Algorithm Engineering Applied To Graph Clustering

Insights and Open Questions in Designing Experimental Evaluations

Marco Gaertler[1]

Faculty of Informatics
Universität Karlsruhe (TH)

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Outline

What is Graph Clustering?

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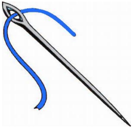
Cluster Analysis is the mathematical study of methods for recognizing natural groups within a class of entities.

What are interesting patterns or natural groups?

classification

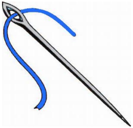
+



classification

partitioning

+



versus

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classification

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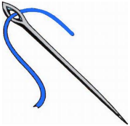
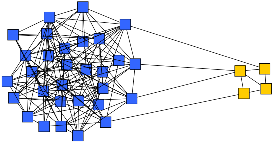


$\approx$



partitioning

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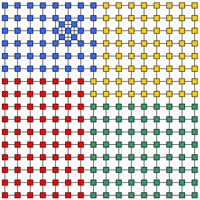

Framework?

Questions:

- What are suitable models / paradigms for clusterings?
  $\longrightarrow$ formalization of clustering / quantification of quality
- How can we objectively evaluate clustering algorithms?
  $\longrightarrow$ theoretical guarantees versus experimental validation

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Outline

General

Task

experimental evaluation of clustering algorithms

testbed:

application-oriented:

- large relevance
- not always available

generated data:

- easy to produce
- need not be realistic

Setup for Statistical Evaluation

generate data

↓

algorithms

↓

quality assessment

↓

statistical summary

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generator: random graph model with clustering information

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generator: random graph model with clustering information

algorithms: sets of technique to test

quality: quantification of achieved quality

summary: statements of average behavior

Advantages & Disadvantages

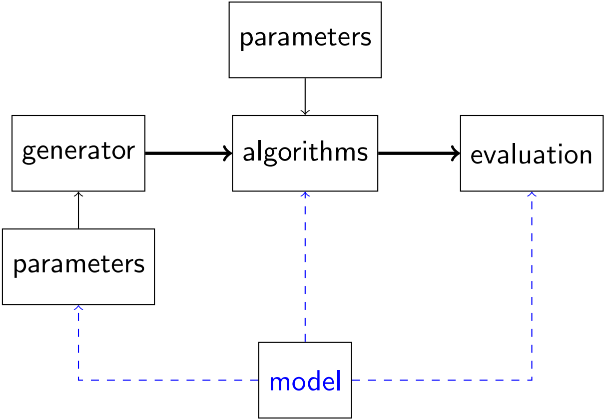
advantages:

- easy to setup and perform
- "average"-case analysis
- benchmark-like behavior
  - reproducible (without having the implementation)
  - comparable with former/future evaluations

disadvantages:

- worst cases can be arbitrary bad
- hidden dependencies between generator, algorithms and quality measures can lead to wrong conclusions

Detail Setup



clustering model implicitly affects

- generator
- algorithms
- quality evaluation

Questions:

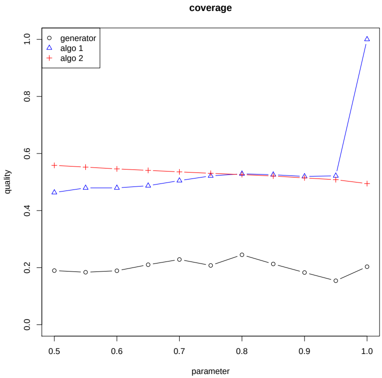
1. How severe are the (hidden) dependencies between generator, algorithms and quality measures?
2. What kind of graph generator do we need?

Hidden Dependencies

setting:

- (uniform) random graph
- two arbitrary clustering algorithms

Hidden Dependencies



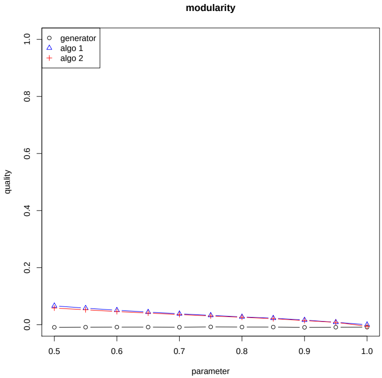
setting:

- (uniform) random graph with random equi-partition
- two arbitrary clustering algorithms

observations:

- both algorithms perform fairly good

Hidden Dependencies



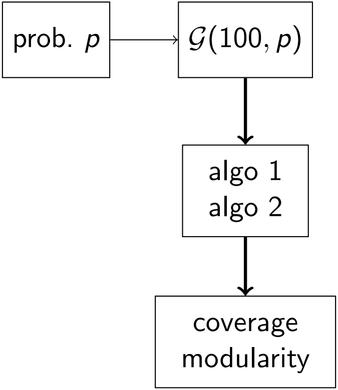
setting:

- (uniform) random graph with random equi-partition
- two arbitrary clustering algorithms

observations:

- both algorithms perform fairly good
- or not?!

Explanation



- $\mathcal{G}(n, p)$ does not generally have a clustering structure (for large p)
- *coverage* of ≈ 0.5 means half of the edges are inside clusters
  $\longrightarrow$ not very good for dense graphs
- *modularity* of ≈ 0 means the clustering structure is not significant (compared to random rewiring)

$\xrightarrow{!}$ due to the 'structure' of the generator and the selected evaluation mechanism this outcome was to be expected

Generators

What are suitable graph generators?

preferred properties:

- efficient computation
- direct correspondence to a clustering model/paradigm
- parameters control the significance of the clustering

Do we need an associated clustering?

Yes/No, but it serves as indicator for the clusterability of the generated graph

Key Question

If we come up with a generator, how do we know that it is suitable for evaluation?

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more generally:

How to design suitable components for (statistical) experimental evaluation?
Every combination of two suitable components can be used to evaluated the missing third one.

Cyclic Dependency

How to break this cyclic dependency?

bad news: no chance, all components formalize the model

good news: can break the dependencies into smaller/easier blocks
$\longrightarrow$ concept of unit tests

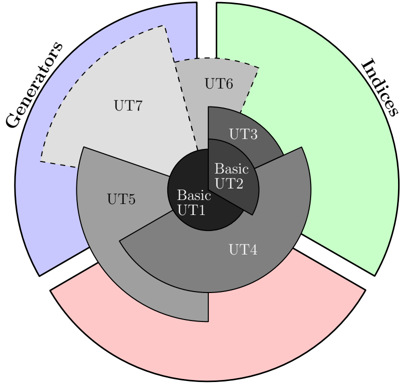
Unit Test

general:
a simple rule describing a behavioral pattern of a component

example for generators:
as the level of perturbation increases (modeled by parameters) the coverage of the clustering should not increase

$$\text{coverage} = \frac{\#\text{ intra-cluster edges}}{\# edges}$$

Collection of Unit Tests



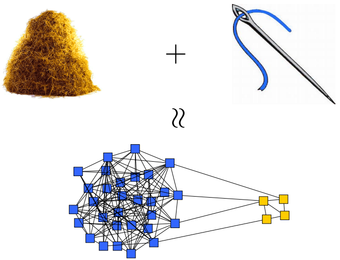
desired outcome:

- basic rules for general behavioral patterns
- advanced rules building on tested components
- application-specific requirements as constraints

Outline

Random Clustered Graph Generator

classification model



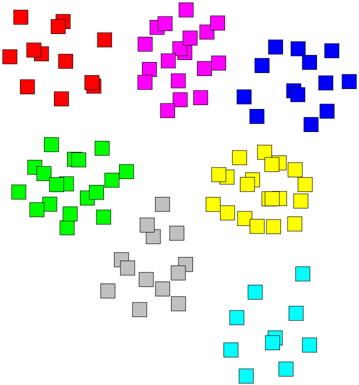
generator:

- create n nodes
- partition nodes in k clusters
- create edges inside of clusters with probability p_{in}
- create edges between clusters with probability p_{out}

overall:

- random graph with clustering structure
- significance of clustering depends on probabilities p_{in} and p_{out}

Example: $\mathcal{G}((12, 18, 13, 18, 20, 13, 10), 0.85, 0.01)$



- node partitioning in 7 clusters

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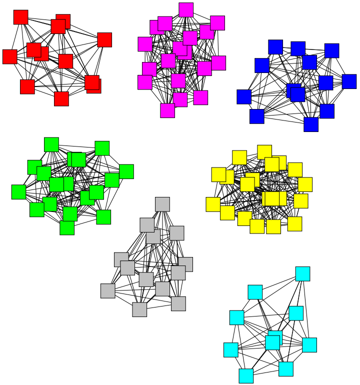

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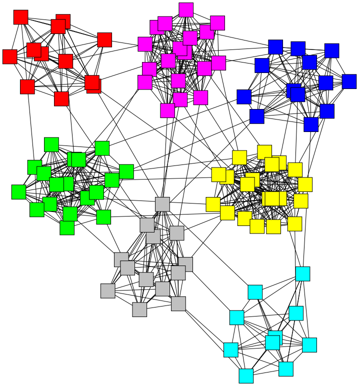

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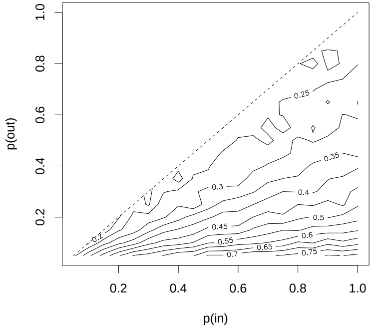
Validation via Basic Unit Test



- increases in perturbation implies non-increase in coverage: ✓
- increases in perturbation implies non-increase in modularity: ✓

overall measuring perturbation vs. quality: ✓

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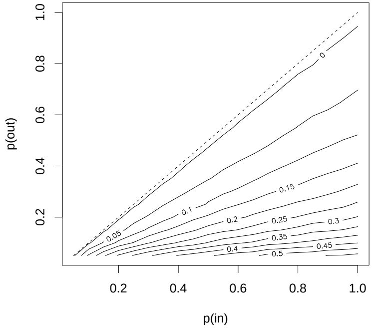

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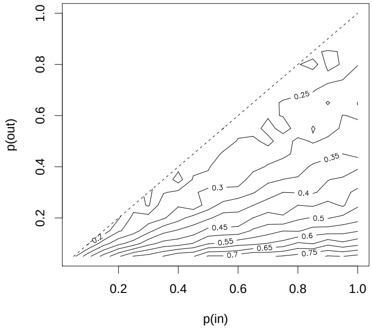
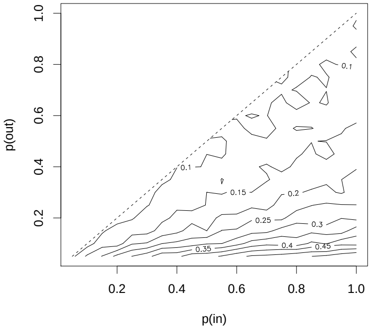
Scalability?



$n = 100$



$n = 1000$

ratio of intra- and inter-cluster edges depends on $p_{\text{in}}, p_{\text{out}}$ and n

Scalability?

questions:

- what is the dependency of number and size of clusters and n?
- should the ration (intra- vs. inter-cluster edges) be independent of n?
- what about other properties? quality?

Tuning Parameters

choosing p_{out} individually according to k, p_{in} and the ratio of (expected) intra- versus inter-cluster edges

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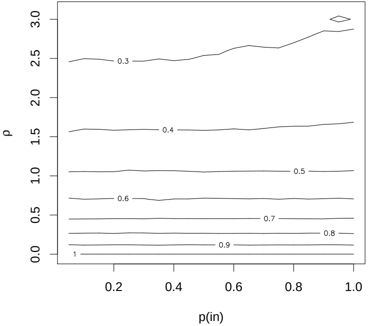

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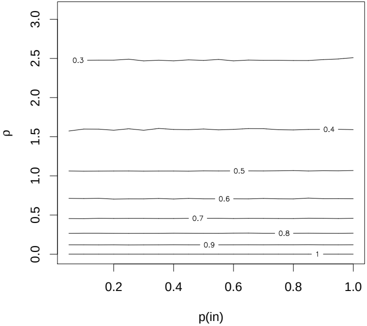

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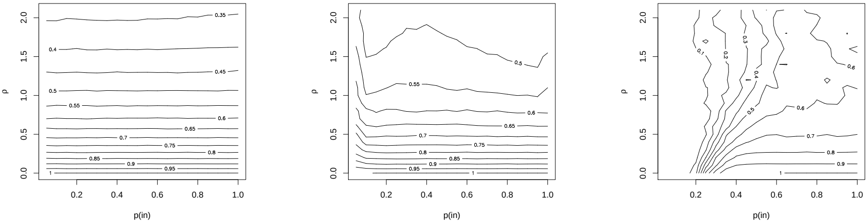
Comparing Algorithms

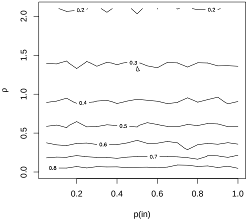
comparing coverage:



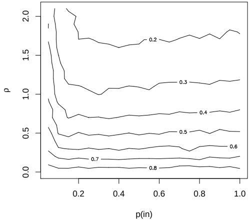
generator greedy optimization iterative pruning

Comparing Algorithms

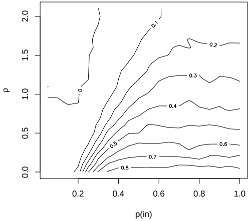
comparing modularity:



generator



greedy optimization



iterative pruning

Observations

greedy optimization:

- general good performances (wrt. generator)
- minor artifacts for very very sparse graphs

iterative pruning:

- good performance for small-perturbed instances
- artifacts for sparse graphs ($p_{\text{in}} \leq 0.2$)

Outline

Summary

experimental evaluation:

- good and flexible mean for average-case analysis
- easy to reproduce and compare with each other
- implicit assumption of the model can have a large impact
- not all combination of generators, algorithms and quality measures makes sense
- designing and evaluating good components is non-trivial

Summary

concept of unit test:

- engineering approach to systematic evaluations
- formalization of rules of thumb
- easy integration of application specifics
- knowledge of basic building blocks required
  (e.g. formalization of model as quality index)
- results target only "average" cases

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