```

$$\delta = .1 / (\log n)^{1/p}$$
  - Compute nearest distances between all pairs of exemplars
  - Fit exponential distribution to upper tails nearest-neighbor distances
  - Flag members associated with exemplars exceeding distance cut-off (1-0.05 from CDF of previous step) from other exemplars as outliers

## hdoutliers



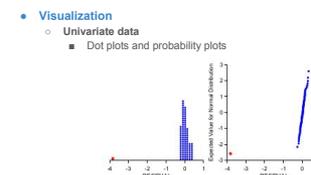
## hdoutliers

- Visualization**

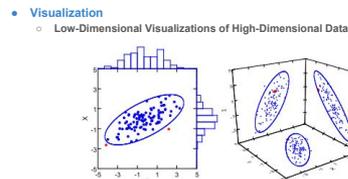
Core principles:

  - Probability-grounded algorithm necessary for reliable outlier detection
    - Risk of outlier classification unknown without statistical foundation
  - Visual analysis necessary to derive meaning from algorithmic detection
    - Highlighting cases based on probabilistic detection guides discovery

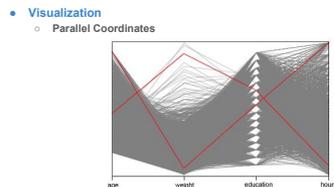
## hdoutliers



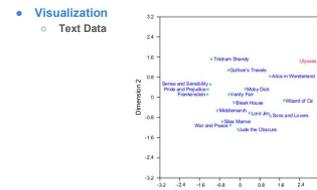
## hdoutliers



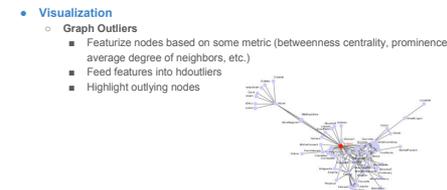
## hdoutliers



## hdoutliers



## hdoutliers



## Conclusions

- Identification of outliers is only valuable if the assumptions that differentiate them from a sample are valid
- Methods that include outliers in estimation of parameters for a given distribution are circular and unreliable
- The risk of excluding outliers is unknown if the probability of accurate detection is not calculated
- Visualization of outliers in context, particularly for high-dimensional data, is essential for extracting information regarding the features which set them apart