## Robust Information-theoretic Clustering

#### Simon Lackerbauer

Institut für Informatik Ludwig-Maximilians-Universität München lackerbauer@lrz.mwn.de

Seminar Information Theoretic Data Mining im WS 2015/16

### Clustering Problems

Solution: The iterative approach

VAC – Volume After Compression

RF – Robust Fitting

CM – Cluster Merging

Example: Cat Retina Images

Summary

## Clustering Problems

Solution: The iterative approach
VAC – Volume After Compression
RF – Robust Fitting
CM – Cluster Merging

Example: Cat Retina Images

Summary

## Clustering Problems

- ▶ There exist a wide range of possible clustering algorithms.
- Many need user input or assume only Gaussian clusters
- We want an algorithm without user input that automatically selects appropriate cluster functions

# Clustering Problems

Example: How not to do it

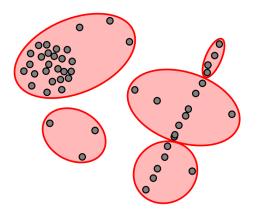


Figure 1: Example of "Bad" Clustering[1]

# **Clustering Problems**

Example: Reasonable reduction

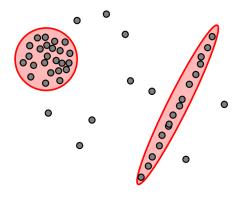


Figure 2: Example of "Good" Clustering[1]

## Comparison of examples

### What makes the second pattern better than the first?

- ▶ It's more descriptive of the interesting patterns in the data, because outliers have been "omitted".
- ► The clusters in the "good" example are those a human would immediately recognize as points being associated somehow.

## Measuring Success

This human intuition must be translated into a dependable clustering algorithm, for which two measures for success can be defined:

- ► Goodness of fit
- Efficiency

# Measuring Success

This human intuition must be translated into a dependable clustering algorithm, for which two measures for success can be defined:

- ▶ Goodness of fit
- Efficiency

## Measuring Success

This human intuition must be translated into a dependable clustering algorithm, for which two measures for success can be defined:

- Goodness of fit
- Efficiency

Clustering Problems

Solution: The iterative approach

VAC – Volume After Compression

RF – Robust Fitting

CM – Cluster Merging

Example: Cat Retina Images

Summary

Clustering Problems

Solution: The iterative approach

 $VAC-Volume\ After\ Compression$ 

RF – Robust Fitting

CM – Cluster Merging

Example: Cat Retina Images

Summary

### **VAC** - Volume after Compression

- does not specify good grouping
- ▶ specifies for two groupings x, y which one is better (e.g., because  $VAC(x) < VAC(y) \rightarrow x$  is a better grouping)
- size of total, lossless compression

Integer Encoding

- point coordinates are always integers
- self-delimiting encoding of integers: Elias (gamma) codes
- smaller integers require fewer bytes

Cluster Encoding

- uses Huffman encoding for positioning points with probability distribution according to assumed cluster pdf
- such, if we assume the correct distribution for the cluster, core points will be more efficiently encoded

Cluster Encoding

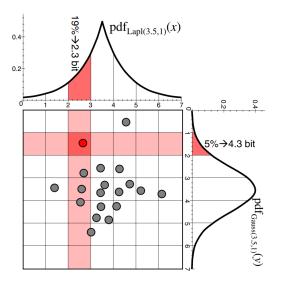


Figure 3: Example of VAC[1]

Cluster encoding

## Definition (VAC of point $\vec{x}$ )

Let  $\vec{x} \in \mathbb{R}^d$  be a point of a cluster C and  $\overrightarrow{pdf}(\vec{x})$  be a d-dimensional vector of probability density functions which are associated to C. Each  $pdf_i(x_i)$  is selected from a set of predefined probability density functions with corresponding parameters, i.e.

 $PDF = \{pdf_{Gauss(\mu_i,\sigma_i)}, pdf_{uniform(Ib_i,ub_i)}, pdf_{LapI(a_i,b_i)}, \ldots\},$   $\mu_i, Ib_i, ub_i, a_i \in \mathbb{R}, \sigma_i, b_i \in \mathbb{R}^+$ . Let  $\gamma$  be the grid constant (distance between grid cells). The  $VAC_i$  of coordinate i of point  $\vec{x}$  corresponds to

$$VAC_i(x) = \log_2 \frac{1}{pdf_i(x_i) \cdot \gamma}$$

The VAC of point  $\vec{x}$  corresponds to

$$VAC(x) = \left(\log_2 \frac{n}{|C|}\right) + \sum_{0 \le i < d} VAC_i(x)$$

Cluster Encoding and Decorrelation

- $ightharpoonup \gamma$  is a measure of granularity of grid cells
- absolute VAC changes with grid resolution, but relative VAC stays the same
- ▶ to choose optimal parameter settings for clusters, we use the statistical parameter of the dataset
- if data is correlated amongst itself, define a decorrelation matrix iff the VAC savings at least compensate for saving the decorrelation matrix

Clustering Problems

Solution: The iterative approach

VAC – Volume After Compression

 $\mathsf{RF}-\mathsf{Robust}\ \mathsf{Fitting}$ 

CM – Cluster Merging

Example: Cat Retina Images

Summary

# Two helper algorithms Robust Fitting

- ▶ Start: get as input a set of clusters  $C = \{C_1, ..., C_k\}$  by an arbitrary method
- ▶ for every  $C_i$  in C define a similarity measure (decorrelation matrix == ellipsoid)
- use the VAC score to try out decorrelation matrices until the one with the lowest VAC is found

# Two helper algorithms Robust Fitting

#### Decorrelation Matrix:

- contains the vectors that define the space in which points in the cluster reside
- ▶ to improve robustness of cluster center estimation use coordination-wise median instead of arithmetic means
- of the several matrices generated during this step, again partition into core points and noise by choosing the one with best VAC

Robust Fitting

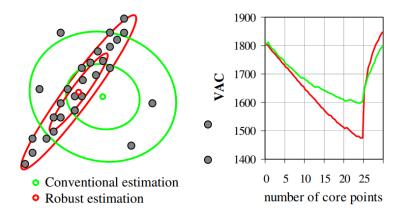


Figure 4: Conventional and robust estimation[1]

Clustering Problems

Solution: The iterative approach

VAC - Volume After Compression

RF – Robust Fitting

 $\mathsf{CM}-\mathsf{Cluster}\ \mathsf{Merging}$ 

Example: Cat Retina Images

Summary

Cluster Merging

- ▶ Start: get as input a set of clusters  $C = \{C_1, ..., C_k\}$  by an arbitrary method
- Purify (of noise) each cluster individually

Cluster Merging

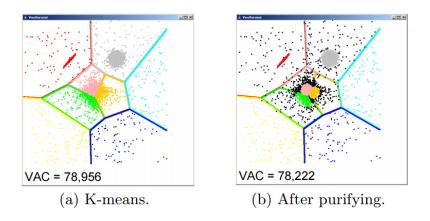


Figure 5: Clustering by using K-means and then purifying[1]

Cluster Merging

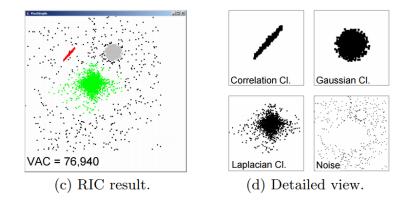


Figure 6: After merging[1]

Clustering Problems

Solution: The iterative approach

VAC – Volume After Compression

RF – Robust Fitting

CM – Cluster Merging

Example: Cat Retina Images

Summary

- ightharpoonup 219 blocks of retinal images, 96 tiles per image ightarrow 22,024 tiles in total (example tiles in figure 7)
- ▶ each tile is represented as vector of 7 features (figure 8(a))
- RIC finds 13 clusters, color coded in figure 8(b)
- Example clusters in figures 9(a)-(f)

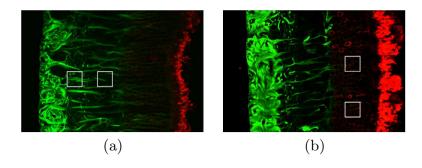


Figure 7: Examples of tiles[1]

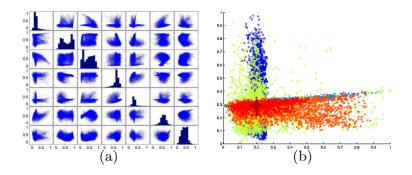


Figure 8: Visualization of cat retina data[1]

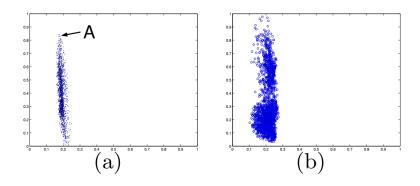


Figure 9: Example clusters[1]

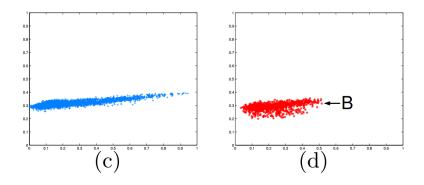


Figure 8: Example clusters[1]

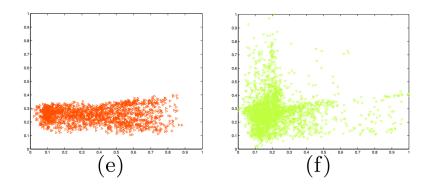


Figure 8: Example clusters[1]

### Clustering Problems

Solution: The iterative approach
VAC – Volume After Compression
RF – Robust Fitting
CM – Cluster Merging

Example: Cat Retina Images

Summary

## Summary

- The VAC criterion provides a stable measure of goodness of fit.
- ► The RIC framework is very flexible, does not rely on user input and can handle any distribution that can be described by a pdf
- Anytime a new, better clustering algorithm is introduced, RIC can improve on it by running its parts (CM and RF) with the better algorithm as a starting point

### Clustering Problems

Solution: The iterative approach
VAC – Volume After Compression
RF – Robust Fitting
CM – Cluster Merging

Example: Cat Retina Images

Summary

### References

[1] Christian Böhm, Christos Faloutsos, Jia-Yu Pan, and Claudia Plant. Robust information-theoretic clustering. In *Proceedings of the 12th ACM SIGKDD international conference on Knowledge discovery and data mining*, pages 65–75. ACM, 20 August 2006.