

HelmholtzZentrum münchen

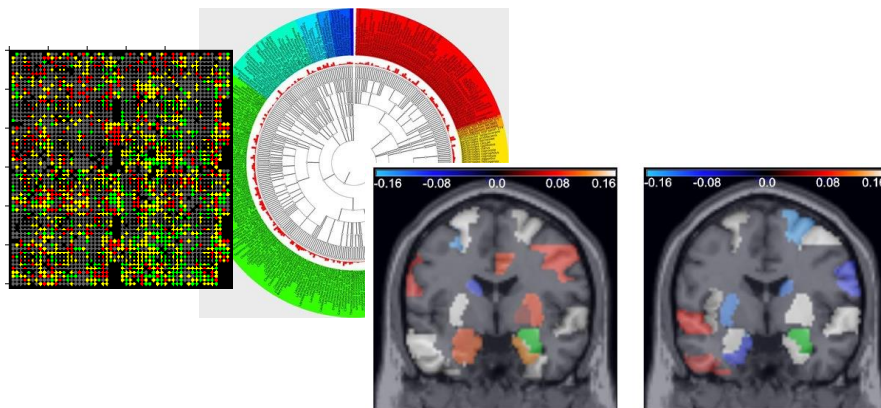
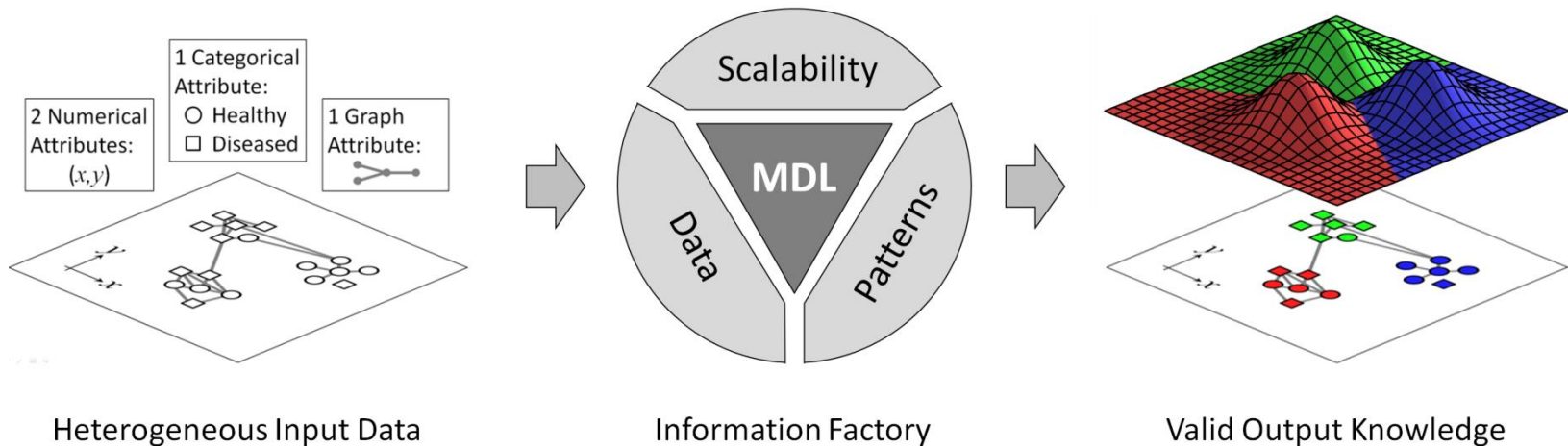
Deutsches Forschungszentrum für Gesundheit und Umwelt

# Current Topics in Information-theoretic Data Mining

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# Helmholtz-Hochschul research group iKDD



**Applications:**  
Neuroscience,  
Diabetes research.

# Outline

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1. Introduction
2. General Information
3. Short Presentation of Topics
4. Selection of Topics

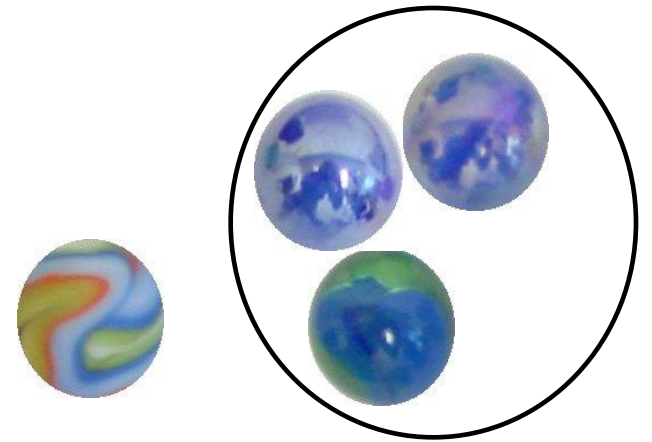
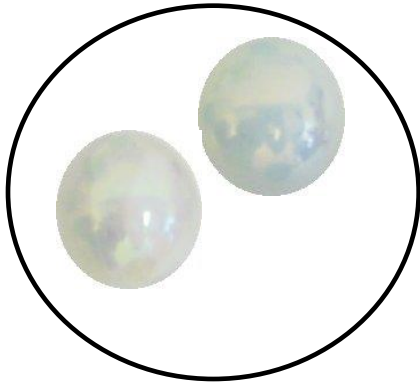
# Information-theoretic Data Mining

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INTRODUCTION

# Example Clustering:

Find a natural grouping of the data objects.

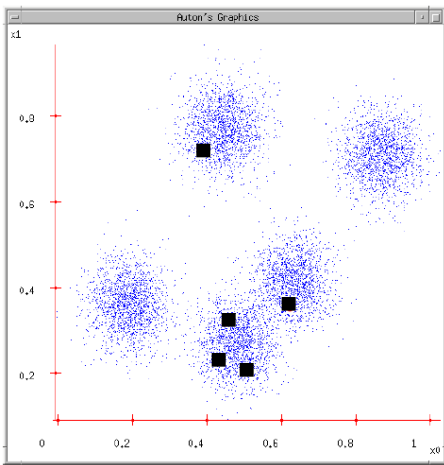


How many clusters?

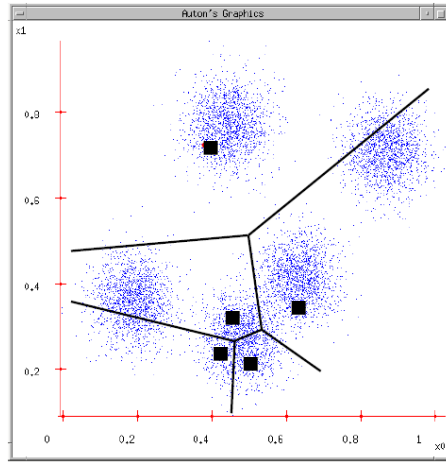
What to do with outliers?



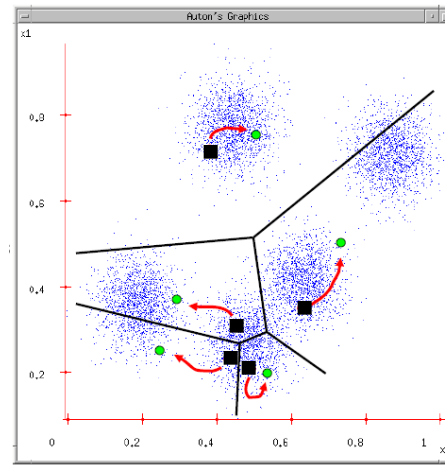
# The Algorithm K-Means



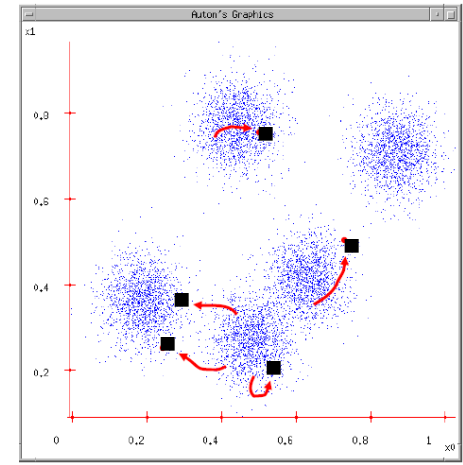
1) **Initialize**  
K cluster centers  
randomly.



2) **Assign** points to  
the closest center.



3) **Update**  
centers.

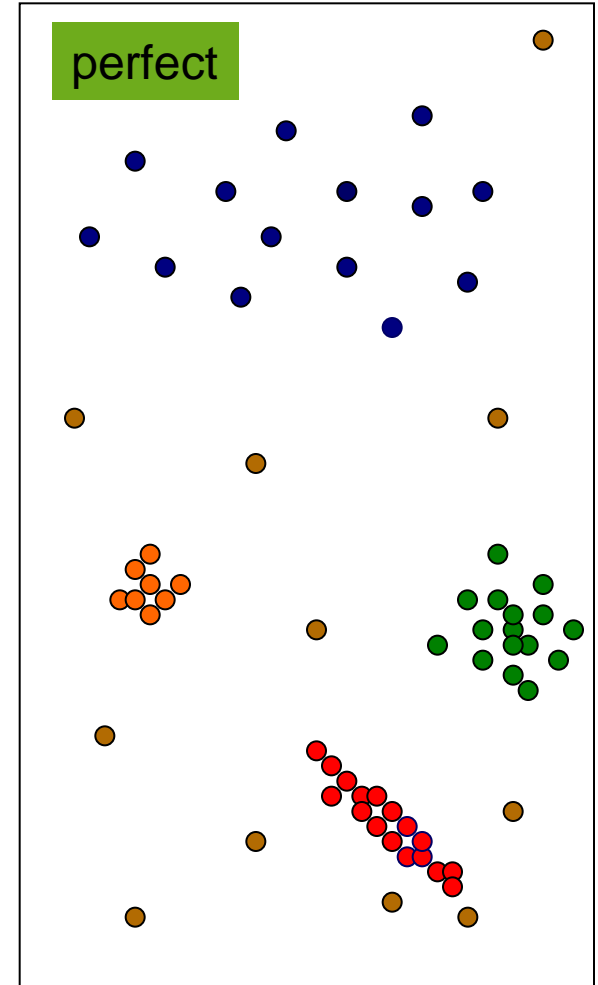
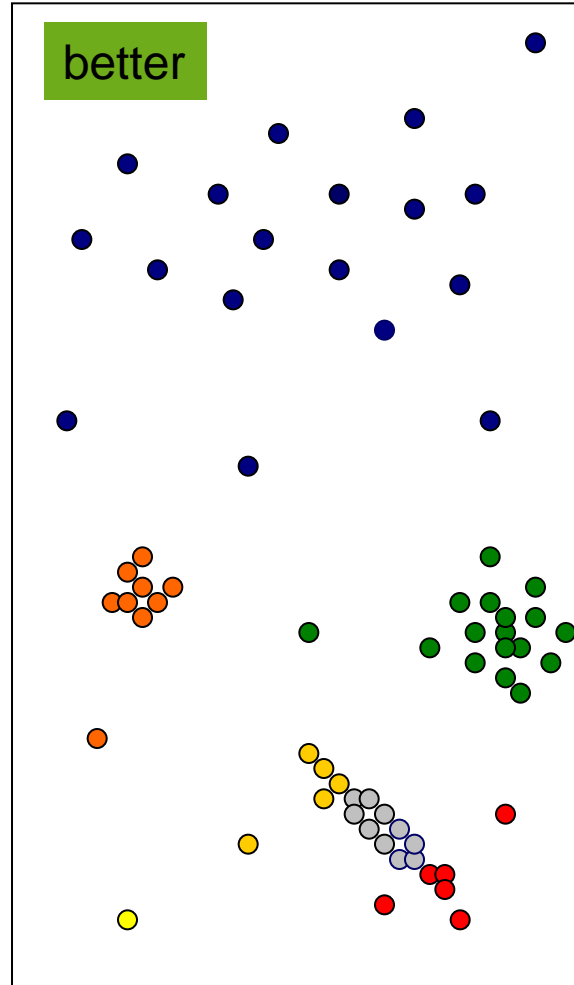
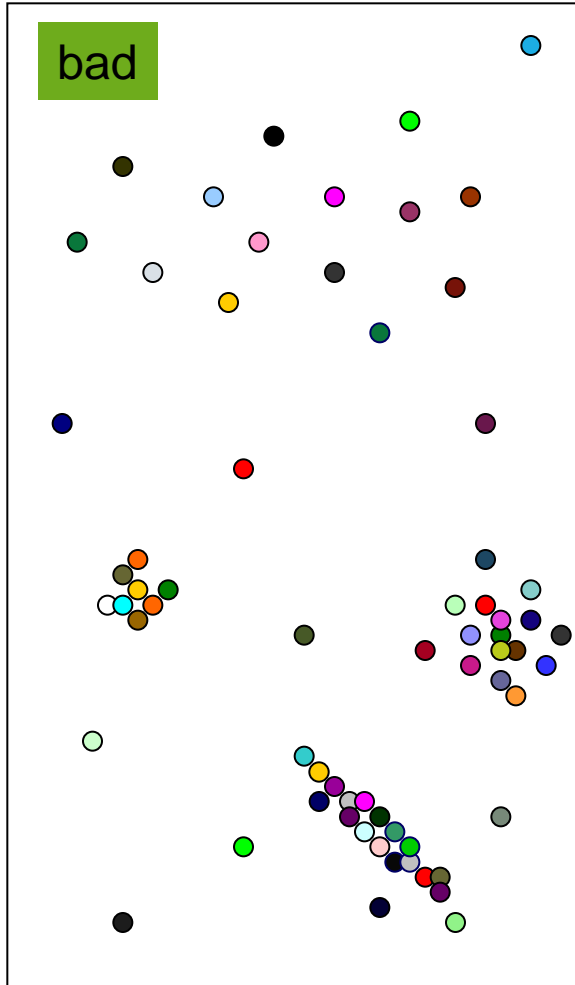


4) **Iterate**  
2) und 3) until  
convergence.

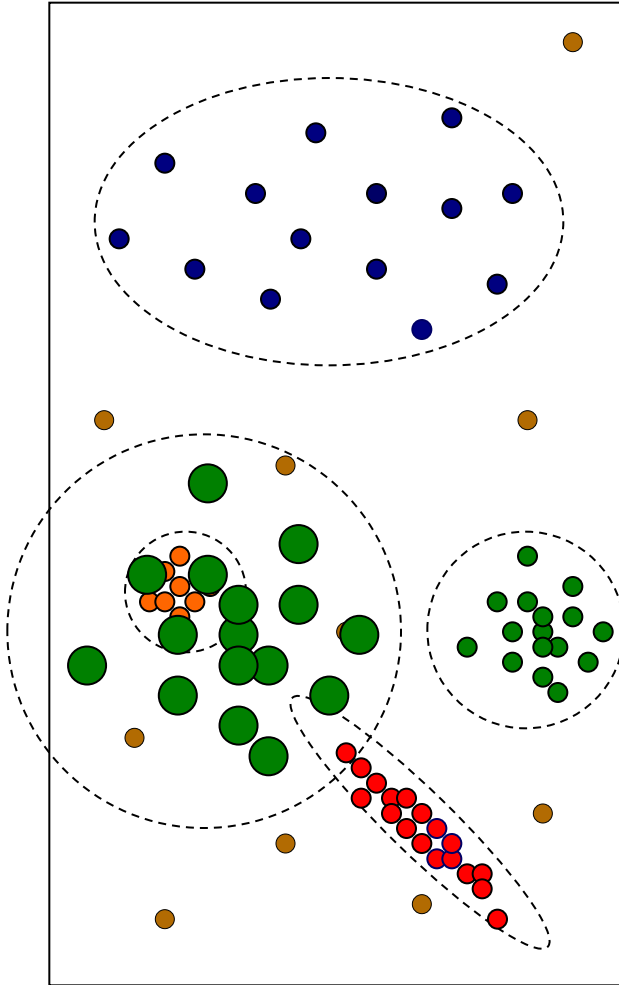
- + fast convergence,
- + well-defined objective function,
- + gives a model describing the result.

$$J = \sum_{j=1}^k \sum_{i=1}^n \left\| x_i^{(j)} - c_j \right\|^2$$

# We need a quality criterion for clustering



# Measuring Clustering Quality by Data Compression



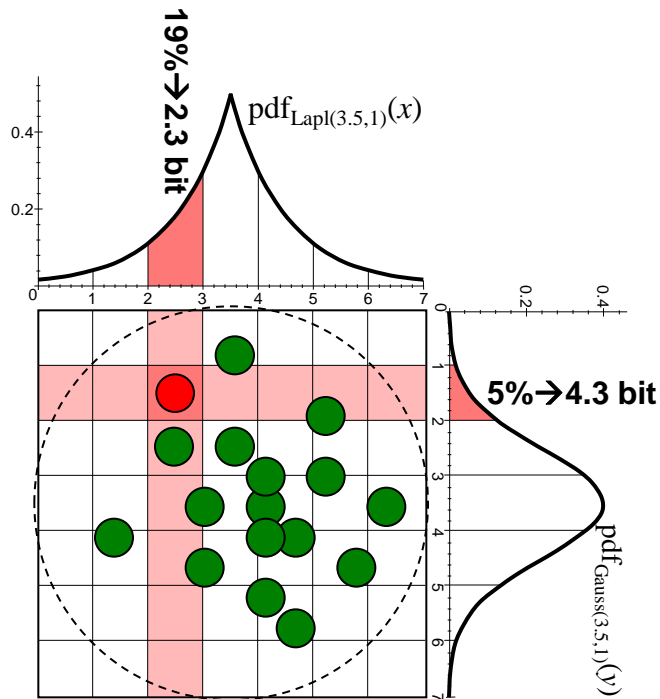
**Data compression is a good criterion for...**

- the required number of clusters
- the goodness of a cluster structure
- the quality of a cluster description

**How can a cluster be compressed?**



# Measuring Clustering Quality by Data Compression



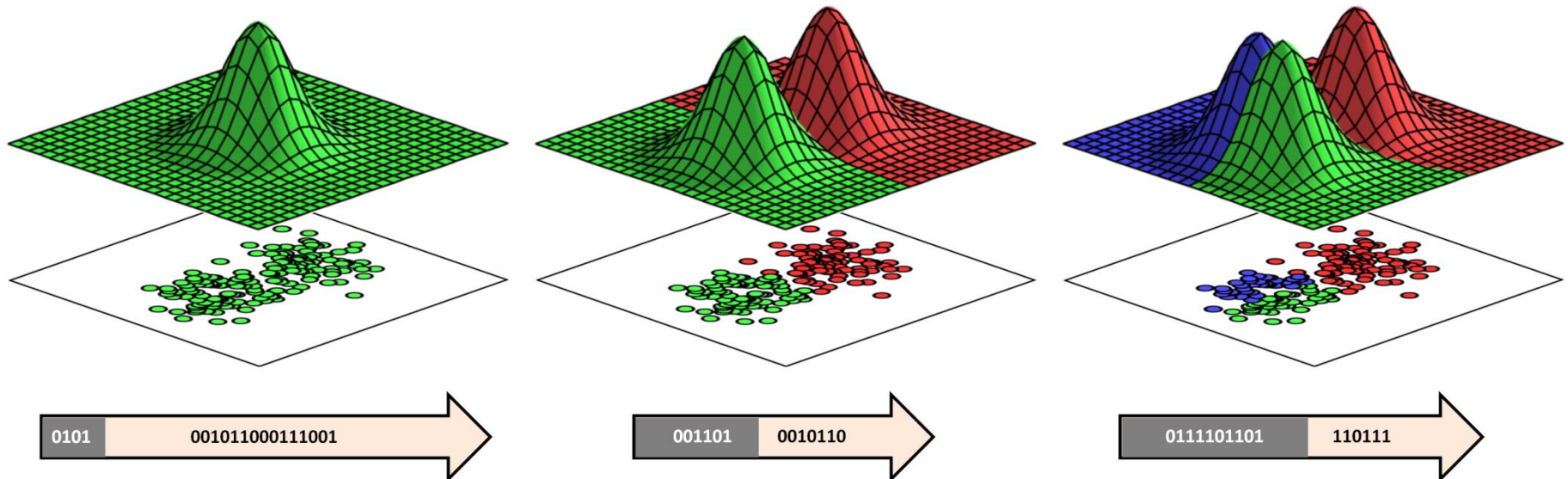
**Data compression is a good criterion for...**

- the required number of clusters
- the goodness of a cluster structure
- the quality of a cluster description by a pdf

**How can a cluster be compressed?**

Minimum Description Length (MDL) Principle:  
Automatic balance of  
Goodness-of-fit and model complexity

# Key Idea



**Data compression is a very general measure for:**

- The amount of any kind of non-random information in any kind of data,
- The success of any kind of data mining technique.

# General Information

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ABOUT THE SEMINAR

# Goals of the Seminar

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Learn how to:

- Read scientific papers
- Discover the state-of-the-art on a specific topic
- Write a scientific report
- Do a scientific presentation

# The Seminar in Practice

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- **ECTS:** 3 Credits (Bachelor), 6 Credits (Master)
- Master students get the harder papers ;)
- **Presentation:** 20 min presentation/10 min questions. Download the template from the seminar web page
- Write a **report (max 8 pages)**.
  - 3-4 pages Bachelor students
  - 5-6 pages Master students
- **Attendance and participation** of the seminar meetings
  - ASK the lecturers ;)
- **Seminar days: February 19 -20, time to be announced at the website.**

# Contents of the Report

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Follow the structure of a scientific publication.

- **Abstract and Introduction**
  - General motivation.
- **State of the Art and Contributions**
  - How is this paper different from (SoA)? e.g What is new? What is better? What is faster?
- **Problem statement**
  - Mathematical formulation
- **Method**
  - Overview: input, output.
  - Method/Algorithm.
- **Results**
  - Summary of experiments and results (what type of data and validation).
  - **YOUR CRITIQUE** of the methodology, set-up and validation (what else could have been done?, is it enough to demonstrate the contribution?, is the data biased?, are there non mentioned assumptions?, can it be easily reproduced?)
- **Conclusion**
  - **YOUR PERSONAL CONCLUSION & IDEAS**
- **References**

# Contents of the Presentation

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As a rule of thumb: max 1 slide per minute (max 20 slides for 20 mins)

- **Present the paper**
  - Type and year of publication: journal, conference, workshop, etc.
  - Authors/Institution
- **Motivation and Goal**
  - What is the problem that the authors try to solve?
  - Name potential applications: what for?
  - General motivation: why is it interesting?
- **Related Work (state of the art)**
  - Mention most similar approaches and explain how your paper is different from them?
  - Citing/Referencing other people's work [Lastname-Conference-Year].
- **Method**
  - Overview (1 or 2 slides): input, output, contribution (the proposed new elements).
  - Method/Algorithm (Only key ideas).
- **Results (short version)**
  - Explain the type of **data** used.
  - Validation: what is being validated and how.
- **Conclusion (include your own conclusions!!)**

# Topic Selection

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FIND YOUR OWN PAPER



# Mining Numerical and Mixed Data

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BASIC CLUSTERING

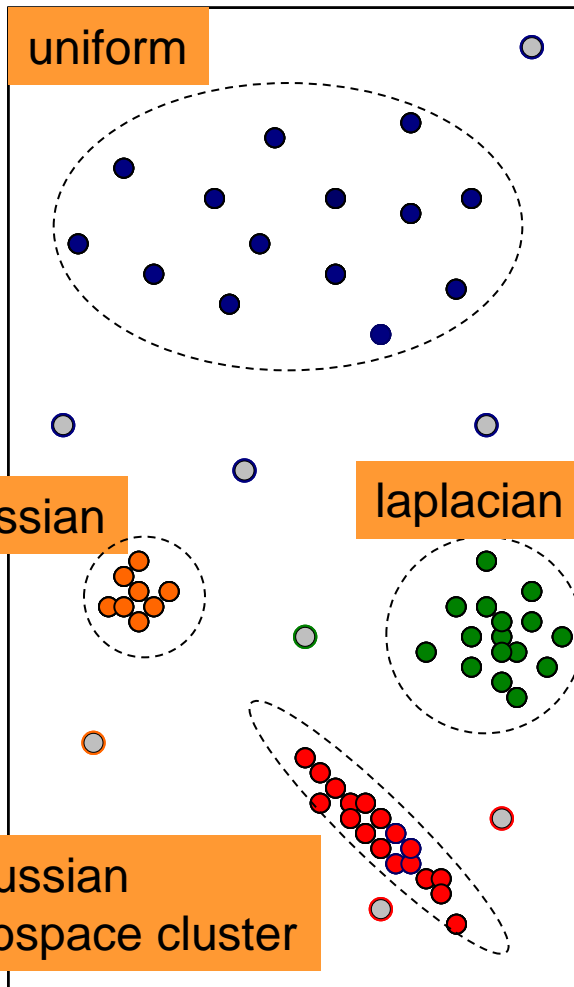
FINDING ALTERNATIVE CLUSTERINGS

MIXED (NUMERICAL, CATEGORICAL DATA)

# Algorithm RIC:

## Robust Information-theoretic Clustering (KDD 2006)

Easy



Start with an arbitrary partitioning

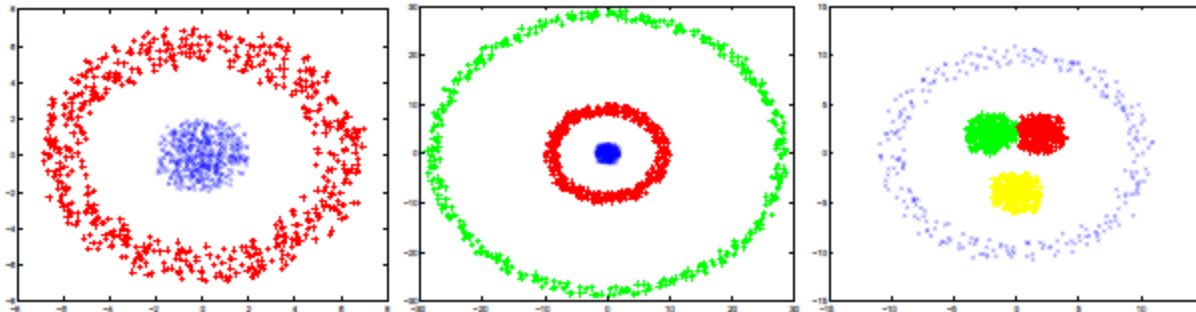
1. Robust Fitting (RF):  
Purifies individual clusters from noise, determines a stable model.
2. Cluster Merging (CM):  
Stiches clusters which match well together.

Additional value-add:  
Description of the cluster content by assigning model distribution functions to the individual coordinates.

**Free from sensitive parameter settings !**

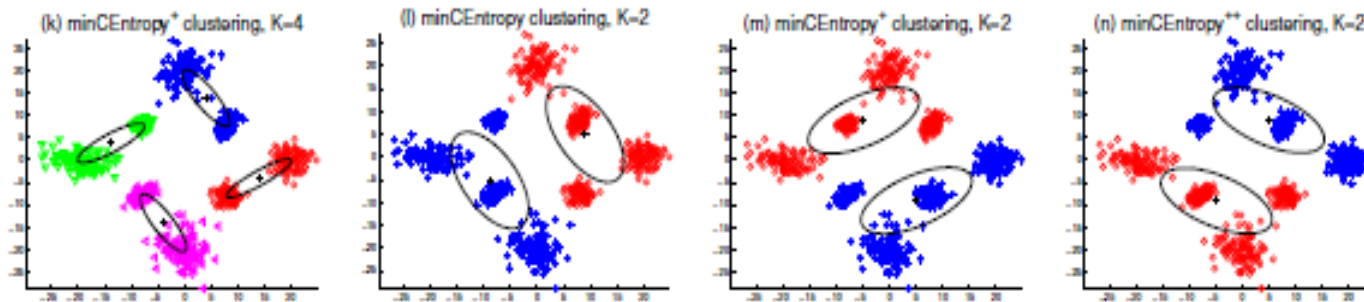
# A Nonparametric Information-Theoretic Clustering Algorithm

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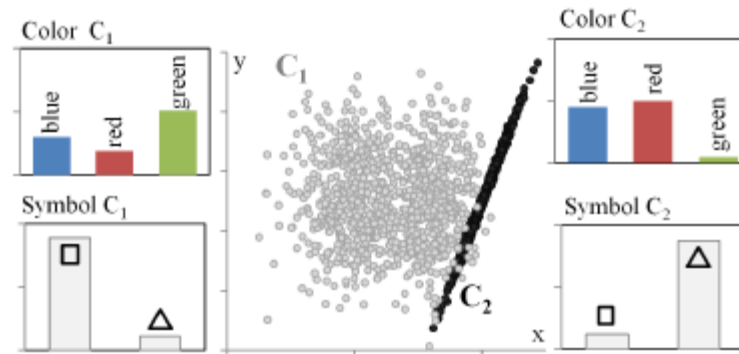
- first google pick for information theoretical clustering ;)
- close to **machine learning**
- uses entropy and **mutual information** as quality function
  - ➔ a bit different than our MDL-based approaches!

# minCEntropy: a Novel Information Theoretic Approach for the Generation of Alternative Clusterings



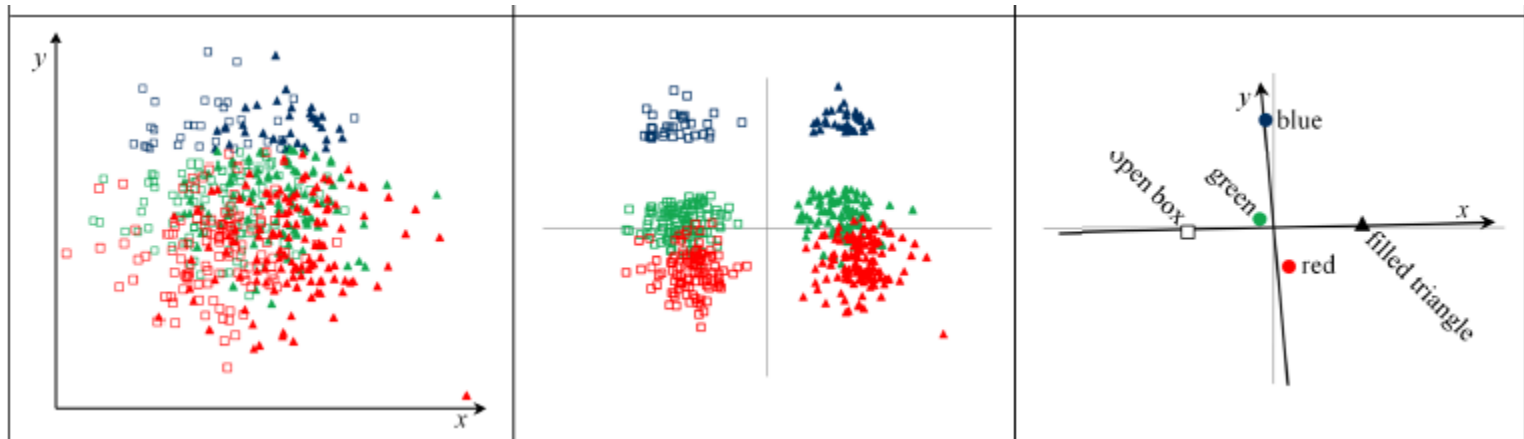
- Aims at finding different **alternative clusterings** for the same data set
- Uses a **general entropy** as objective function (not Shannon)
- can also be used semi-supervised (close to machine learning topics)

# INCONCO: Interpretable Clustering of Numerical and Categorical Objects



- Uses Minimum Description Length (MDL) ;)
- Tackles mixed-type attributes: numerical, categorical data
- Clusters by revealing „dependency patterns“ among attributes by using and extended Cholesky decomposition

# Dependency Clustering across measurement scales



- Uses MDL ;)
- supports mixed-type attributes
- finds **attribute dependencies** regardless the measurement scale

# Relevant overlapping subspace clusters on categorical data

a <sub>1</sub>	b <sub>1</sub>	c <sub>1</sub>	d <sub>3</sub>	e <sub>3</sub>	f <sub>3</sub>	g <sub>1</sub>	h <sub>1</sub>
a <sub>1</sub>	b <sub>1</sub>	c <sub>1</sub>	d <sub>2</sub>	e <sub>2</sub>	f <sub>2</sub>	g <sub>2</sub>	h <sub>2</sub>
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Subspace clustering  
6076 bits

a <sub>1</sub>	b <sub>1</sub>	c <sub>1</sub>	d <sub>3</sub>	e <sub>3</sub>	f <sub>3</sub>	g <sub>1</sub>	h <sub>1</sub>
a <sub>1</sub>	b <sub>1</sub>	c <sub>1</sub>	d <sub>2</sub>	e <sub>2</sub>	f <sub>2</sub>	g <sub>2</sub>	h <sub>2</sub>
a <sub>1</sub>	b <sub>1</sub>	c <sub>1</sub>	d <sub>1</sub>	e <sub>1</sub>	f <sub>1</sub>	g <sub>3</sub>	h <sub>3</sub>
a <sub>1</sub>	b <sub>2</sub>	c <sub>3</sub>	d <sub>1</sub>	e <sub>1</sub>	f <sub>1</sub>	g <sub>1</sub>	h <sub>2</sub>
a <sub>2</sub>	b <sub>3</sub>	c <sub>1</sub>	d <sub>1</sub>	e <sub>1</sub>	f <sub>1</sub>	g <sub>3</sub>	h <sub>1</sub>
a <sub>3</sub>	b <sub>1</sub>	c <sub>2</sub>	d <sub>3</sub>	e <sub>2</sub>	f <sub>2</sub>	g <sub>2</sub>	h <sub>2</sub>
a <sub>1</sub>	b <sub>2</sub>	c <sub>3</sub>	d <sub>2</sub>	e <sub>3</sub>	f <sub>2</sub>	g <sub>2</sub>	h <sub>2</sub>
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a <sub>3</sub>	b <sub>3</sub>	c <sub>2</sub>	d <sub>2</sub>	e <sub>2</sub>	f <sub>3</sub>	g <sub>3</sub>	h <sub>2</sub>
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Full-D clustering  
6147 bits

a <sub>1</sub>	b <sub>1</sub>	c <sub>1</sub>	d <sub>3</sub>	e <sub>3</sub>	f <sub>3</sub>	g <sub>1</sub>	h <sub>1</sub>
a <sub>1</sub>	b <sub>1</sub>	c <sub>1</sub>	d <sub>2</sub>	e <sub>2</sub>	f <sub>2</sub>	g <sub>2</sub>	h <sub>2</sub>
a <sub>1</sub>	b <sub>1</sub>	c <sub>1</sub>	d <sub>1</sub>	e <sub>1</sub>	f <sub>1</sub>	g <sub>3</sub>	h <sub>3</sub>
a <sub>1</sub>	b <sub>2</sub>	c <sub>3</sub>	d <sub>1</sub>	e <sub>1</sub>	f <sub>1</sub>	g <sub>1</sub>	h <sub>2</sub>
a <sub>2</sub>	b <sub>3</sub>	c <sub>1</sub>	d <sub>1</sub>	e <sub>1</sub>	f <sub>1</sub>	g <sub>3</sub>	h <sub>1</sub>
a <sub>3</sub>	b <sub>1</sub>	c <sub>2</sub>	d <sub>3</sub>	e <sub>2</sub>	f <sub>2</sub>	g <sub>2</sub>	h <sub>2</sub>
a <sub>1</sub>	b <sub>2</sub>	c <sub>3</sub>	d <sub>2</sub>	e <sub>3</sub>	f <sub>2</sub>	g <sub>2</sub>	h <sub>2</sub>
a <sub>2</sub>	b <sub>3</sub>	c <sub>2</sub>	d <sub>2</sub>	e <sub>2</sub>	f <sub>2</sub>	g <sub>2</sub>	h <sub>2</sub>
a <sub>3</sub>	b <sub>3</sub>	c <sub>2</sub>	d <sub>2</sub>	e <sub>2</sub>	f <sub>3</sub>	g <sub>3</sub>	h <sub>2</sub>
a <sub>2</sub>	b <sub>2</sub>	c <sub>2</sub>	d <sub>2</sub>	e <sub>2</sub>	f <sub>1</sub>	g <sub>1</sub>	h <sub>3</sub>

No clustering  
6671 bits

- Focus on subspace clustering on **categorical** data.
- Non redundant approach
- Parameter free /automized

# Graph Mining

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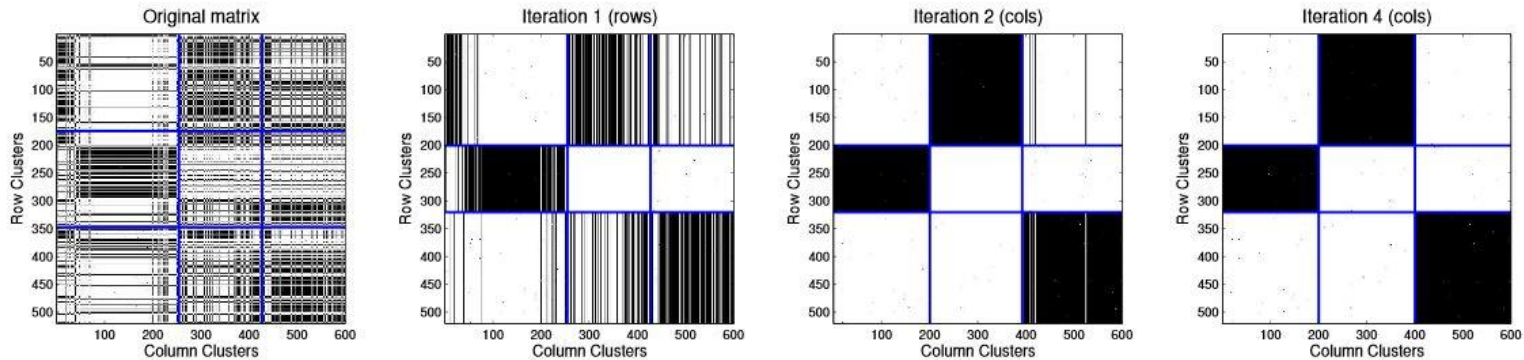
CLUSTERING

WEIGHTED GRAPHS

SUMMARIZATION, STRUCTURE MINING

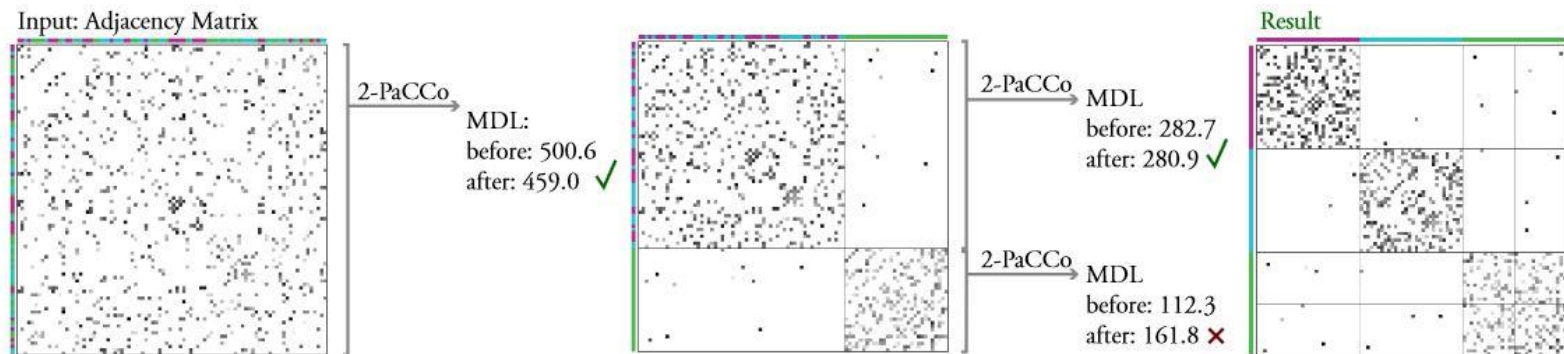


# Fully Automatic Cross-Associations



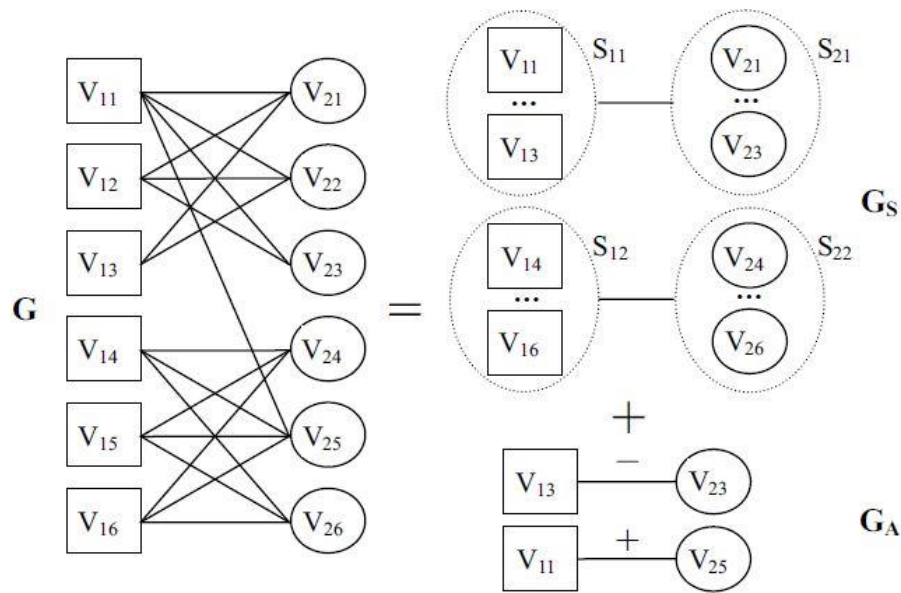
- Finding structures in datasets (parameter-free, fully automatic, scalable to very large matrices)
- Input data: binary matrix (for example gained by graph data)
- Rearrangement of rows and columns according to the smallest coding costs suggested by MDL

# Weighted Graph Compression for Parameter-free Clustering With PaCCo



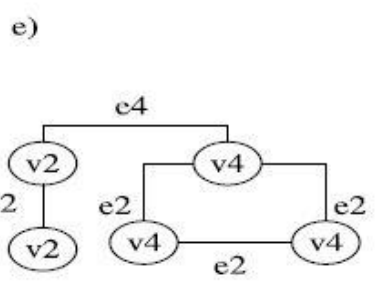
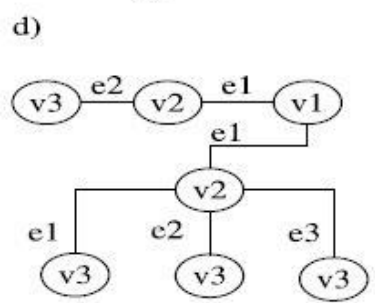
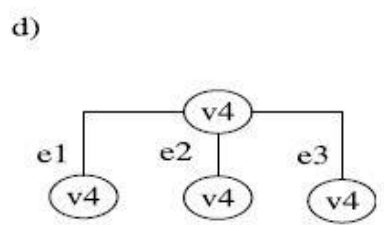
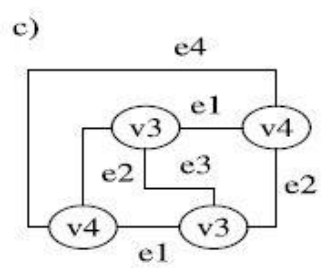
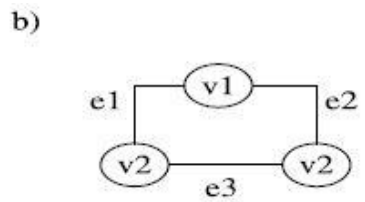
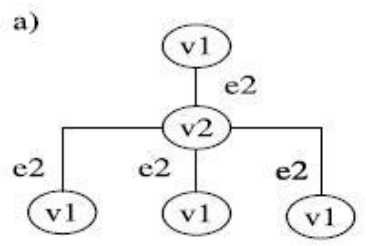
- Clustering weighted graphs (parameter-free, fully automatic, reduced runtime)
- Input data: adjacency matrix (containing weight information)
- Downsampling of the clusters according to the smallest coding costs suggested by MDL

# Summarization-based Mining Bipartite Graphs



- Mining bipartite graphs
- Transforming the original graph into a compact summary graph controlled by MDL
- Contributions: Clustering, hidden structure Mining, link prediction

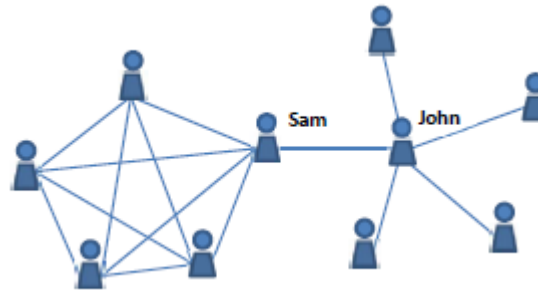
# Subdue: Compression-Based Frequent Pattern Discovery in Graph Data



- Discovering interesting patterns
- Input data: single graph or set of graphs (labeled or unlabeled)
- Outputting substructures that best compress the input data set according to MDL

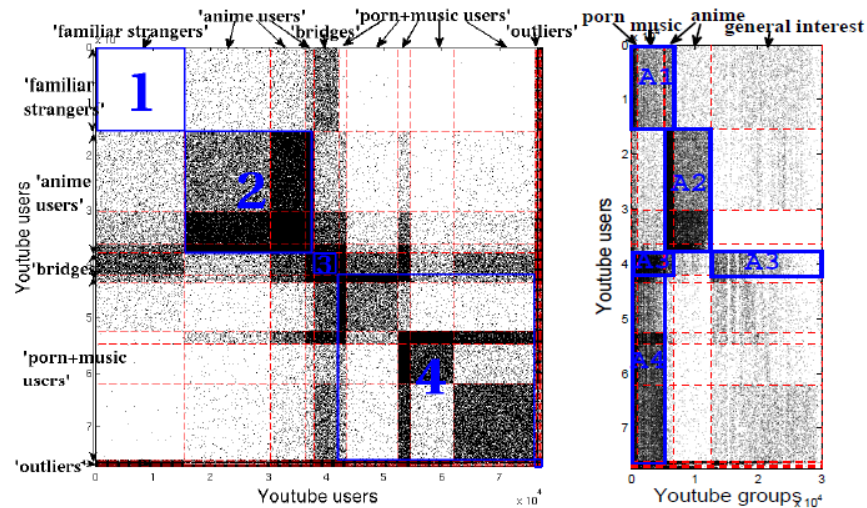
# Compression-based Graph Mining Exploiting Structure Primitives

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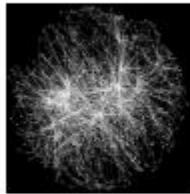
- Graph clusterer that distinguishes different pattern in graphs
- Suitable for sparse graphs
- Minimum Description Length compression leads to favorizing „stars“ or „cliques“

# PICS: Parameter-free Identification of Cohesive Subgroups in Large Attributed Graphs

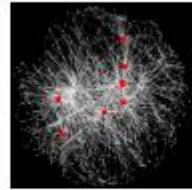


- Summarizes Graphs with node Attributes
  - Fully Automatic
  - Linear runtime

# VOG: Summarizing and Understanding Large Graphs



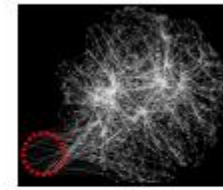
(a) Original Wikipedia Controversy graph (with 'spring embedded' layout [15]). No structure stands out.



(b) VOG: 8 out of the 10 most informative structures are stars (their centers in red - Wikipedia editors, heavy contributors etc.).



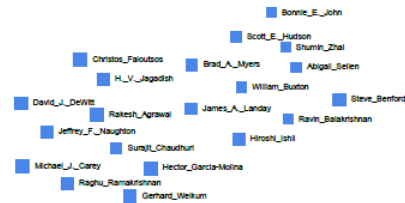
(c) VOG: The most informative bipartite graph - 'edit war' - warring factions (one of them, in the top-left red circle), changing each-other's edits.



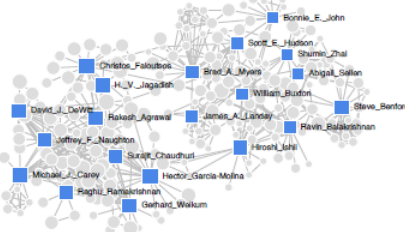
(d) VOG: the second most informative bipartite graph - another 'edit war', between vandals (bottom left circle of red points) vs responsible editors (in white).

- Compressing a graph with structure patterns: cliques, hubs, chains
- near linear runtime
- Newest paper on the line ;)

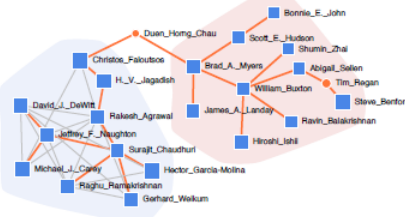
# Mining Connection Pathways for Marked Nodes in Large Graphs



(a) What to say about this “list” of authors?



(b) Any patterns? “Too many” connections.



(c) The “right” connections → Better sensemaking

- determining connection pathways → different ways of link analysis
- NP hard problem (travelling salesman)
- Uses minimum description length



Vielen Dank für die  
Aufmerksamkeit

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