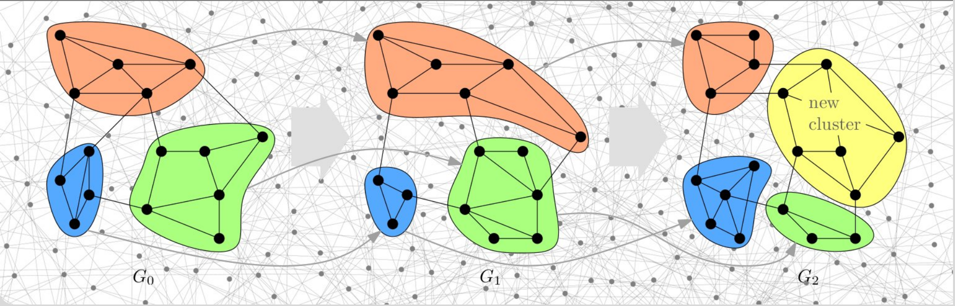
Algorithm Engineering for Graph Clustering

School on Graph Theory, Algorithms and Applications

Dorothea Wagner | Erice, Italy, 25. September – 3. October, 2011

KARLSRUHE INSTITUTE OF TECHNOLOGY – INSTITUTE OF THEORETICAL INFORMATICS

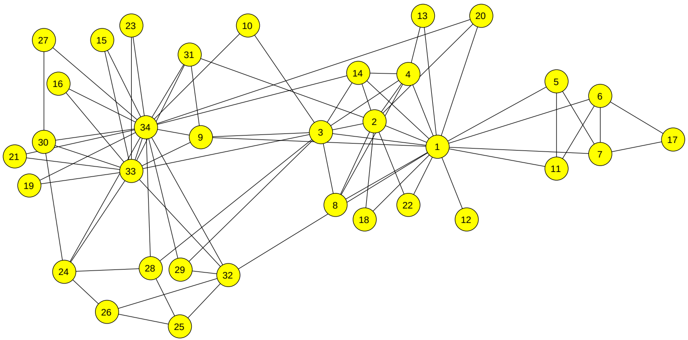


Structure

Structure

Scenario of Network Analysis

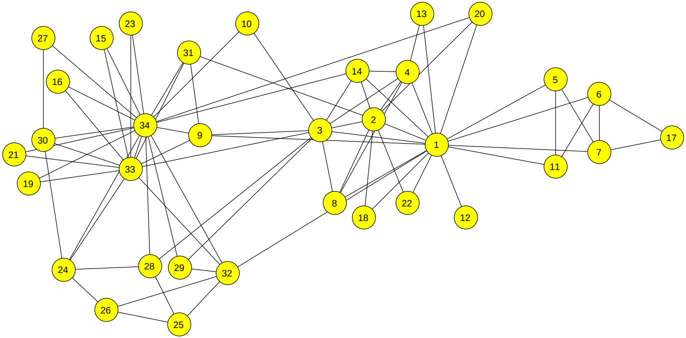
Given a network . . .



- explore the instance
- derive its structure
- identify its properties

Scenario of Network Analysis

Given a network . . .



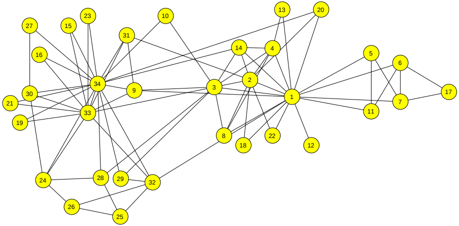
- explore the instance
- derive its structure
- identify its properties

How can we learn about the instance?

Structure

An Archetypal Example

"Zachary's Karate Club", a real, social network

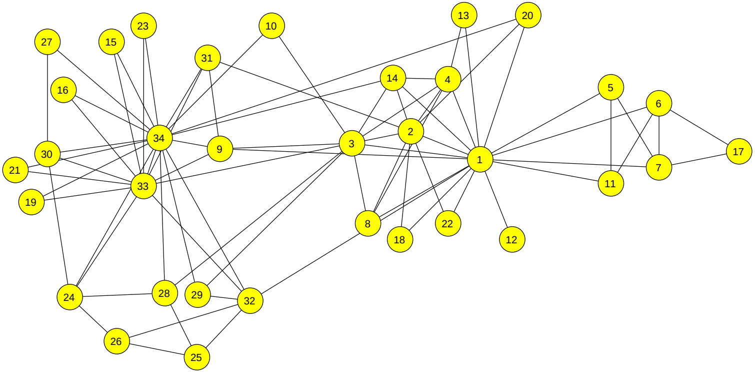


- 2 years of observation
- 34 vertices = members
- 78 edges = social ties
- club split up after dispute
- manager vs. trainers
- archon of toy examples

Caused by an *"unequal flow of sentiments and information across the ties"* a *"factional division led to a formal separation of the club"*.

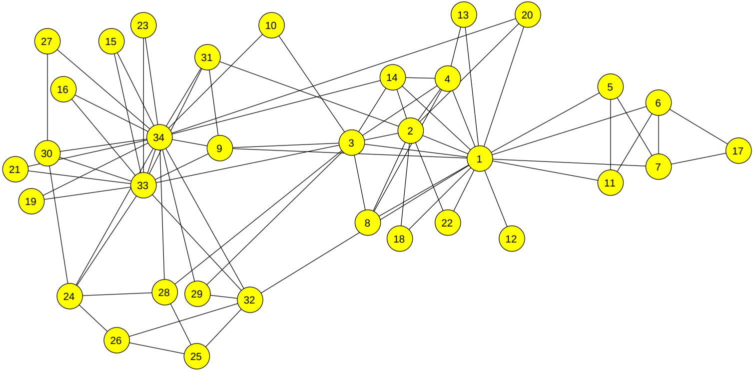
[Wayne Zachary: An Information Flow Model for Conflict and Fission in Small Groups, '77]

A Glimpse of Network Analysis



A Glimpse of Network Analysis

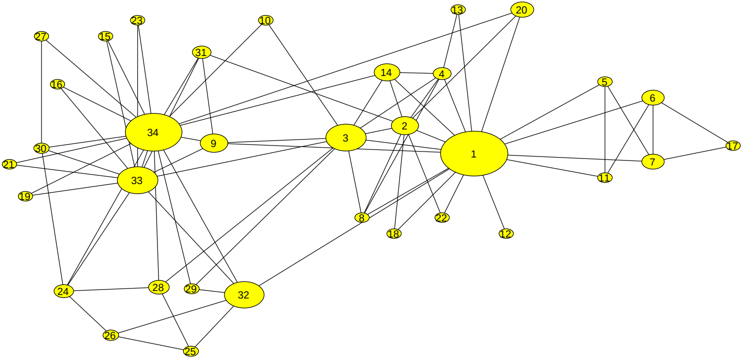
size, density,



#vertices = 34, #edges = 78, ∅-degree = 4.6

A Glimpse of Network Analysis

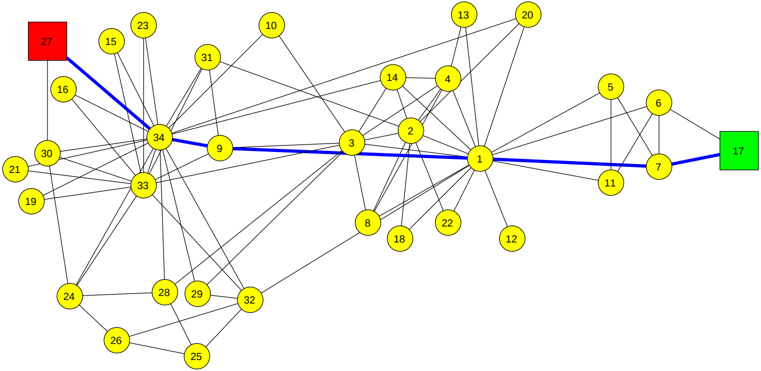
size, density, centrality / importance,



size = importance

A Glimpse of Network Analysis

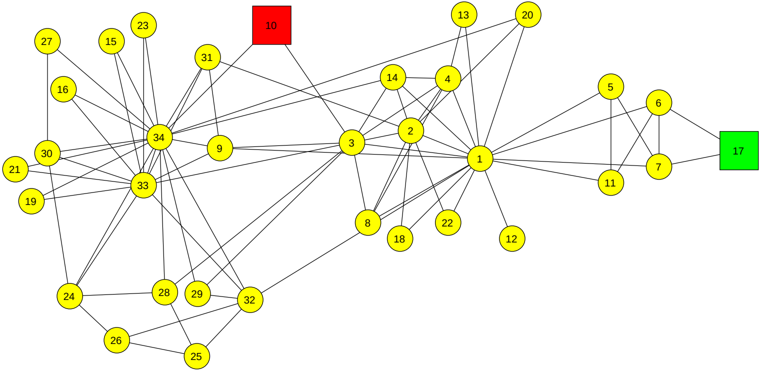
size, density, centrality / importance, distances,



distance between red and green

A Glimpse of Network Analysis

size, density, centrality / importance, distances, maximum flow,



flow from red to green

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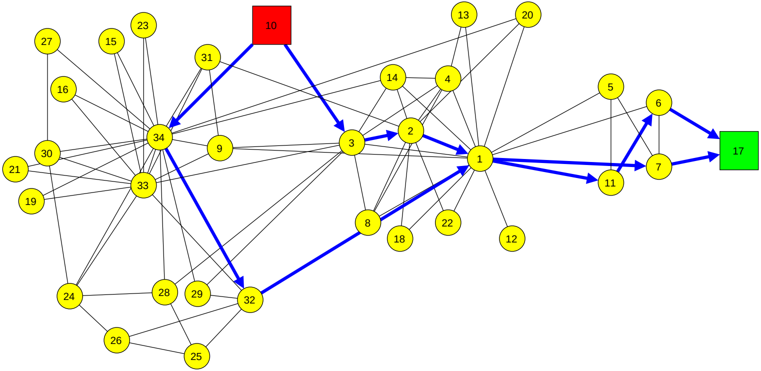
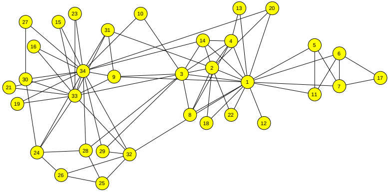
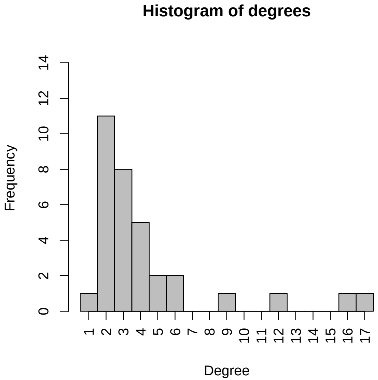


flow from red to green

Degree Distribution





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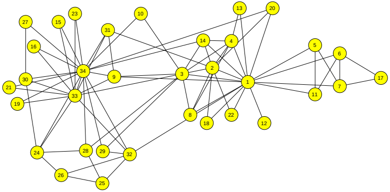

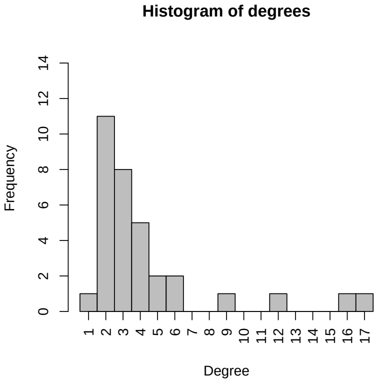

typical:
- (very few very-low-degree vertices)
- exponential-like distribution
- long tail or rare high degrees

Two Basic Models and their Degrees

Question: What is a reasonable random model emulating real networks?

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Gilbert's model $G(n, p)$ / Erdős-Rény model $G(n, m)$

1. introduce n vertices
2. for each pair $\{u, v\} \in \binom{V}{2}$, connect $\{u, v\}$ with probability p

degree distribution (binomial): $P(d) = \binom{n-1}{d} \cdot p^d (1-p)^{n-1-k}$

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Cumulative Advantage / Preferential Attachment (n,a)

for vertices $v_1,\ldots,v_n$ do
    add vertex v_i to graph
    for v_i's edges $e_1,\ldots,e_a$ do
        connect v_i to (other) (non-adjacent) vertex u, with prob.$\sim \deg(u)$

degree distribution: $P(d) \sim d^{-\gamma}$ (with $\gamma = 3$ for this specific setup)

Core-Decomposition: Definition

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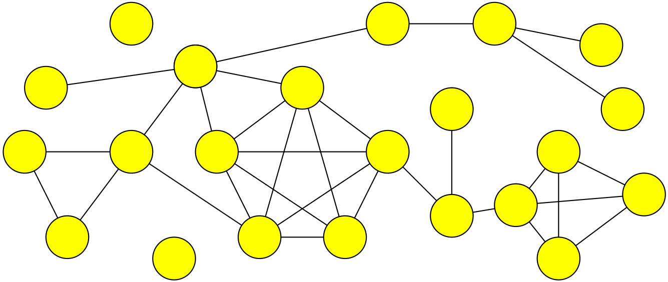
Definition (k-core of a graph)

Maximum subset of vertices $V_k \subseteq V$ such that each $v \in V_k$ has at least k neighbors in V_k (i.e.: $\forall v \in V_k : |N(v) \cap V_k| \geq k$).



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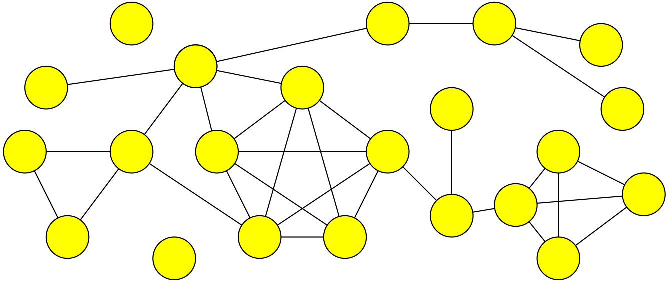

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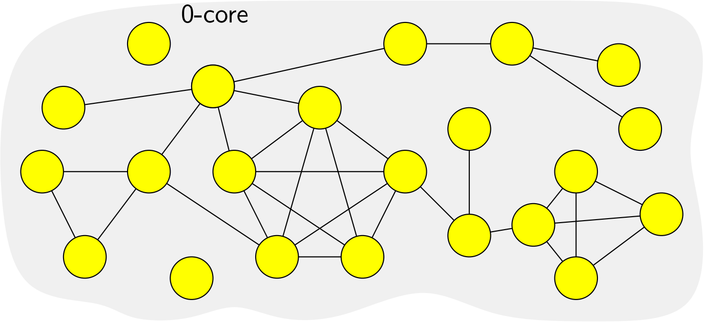

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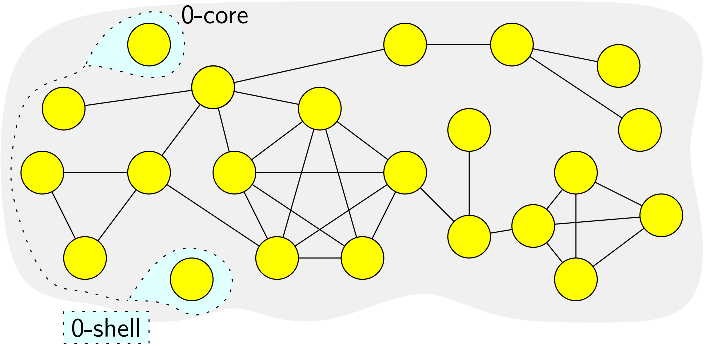

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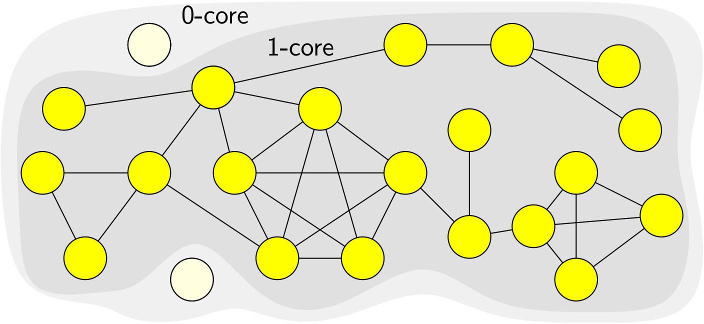

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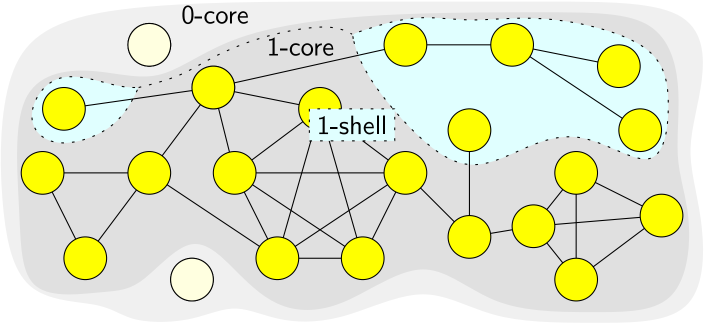

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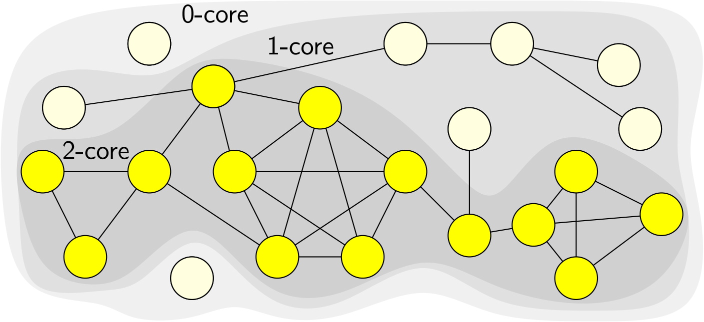

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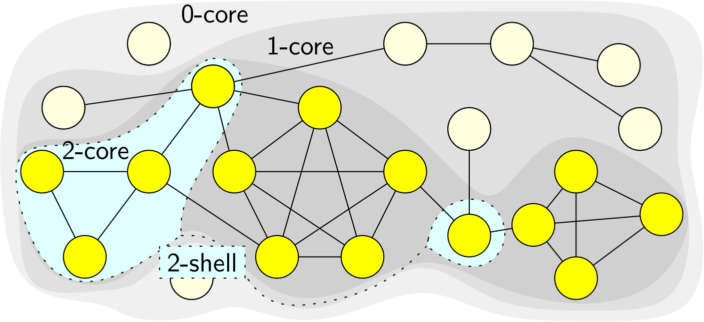

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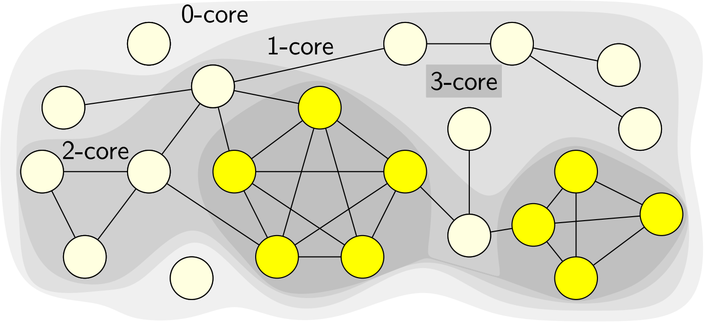

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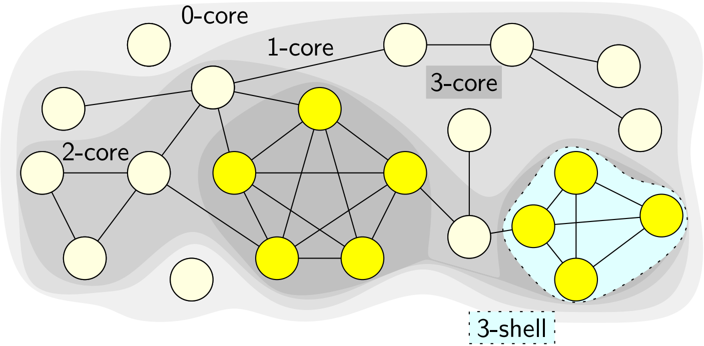

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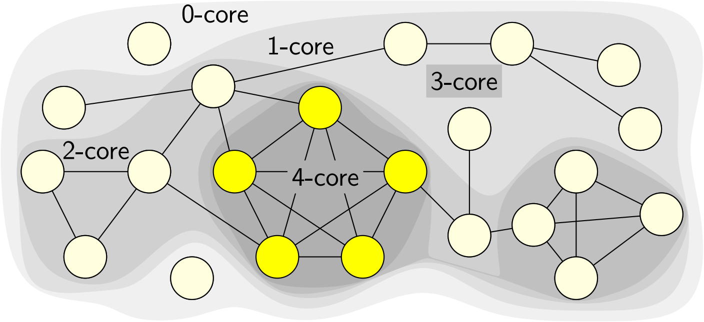

Centrality

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Idea: "[quantify intuition that some vertices are more central than others]"[1]
(note: *coreness* and *degree* are special measures for centrality)

[1] [[Brandes, Erlebach (eds.) '05, Network Analysis, Methodological Foundations]]

Centrality

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Idea: “[quantify intuition that some vertices are more central than others]”[1]
(note: *coreness* and *degree* are special measures for centrality)
Other important centrality measures are:

- *eccentricity:* $1/$ distance to farthest vertex in G
- *closeness:* $1/$ sum of distances to all vertices in G
- *stress:* total number of shortest paths requiring vertex v
- *betweenness:* sum of ratios of shortest paths requiring vertex v (over all pairs $s, t \neq v$)
- *reach:* maximum over all shortest s-t-paths v participates in: $\min\{\text{distance}(s, v), \text{distance}(v, t)\}$
- *Katz:* spectral, random walk, PageRank TODO

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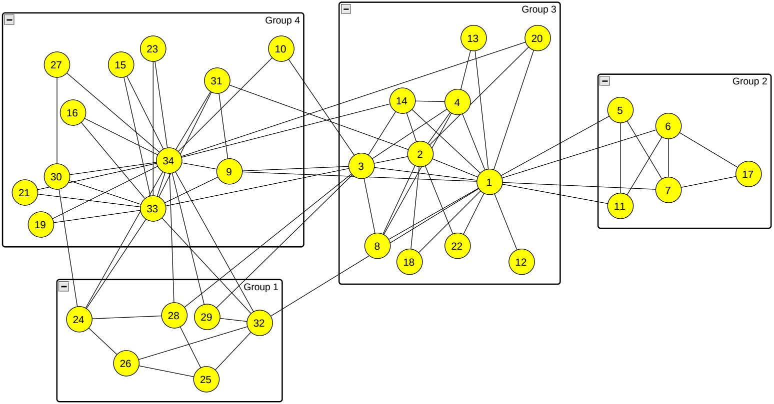
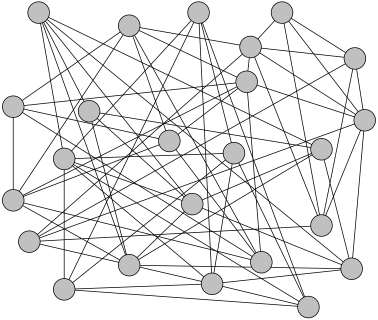
A Glimpse of Network Analysis

graph clustering / detecting communities



box = cluster

Why Graph Clustering?



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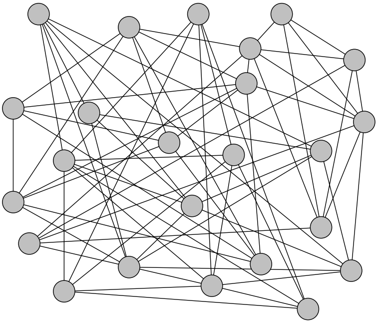

=

nodes	24
edges	57
cyclic	yes
planar	no
components	1
density	0.2065
avg. degree	4.75
core depth	4
triples	233
triangles	40
transitivity	0.515
clust. coeff.	0.6157

diverse field of network analysis

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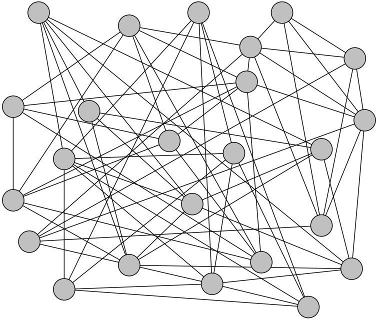

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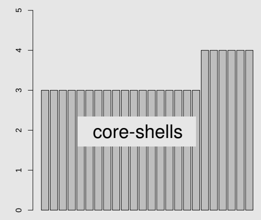

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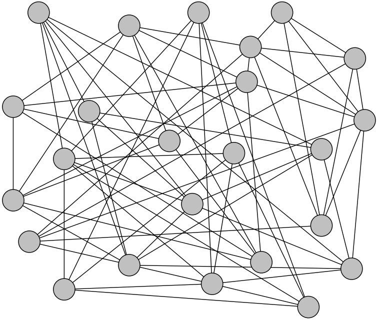

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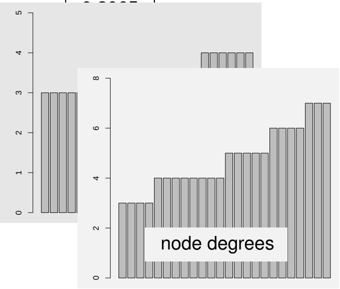

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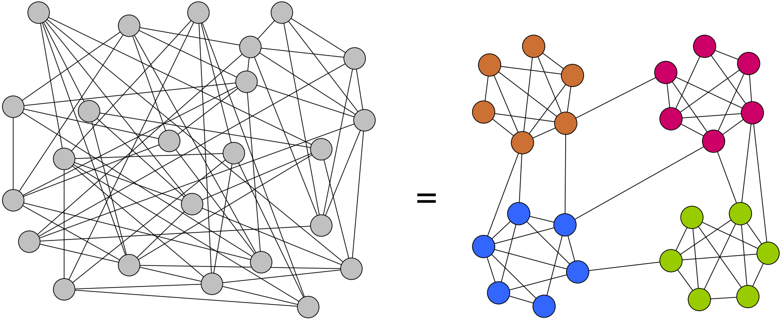
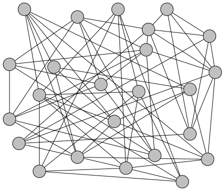


diverse field of network analysis
graph clustering = search for structure in networks

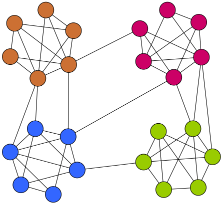
Structure

1. Introduction
   - Scenario: Network Analysis
   - Paradigm of Clustering
   - Example Applications
2. Formalization of Aims and Objectives
   - Objective Functions
3. Algorithmic Approaches
   - Greedy Merge
   - Local Moving and Multilevel
   - Clustering with Minimum-Cut Tree
   - Integer Linear Programs
   - Other Algorithmic Approaches
4. Experimental Evaluation
   - The Role of Test Data in Algorithm Engineering
   - Comparing Clusterings
5. Dynamic Graph Clustering
   - Online Dynamic Clustering
   - Offline Dynamic Clustering
6. Appendix

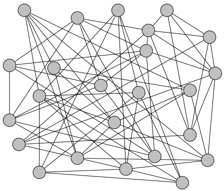
Clustering: Intuition to Formalization



- **Task:** partition graph into natural groups
- **Paradigm:** intra-cluster density vs. inter-cluster sparsity



Clustering: Intuition to Formalization



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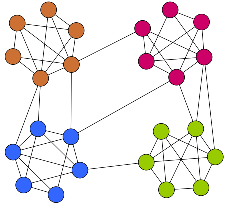


Different approaches exist to formalize this paradigm, usually:

Paradigm of Graph Clustering

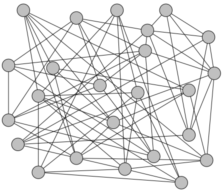
Intra-cluster density vs. inter-cluster sparsity

$\Downarrow$

Mathematical Formalization

quality measures for clusterings

Clustering: Intuition to Formalization



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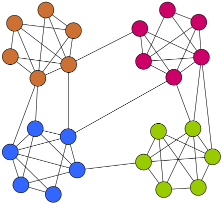

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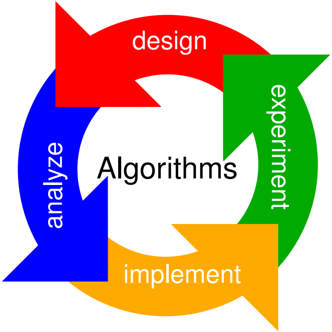
Mathematical Formalization

quality measures for clusterings

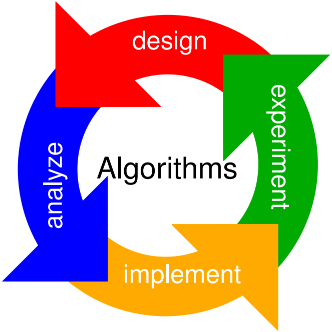
- Many exist, optimization generally (NP-)hard
- There is no single, universally best strategy

Algorithm Engineering



- modelling reality is hard

Algorithm Engineering



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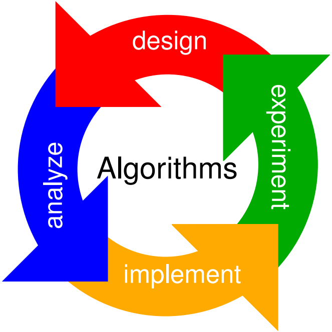

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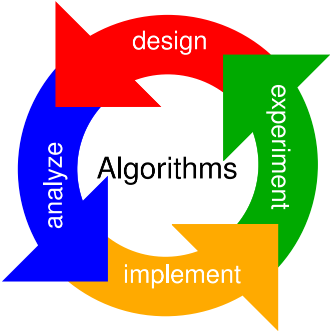

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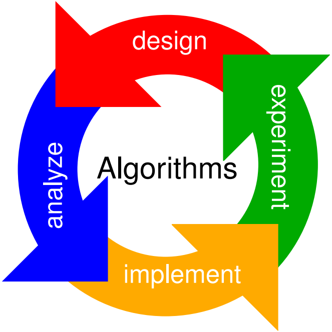
Algorithm Engineering



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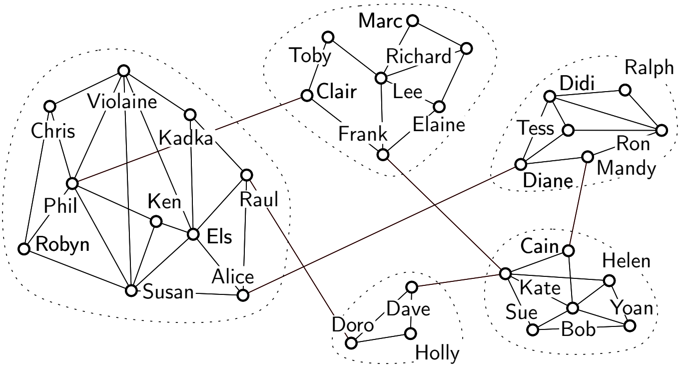
- still, we do need to cluster
- $\Rightarrow$ need good foundation

Formalization via Bottleneck



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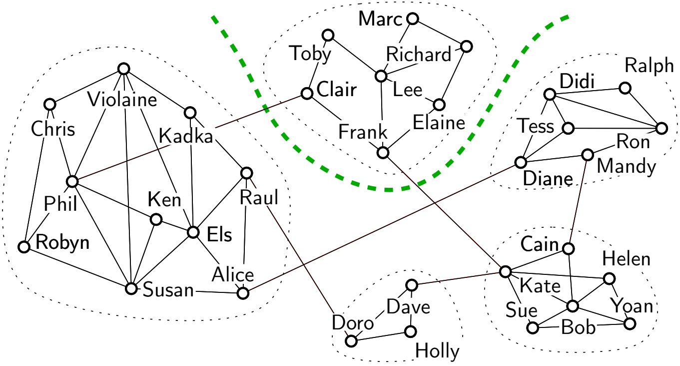
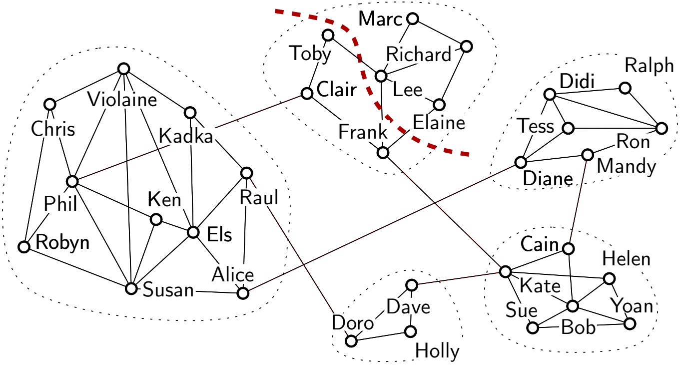


Quality of the clustering, upper cluster:

- inter-cluster sparsity: 2 *edges for cutting off* 7 *nodes* **(cheap)**

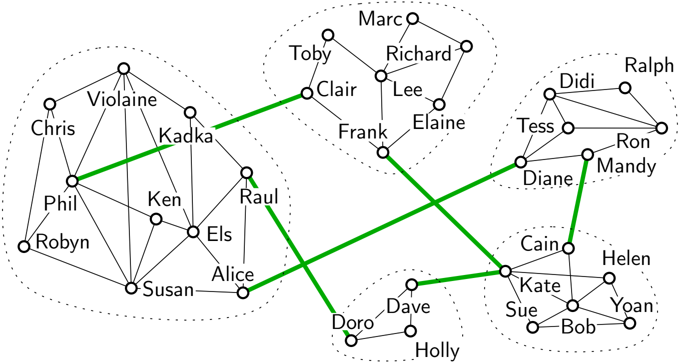
Formalization via Bottleneck



Quality of the clustering, upper cluster:

- inter-cluster sparsity: 2 *edges for cutting off* 7 *nodes* **(cheap)**
- intra-cluster density: best addit. cut:
  3 *edges for cutting off* 4 *nodes* **(expensive)**

Formalization: Counting Edges



Measuring clustering quality by counting edges:

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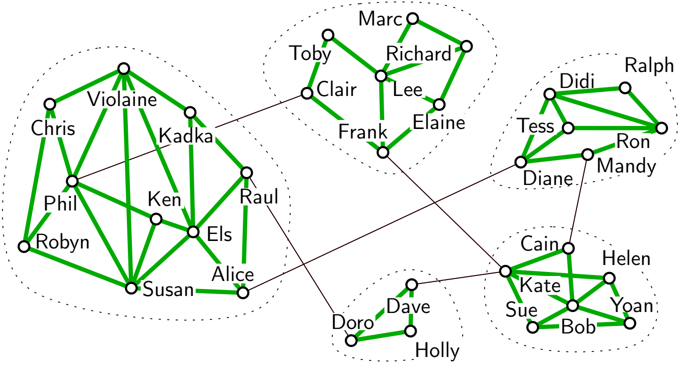

Measuring clustering quality by counting edges:

- inter-cluster sparsity: 6 *edges of ca. 800 node pairs* **(few)**
- intra-cluster density: 53 *edges of* 99 *node pairs* **(many)**

Clustering vs. Partitioning

	clustering	**partitioning**
purpose	analysis (pred.)	handling of instance
. . . and then?	zoom/abstraction	computations on parts
# of parts	open	predefined (upper bound)
size of parts	open	upper bound (or even fixed)
criteria	various (later)	weighted cuts
constraints	often none	see above
applications	various (later)	often: distributed finite element methods on 3d-meshes of objects

Bicriterial Formulations

observations:

1. clusterings often “nice” if balanced (like partition)
2. *intra-density vs. inter-sparsity* is bicriterial

bicriterial (or multi-) measures for clusterings can help:

- constrain sparsity within clusters
- constrain density between clusters
- explicitly formulate desiderata

(more on bicriteria later)

Postulations to a Measure

Given a graph G and a clustering $\mathcal{C}$, a *quality measure should behave as follows:*

- more intra-edges $\Rightarrow$ higher quality

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- less inter-edges $\Rightarrow$ higher quality
- cliques must never be separated
- clusters must be connected
- random clusterings should have bad quality

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Postulations to a Measure

Given a graph G and a clustering $\mathcal{C}$, a *quality measure should behave as follows:*

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- fulfill the desiderata of the application
- ...

exercise: choose desiderata and design a measure!

A Theorem of Impossibility

A warning theorem on the field of data clustering:

Theorem

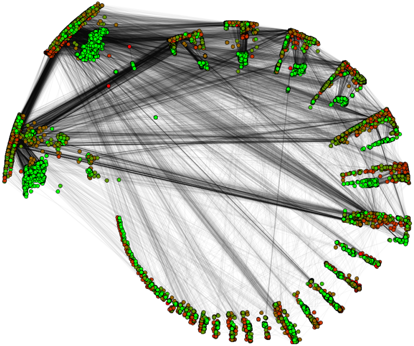
Given set S.
Let $f : d \mapsto \Gamma$ be a function on a distance function d on set S, returning a clustering Γ.
No function f can simultaneously fulfill the following:

- *Scale-Invariance*
  for any distance function d and any $\alpha > 0$, we have $f(d) = f(\alpha \cdot d)$
- *Richness*
  for any given clustering Γ, we should be able to define a distance function d such that $f(d) = \Gamma$
- *Consistency*
  if we build d' from d by reducing intra-distances and increasing inter-distances, we should have $f(d') = f(d)$

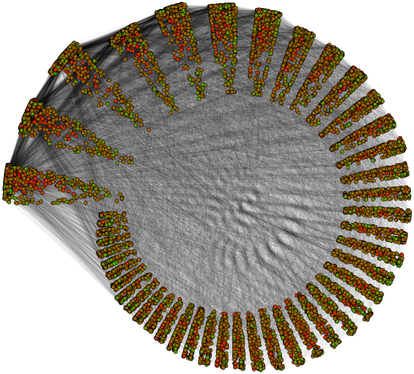
[Jon Kleinerg: An Impossibility Theorem for Clusterings, 2002]

Still, there is structure in networks!

we want/need to find it, and it is doable in practice



AS network, decomposed by a clustering; nodes with a high (low) betweenness are colored red (green)



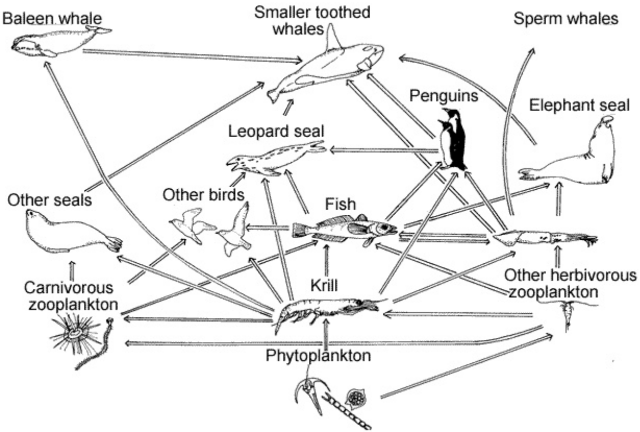
a network created with BRITE, designed to emulate the AS topology

[Görke at al.: LunarVis – analytic visualizations of large graphs, 2008]
[Medina et al.: BRITE – an approach to universal topology generation, 2001]

Structure

1. Introduction
   - Scenario: Network Analysis
   - Paradigm of Clustering
   - Example Applications
2. Formalization of Aims and Objectives
   - Objective Functions
3. Algorithmic Approaches
   - Greedy Merge
   - Local Moving and Multilevel
   - Clustering with Minimum-Cut Tree
   - Integer Linear Programs
   - Other Algorithmic Approaches
4. Experimental Evaluation
   - The Role of Test Data in Algorithm Engineering
   - Comparing Clusterings
5. Dynamic Graph Clustering
   - Online Dynamic Clustering
   - Offline Dynamic Clustering
6. Appendix

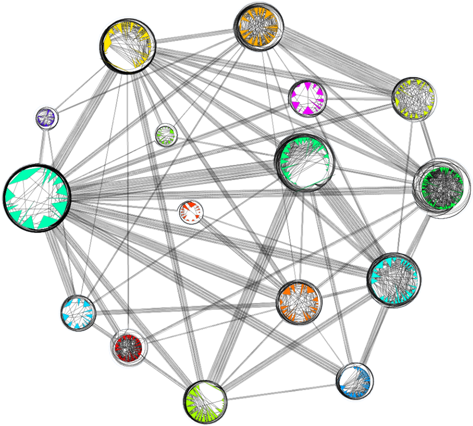
Applications



A simplified ecosystem: the antarctic food web
(source: Antarctica)

cluster ≈ self-sustaining / indivisible subsystem

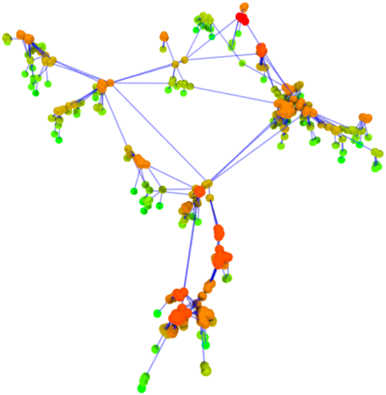
Applications



Company-internal email traffic, groups are departments

(source: )

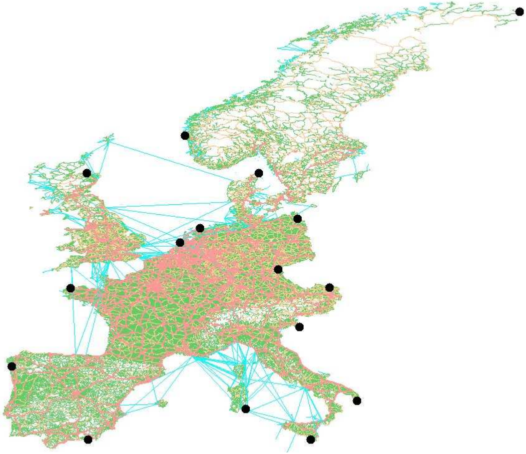
Applications



Excerptof the network of Amazon recommendations, around
"*VW Beetle Repairs*"
(source: [Gaertler 07])

cluster $\approx$ customer profile

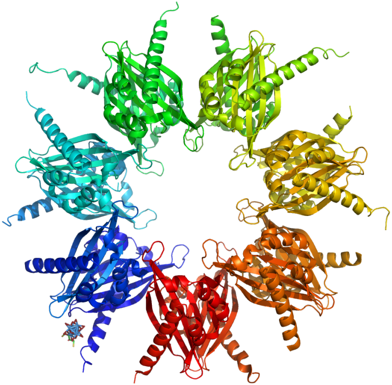
Applications



Road network of Europe, 18M vertices, 42M vertices
(source: PTV)

cluster ≈ urban areas used for preprocessing in route planning

Applications

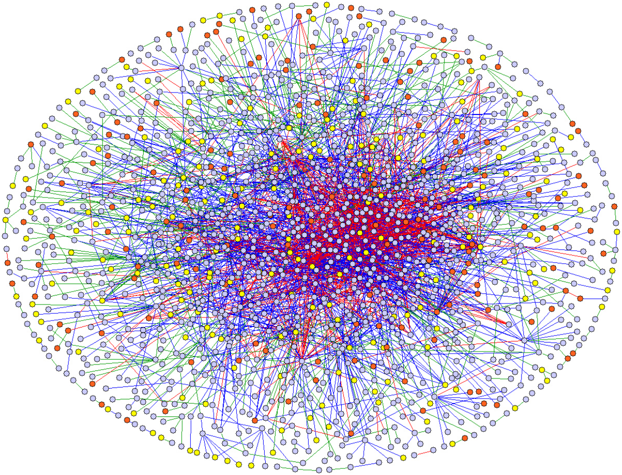


molecular structure of a protein

(Ca^{2+}/Calmodulin-dependent kinase II (CaMKII)
source: protein database www.rcsb.org)

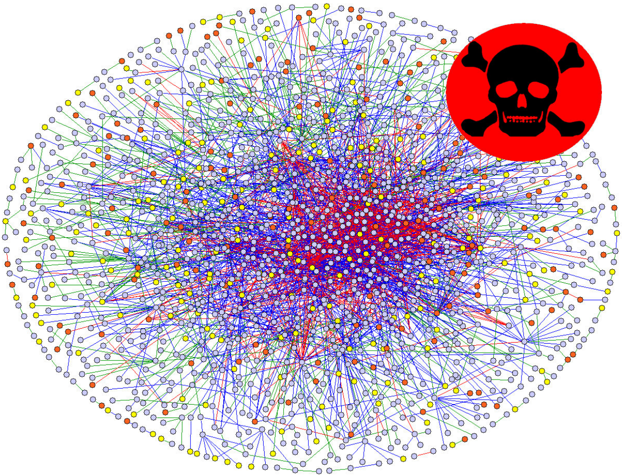
cluster ≈ functional unit (*domain*) of a protein

Applications



protein interactions
(source: Max-Delbrück-Centre for molecular medicine, www.mdc-berlin.de)

Applications



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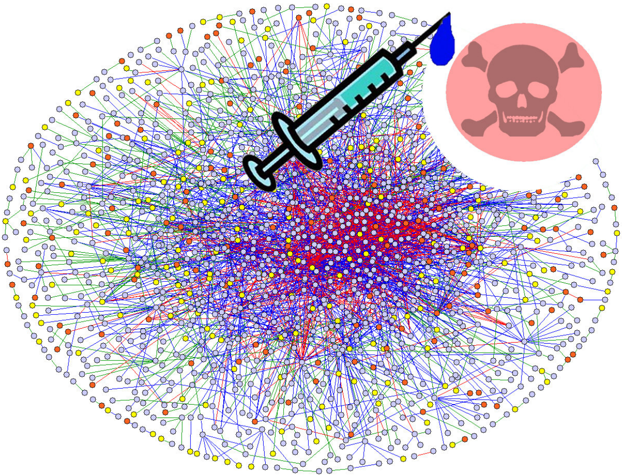
cluster ≈ isolatable seat of disease

Applications



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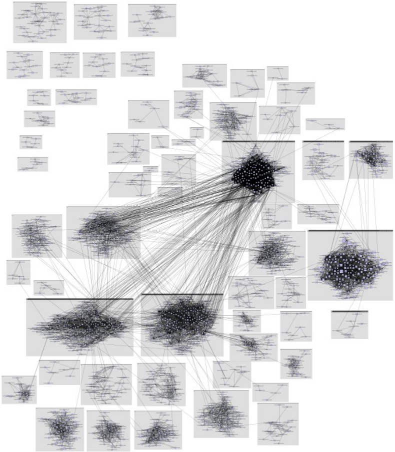
(source: Max-Delbrück-Centre for molecular medicine, www.mdc-berlin.de)

cluster ≈ isolatable seat of disease

Application: Shopping Data

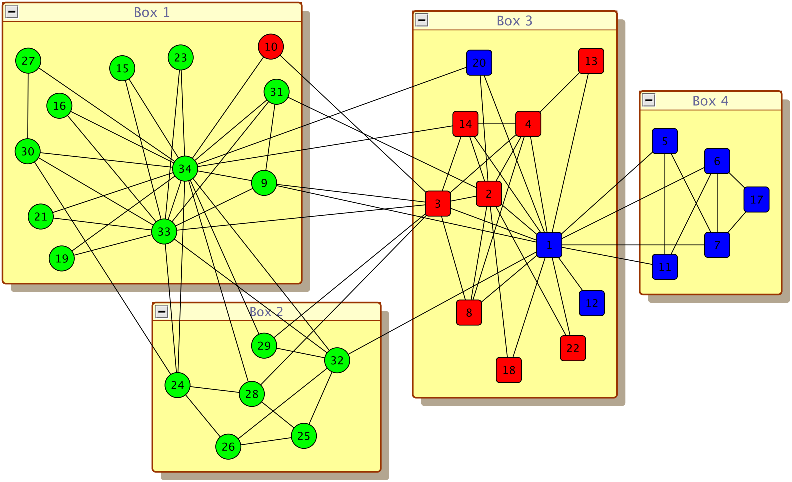
Data:

- **product base**
  product, classification, brand, setup block, . . .
- **store base**
  location, type, size, catchment area, . . .
- **customer base**
  customer number, age, gender, post code, . . .
- **receipts**
  “Who bought what, when and where?”



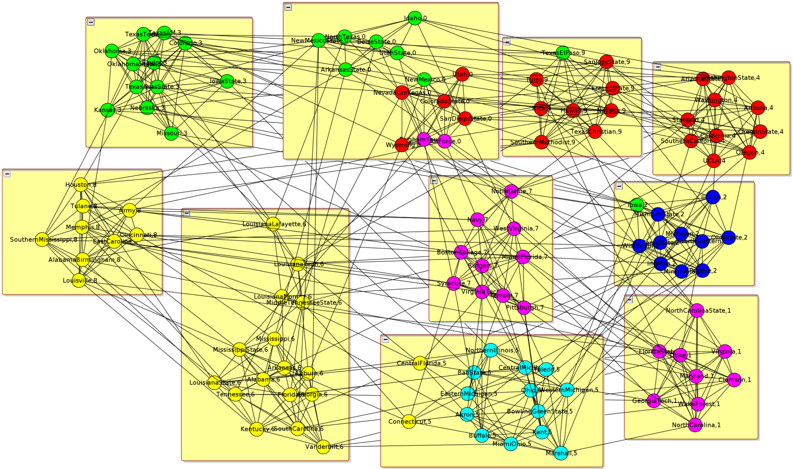
(example network of *receipt-similarity* one store, one month, clustered)

Scaling of Real-World Instances



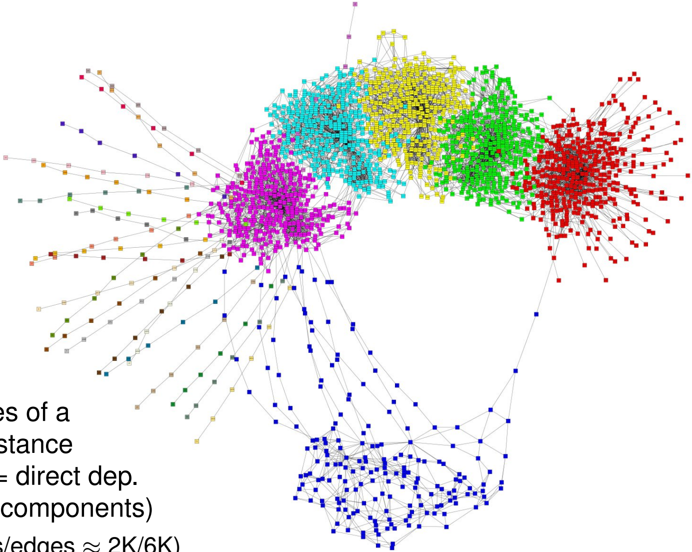
„Zachary's Karate Club")
(vertices/edges = 34/78)

Scaling of Real-World Instances



„US college football“ teams and matches
(vertices/edges = 115/616)

Scaling of Real-World Instances

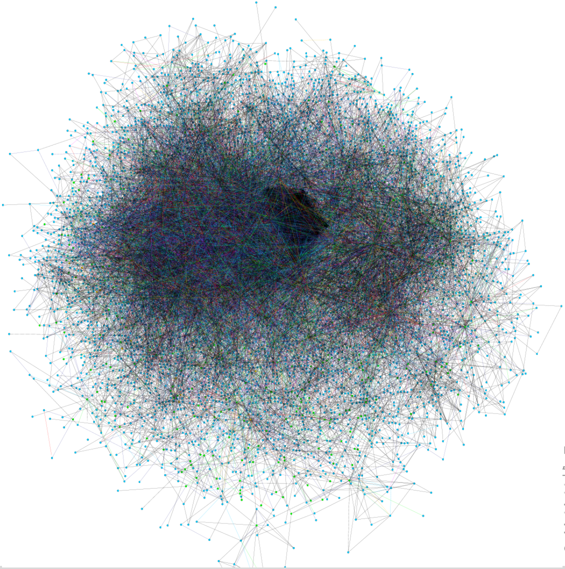


variables of a
SAT-instance
edges = direct dep.
(electr. components)

(vertices/edges ≈ 2K/6K)

Scaling of Real-World Instances

sci. collaborations:
3-hop neighorhood
von D. Wagner
(*DBLP*)
(vertices/edges ≈ 10k/40k)



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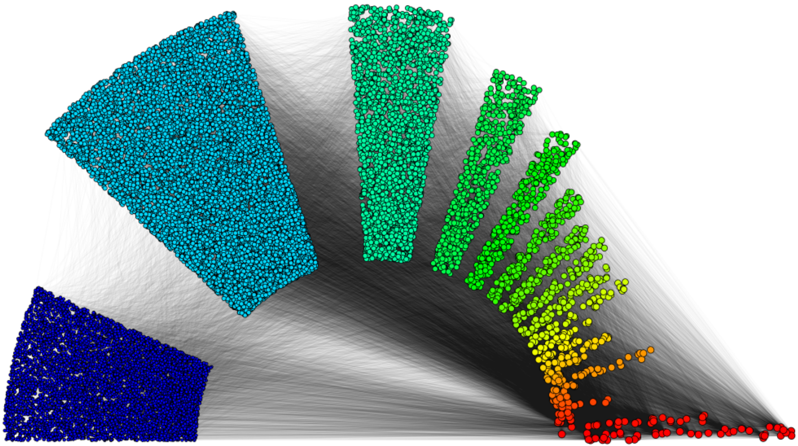


physical Internet: autonomous systemes

(vertices/edges $\approx$ 20K/60K)

Scaling of Real-World Instances

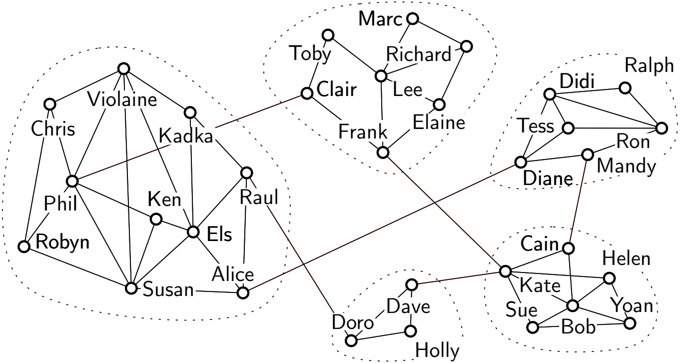
...no limit to be expected...

instance	vertices	edges
coauthors in *DBLP*	300K	1M
roads in the USA	24M	60M
WWW: .UK-domain '02	20M	500M
(neurons in human brain	$\gtrsim 10^{11}$	$\sim 10^{17}$)

Structure

Structure

Formalization via Bottleneck



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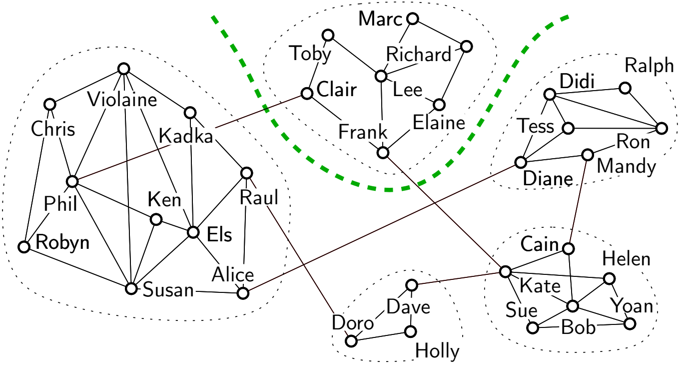
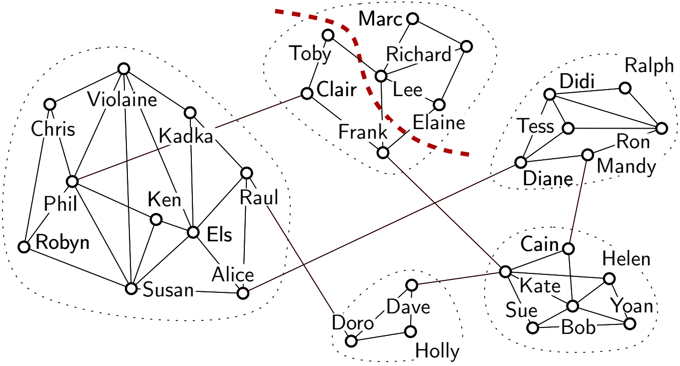


Quality of the clustering, upper cluster:

- inter-cluster sparsity: *2 edges for cutting off 7 nodes* **(cheap)**

Formalization via Bottleneck



Quality of the clustering, upper cluster:

- inter-cluster sparsity: *2 edges for cutting off 7 nodes* **(cheap)**
- intra-cluster density: best addit. cut:
  3 edges for cutting off 4 nodes **(expensive)**

Examples: Conductance, Expansion

generalization to case of weighted edges $\omega(e) \not\equiv 1$
e.g.: $\omega(E') = \sum_{e \in E'} \omega(e)$ or $\omega(v) = \sum_{e \sim v} \omega(e)$

conductance of a cut $(C, V \setminus C)$:

$$\varphi(C, V \setminus C) := \frac{\omega(E(C, V \setminus C))}{\min\left\{\sum_{v \in C} \omega(v), \sum_{v \in V \setminus C} \omega(v)\right\}}$$

(i.e.: thickness of bottleneck which cuts off C)

inter-cluster conductance $(\mathcal{C}) := 1 - \max_{C \in \mathcal{C}} \varphi(C, V \setminus C)$
(i.e.: $1-$ worst bottleneck induced by some $C \in \mathcal{C}$)

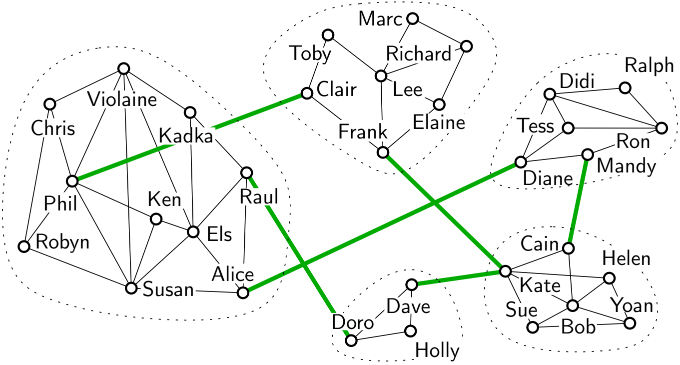
intra-cluster conductance $(\mathcal{C}) := \min_{C \in \mathcal{C}} \min_{P \uplus Q = C} \varphi_{|C}(P, Q)$
(i.e.: best bottleneck still left uncut inside some $C \in \mathcal{C}$)

expansion of a cut $(C, V \setminus C)$:

$$\psi(C, V \setminus C) := \frac{\omega(E(C, V \setminus C))}{\min\left\{|C|, |V \setminus C|\right\}}$$

(i.e.: in φ, replace $\omega(v)$ by 1; *intra-* and *inter-cluster expansion* analogously)

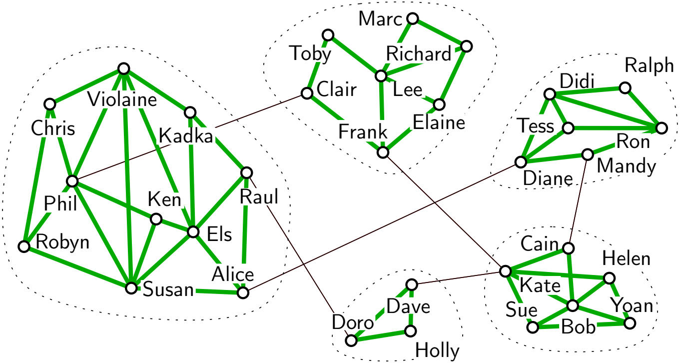
Formalization: Counting Edges



Measuring clustering quality by counting edges:

- inter-cluster sparsity: 6 *edges of ca. 800 node pairs* **(few)**

Formalization: Counting Edges



Measuring clustering quality by counting edges:

- inter-cluster sparsity: 6 *edges of ca. 800 node pairs* **(few)**
- intra-cluster density: 53 *edges of* 99 *node pairs* **(many)**

Example Counting Measures

coverage: $\text{cov}(\mathcal{C}) := \frac{\text{\# intra-cluster edges}}{\text{\# edges}}$

(i.e.: fraction of covered edges)

performance: $\text{perf}(\mathcal{C}) := \frac{\text{\# intra-cluster edges} + \text{\# absent inter-cluster edges}}{\frac{1}{2}n(n-1)}$

(i.e.: fraction of correctly classified pairs of nodes)

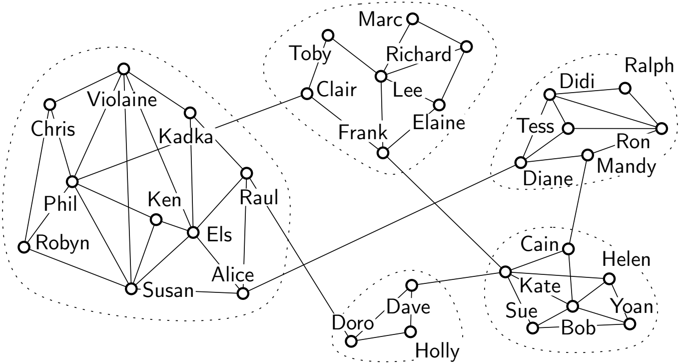
density: $\text{den}(\mathcal{C}) := \frac{1}{2}\frac{\text{\# intra-cluster edges}}{\text{\# possible intra-cluster edges}} + \frac{1}{2}\frac{\text{\# absent inter-cluster edges}}{\text{\# possible inter-cluster edges}}$

(i.e.: fractions of correct intra- and inter-edges)

modularity: $\text{mod}(\mathcal{C}) := \text{cov}(\mathcal{C}) - \mathbb{E}[\text{cov}(\mathcal{C})]$

(i.e.: how clear is the clustering, compared to random network?)

Motivation for Modularity



- *coverage* $= \dfrac{\text{\# intra-cluster edges}}{\text{\# edges}} \approx 0.9$

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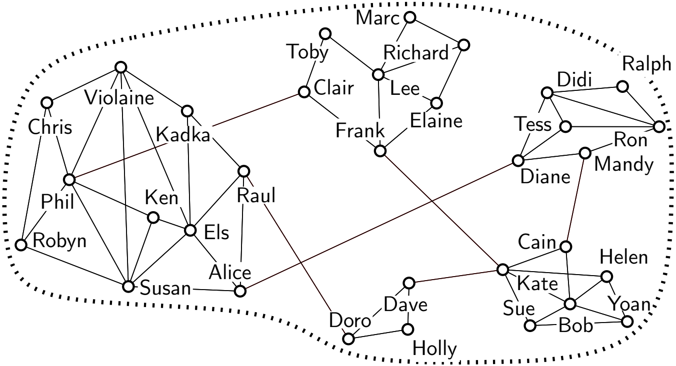

- $\textit{coverage} = \frac{\text{\# intra-cluster edges}}{\text{\# edges}} \approx 0.9$
- **only one cluster $\Rightarrow$ *coverage* = 1.0**

A Promising Remedy

[Girvan and Newman: Finding and evaluating community structure in networks, '04]:

"... if we subtract from [coverage] the ***expected*** *value [...], we do get a useful measure."*

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*"... if we subtract from [coverage] the **expected** value [...], we do get a useful measure."*

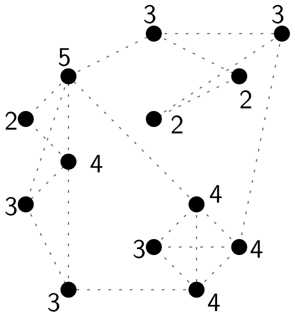
Modularity

$$\begin{aligned} \mathrm{mod}(\mathcal{C}) :=&\ \mathit{cov}(\mathcal{C}) - \mathbb{E}(\mathit{cov}(\mathcal{C})) \\ =&\ \frac{\#\text{ intra-cluster edges}}{|\#\mathit{edges}|} - \frac{1}{4|\#\mathit{edges}|^2} \sum_{C \in \mathcal{C}} \left(\sum_{v \in C} \deg(v) \right)^2 \end{aligned}$$

Probability Space of Modularity

Intuition: Keep expected node degrees, randomly throw in edges

1. start with set V



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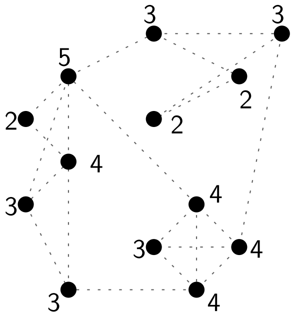

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1. start with set V
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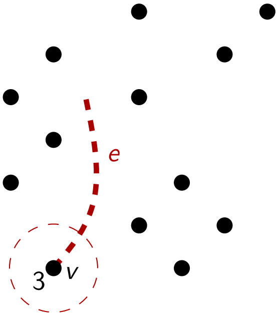
3. edge attaches to node v with $p = \frac{\deg(v)}{2|E|}$



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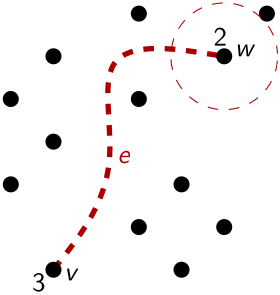

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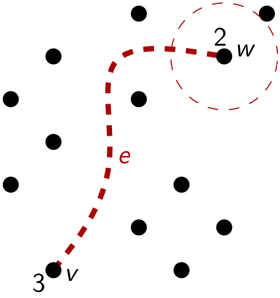
5. forward and backward $\rightsquigarrow$ count twice



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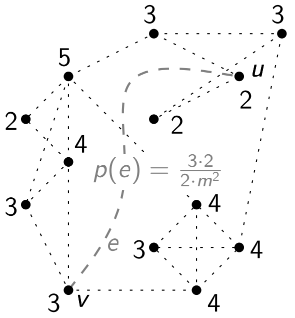

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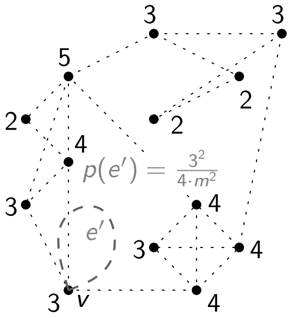

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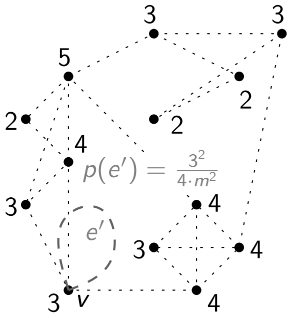

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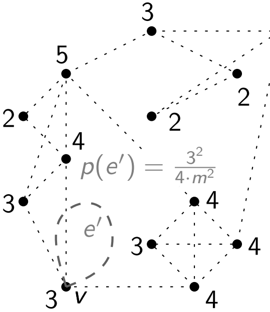
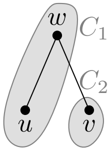
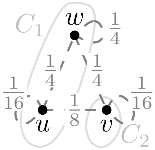




$G, \mathcal{C}(G)$

$\text{cov} = \frac{1}{2}$



(Ω, p),

$\mathbb{E}[\text{cov}] = \frac{5}{8}$

$\text{mod} = -\frac{1}{8}$ (bad!)

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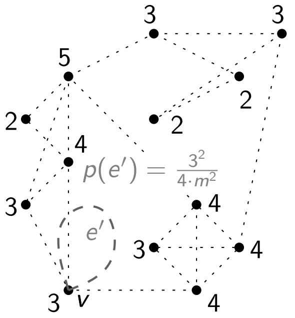

Some thoughts:

- (Ω, p) needs loops + parallel edges
  hazardous: e.g., paper on loop removal uses loop-agnostic formula!

Probability Space of Modularity

Intuition: Keep expected node degrees, randomly throw in edges

1. start with set V
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3. edge attaches to node v with $p = \frac{\deg(v)}{2|E|}$
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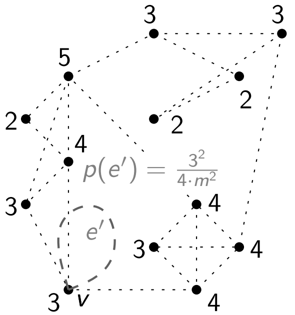

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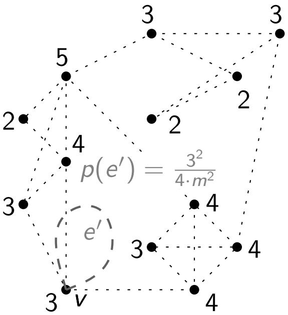

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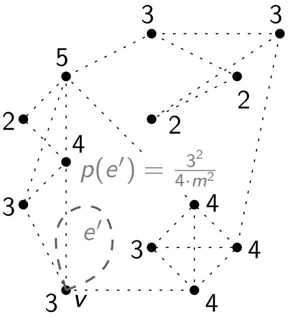

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Modularity in Practice

- easy to use & implement
- reasonable behavior on many practical instances
- $\rightsquigarrow$ heavily used in various fields
  - ecosystem exploration
  - collaboration analyses
  - biochemistry
  - structure of the internet (AS-graph, www, routers)
- close to human intuition of quality
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- scaling behavior (double instance, result differs) [folklore]
- non-locality of optimal clustering [folklore]
- resolution limit (no tiny and large clusters at the same time)
  [Fortunato and Barthelemy '07]
- large sparse graph $\rightsquigarrow$ high values, balanced clusters **exercise** [Good et al.: The performance of modularity maximization in practical contexts, 2009]

Modularity, Algorithmic Theory

The complexity of modularity optimization:

- finding $\mathcal{C}$ with maximum modularity is NP-hard
  $\rightsquigarrow$ reduction from 3-PARTITION
- restriction to $|\mathcal{C}| = 2$ also hard $\Rightarrow$ not FPT wrt. $|\mathcal{C}|$
- greedy maximization (later) does not approximate
- very limited families combinatorially solvable
- ILP-formulation, feasible for $\approx |V| \leq 200$

[Brandes et al.: On modularity clustering, 2008]

- diverse results on approximability on specific classes of graphs

[DasGupta, Devine: On the complexity of newman's community finding approach for biological and social networks, 2011]

Explicitly Bicriterial Approach

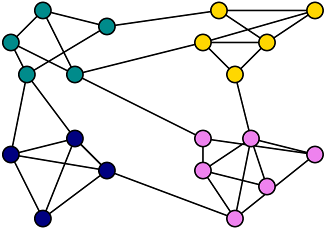
Optimization problem:

- guaranteed intra-cluster density
- good inter-cluster sparsity

Approach:

- systematic collection of sparsity and density measures

Inter-cluster-sparsity: A cut-based point of view



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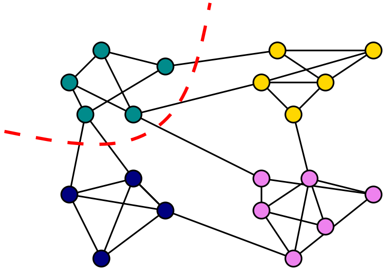

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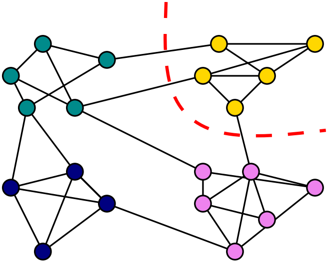

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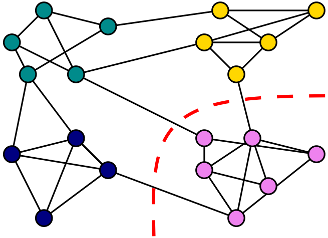

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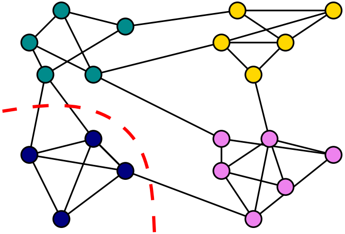

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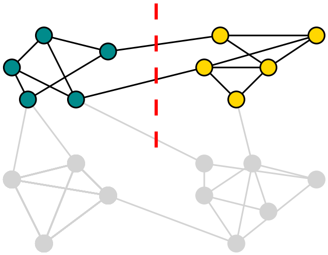

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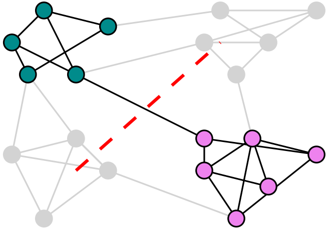

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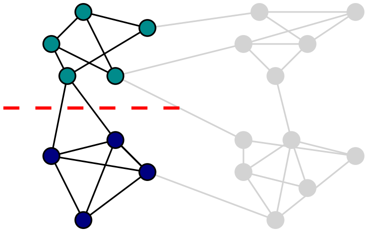

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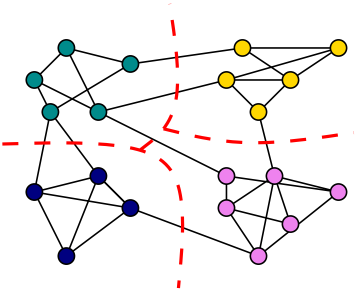

- **Isolated View:** Each cluster induces a cut
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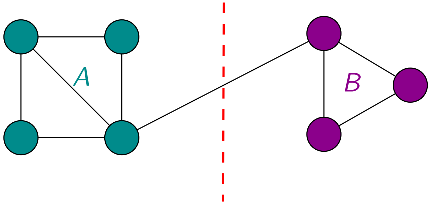
- **Global View:** A clustering with *k* clusters induces a k-way cut

Inter-cluster sparsity: Cut Measures



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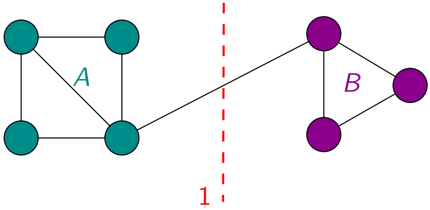

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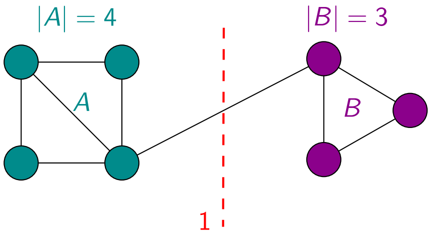

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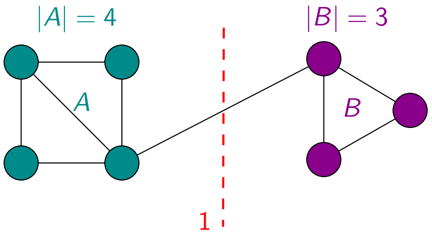

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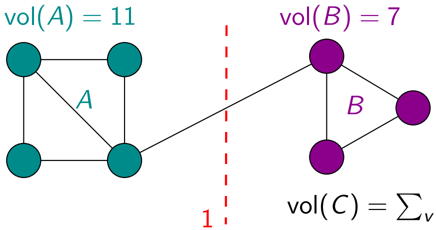

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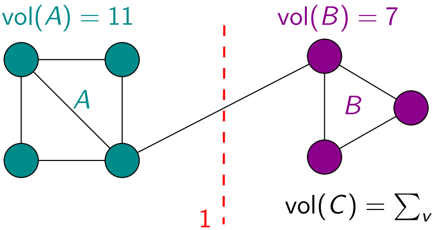

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$\Rightarrow$ Number of cut-edges and density can be generalized to k-way cuts

Inter-cluster Sparsity: Degrees of Freedom

Karlsruher Institut für Technologie

Set of cuts

- isolated (one for each cluster)
- pairwise (one for each pair of clusters)
- global (k-way cut)

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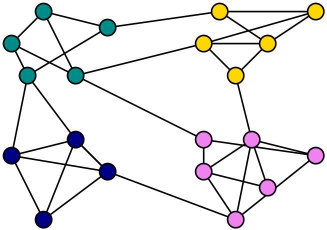

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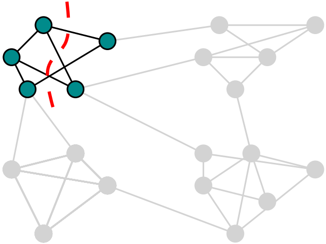

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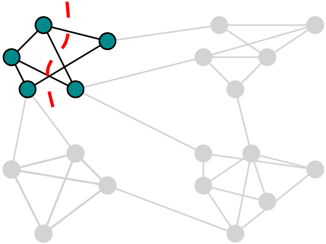

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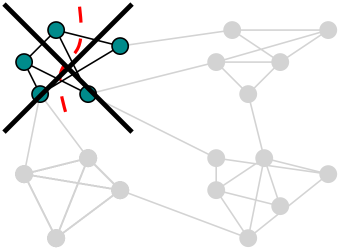

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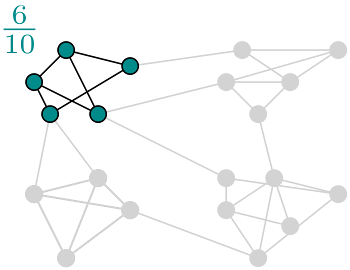

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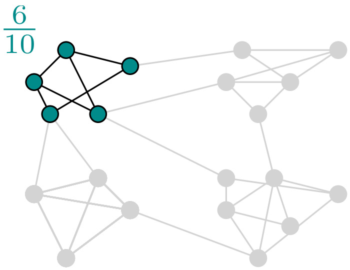

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$\Rightarrow$ **minimum/average/global intra-cluster density**

Problem Statement

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Density-Constrained Clustering[2]

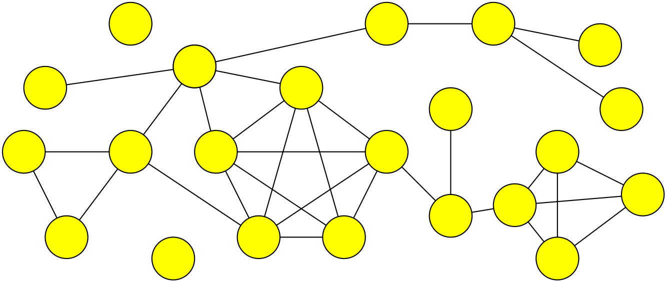
Given a graph $G = (V, E)$, among all clusterings with an intra-cluster density of no less than α, find a clustering $\mathcal{C}$ with optimum inter-cluster sparsity.

- 3 possible intra-cluster density measure
- 14 possible inter-cluster sparsity measures
- $\Rightarrow$ Family of 42 optimization problems

[2] [Schumm et al.: Density-constrained graph clustering, 2011]

Cluster Editing Set

"How many edges must be inserted or deleted to arrive at disjoint cliques?"



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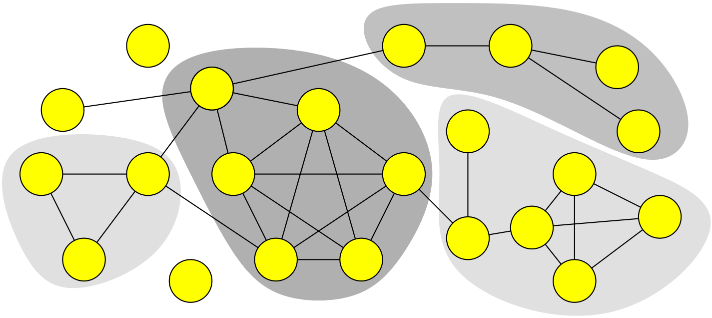

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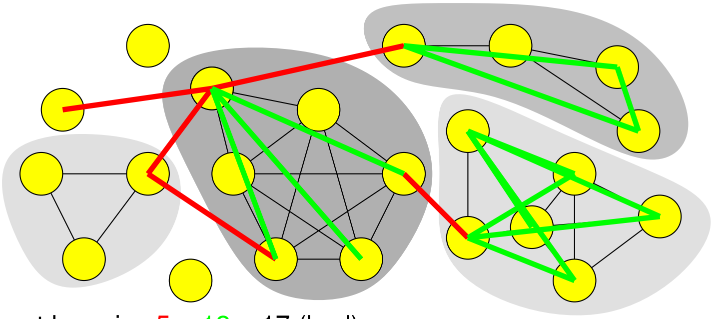

editing set has size 5 + 12 = 17 (bad)

Cluster Editing Set

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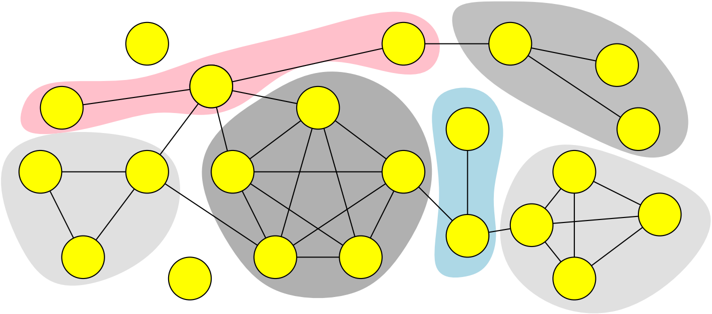

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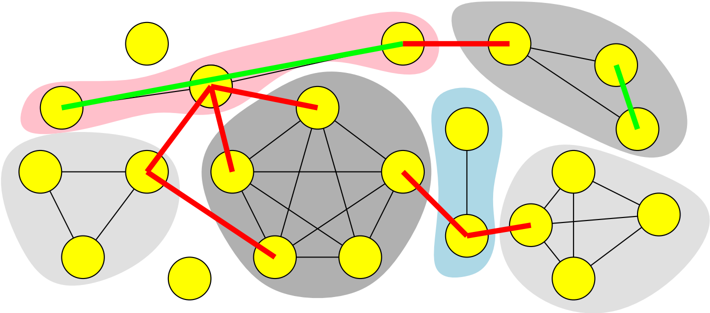

editing set has size 3 + 7 = 10 (better)

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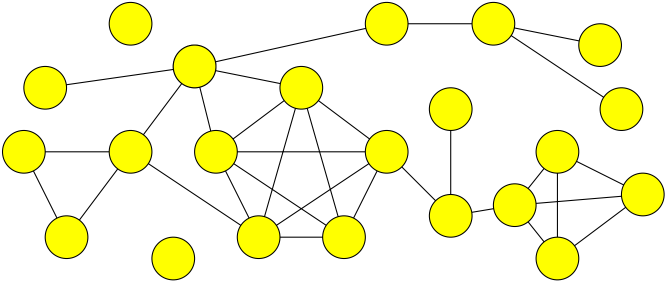

Task: find clustering with minimum cluster editing set

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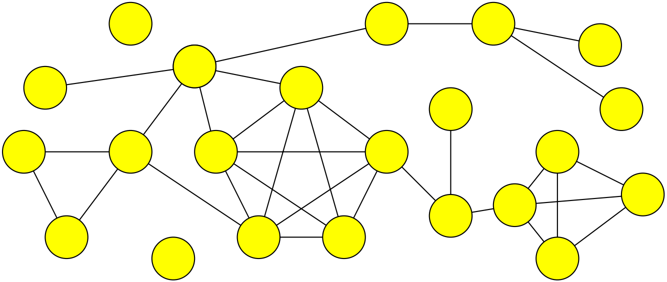

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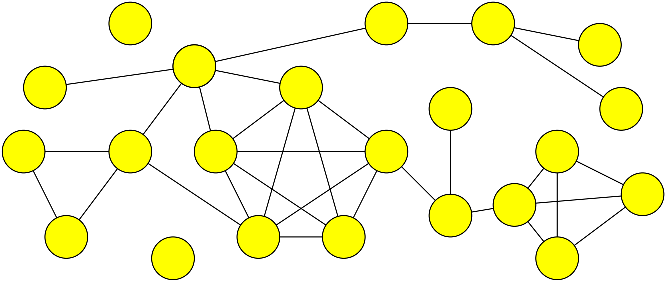
exercise: cluster editing set of Zachary?



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Formal Weaknesses?

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exercise: do the proposed measures violate any desiderata?

Structure

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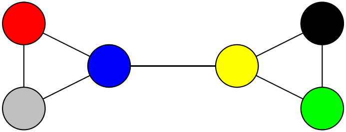

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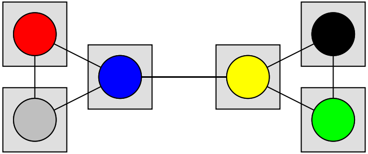

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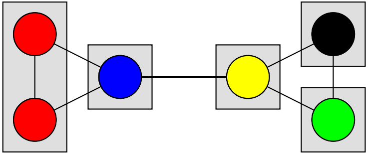

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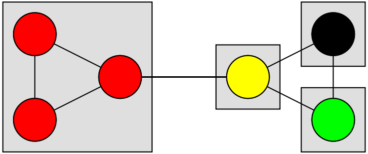

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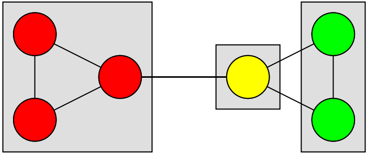

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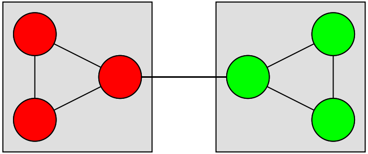

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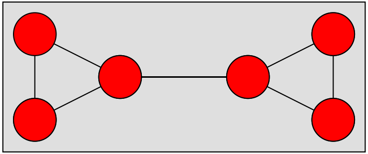

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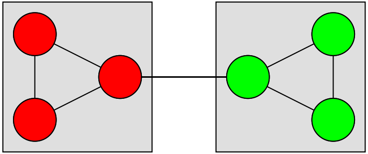

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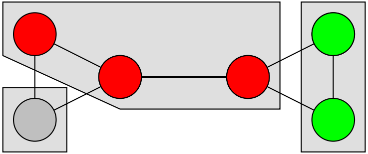

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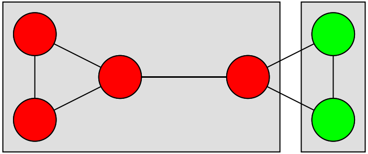

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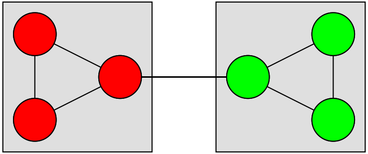

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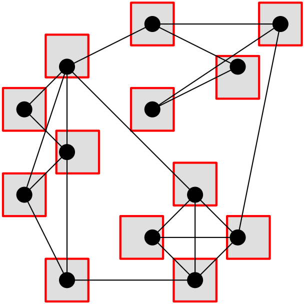
Structure

Greedy Agglomeration / Merge

dendrogram

current clustering



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Greedy Agglomeration / Merge

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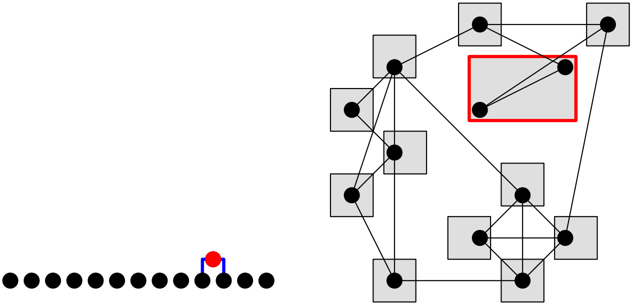

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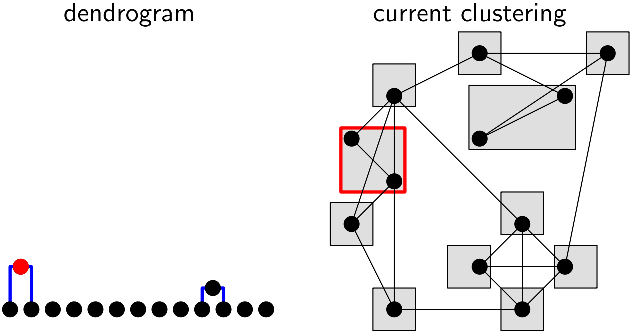

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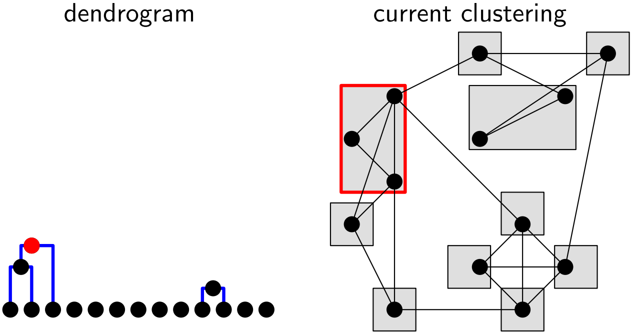

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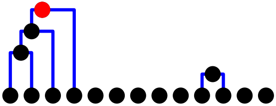

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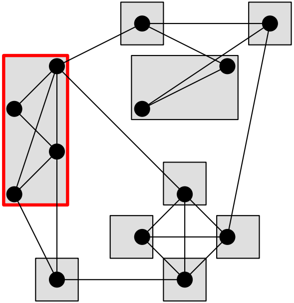

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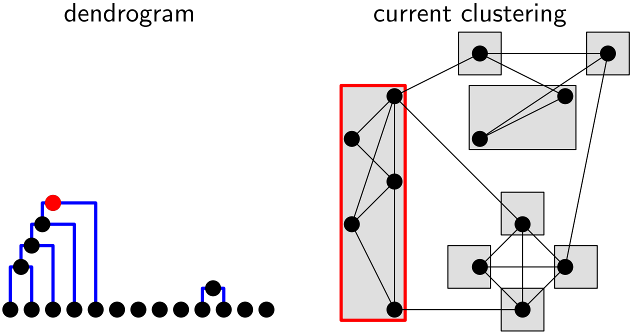

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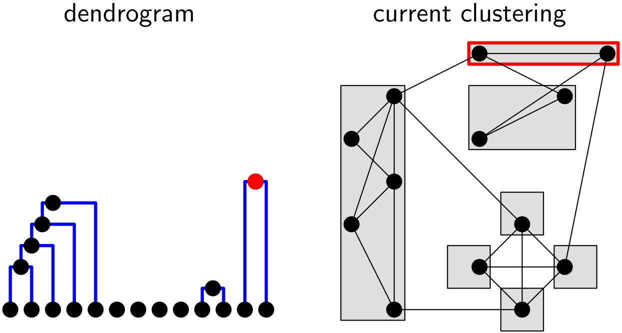

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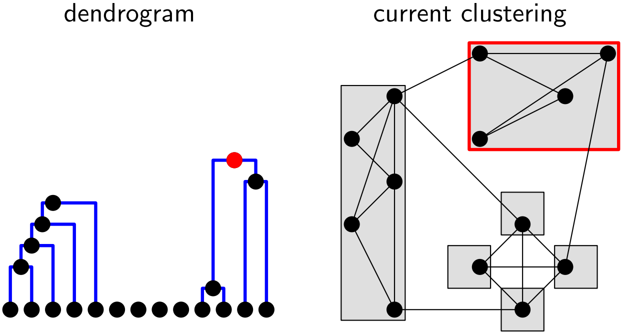

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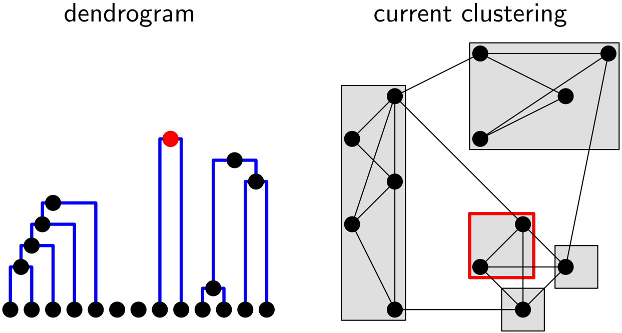

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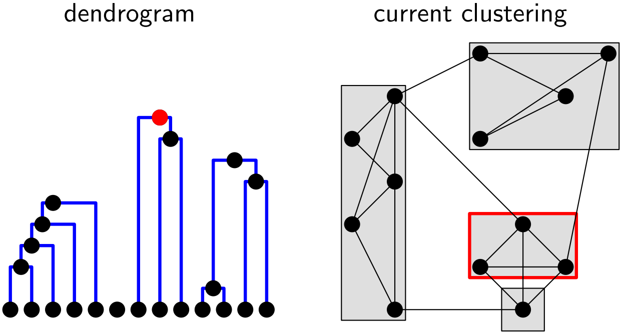

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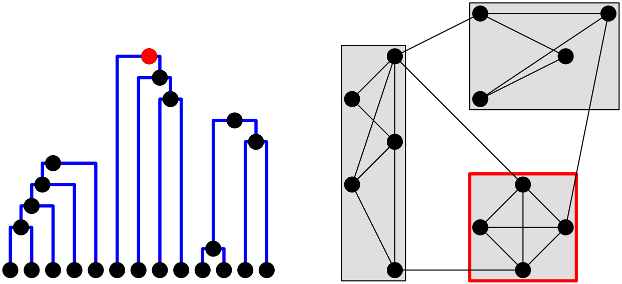
Greedy Agglomeration / Merge

dendrogram current clustering



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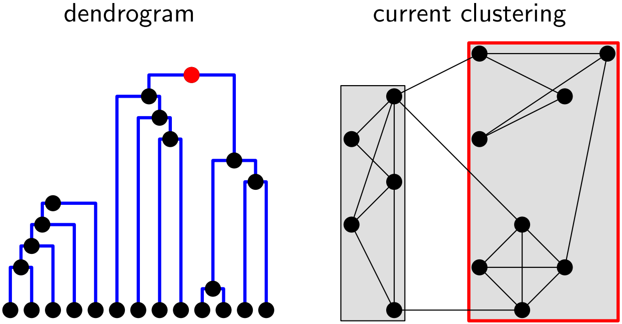

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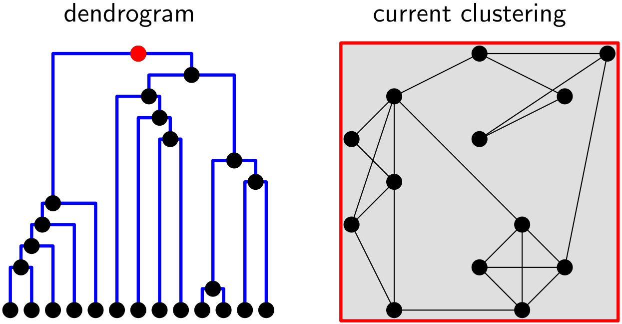

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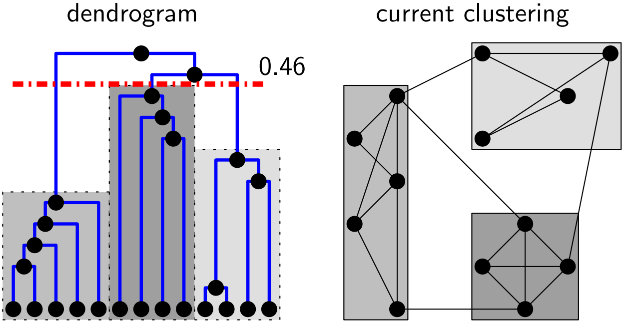

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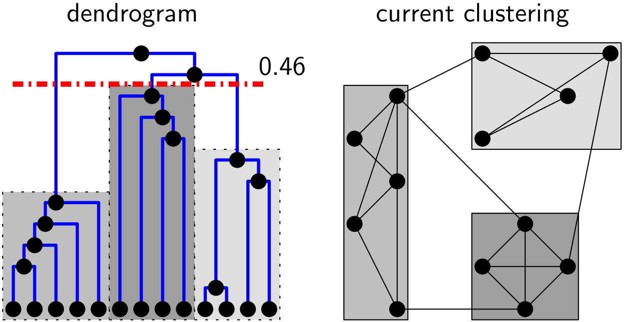

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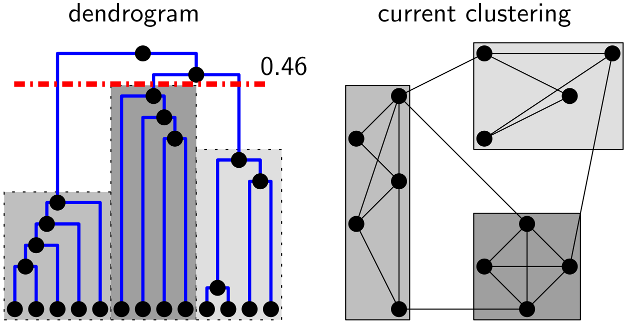

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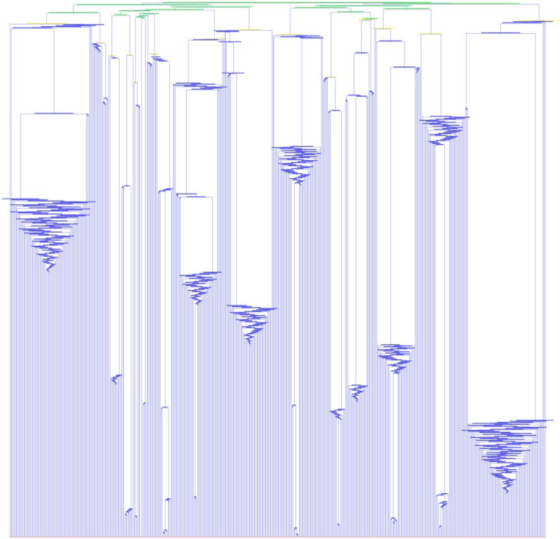
other objective functions, like bicriterial formulations?

Larger Dendrogram



collaboration network, $|V| \approx 1000$

Influence of Measures on Algorithm: Coarseness

Rough Intuition

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Rough Intuition

Question

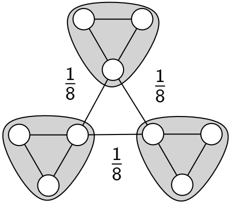
Without constraints, is there always a merge that improves the objective function?

(Un-)Boundedness

Definition

An objective function measure f is *unbounded* if for any clustering $\mathcal{C}$ with $|\mathcal{C}| > 1$ there exists a merge that does not deteriorate f.

Max. pw. inter-cluster conductance
is bounded



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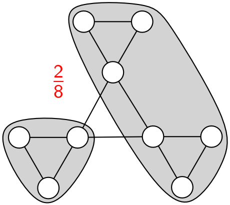

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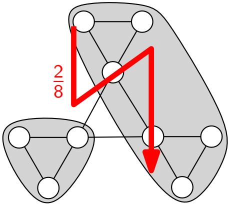

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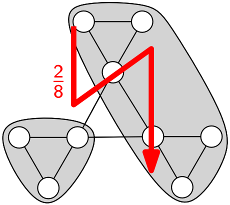

e.g., modularity is bounded

Inter-cluster Sparsity: Degrees of Freedom (Rep.)

Set of cuts

- isolated (one for each cluster)
- pairwise (one for each pair of clusters)
- global (k-way cut)

Measures

- number of cut-edges
- density
- conductance
- expansion

Combinations

- average sparsity
- minimum sparsity

$\Rightarrow$ **14 (reasonable) inter-cluster sparsity measures**

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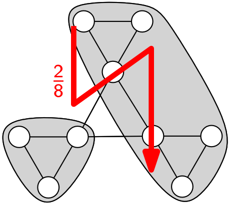

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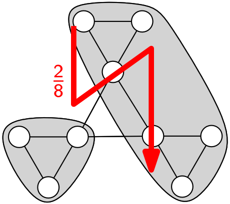

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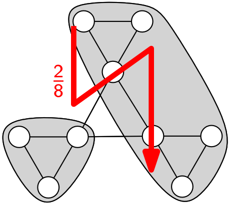

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unbounded

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- gxd
- mixc
- mixd
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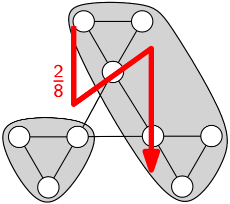

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exercise: reachability, proofs for (un)boundedness

Greedy Merge and Modularity

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- greedy maximization does not approximate $\begin{array}{l} \texttt{nan} \\ > 2 \end{array}$ $\begin{array}{l} \text{worst tie-breaking} \\ \text{best tie-breaking} \end{array}$

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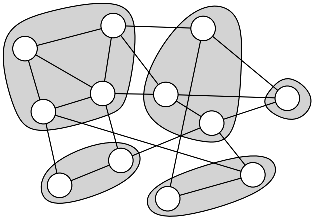
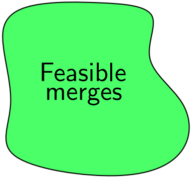
Data structure and maintained information for efficient greedy agglomeration?

Influence of Measures on Efficiency

In a bicriterial setting with constraints:





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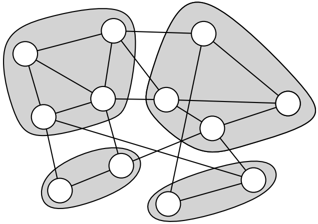

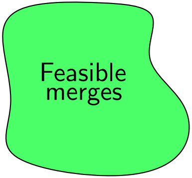

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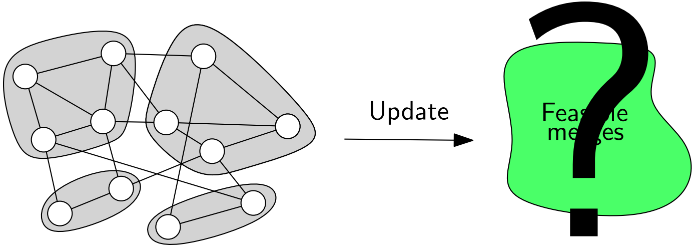

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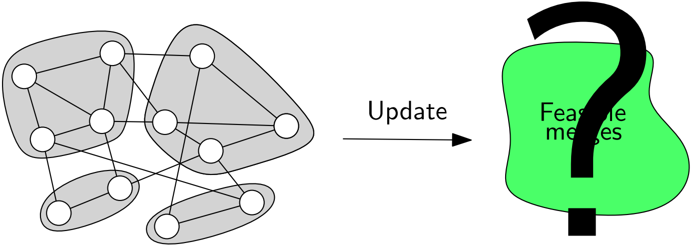

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$\Rightarrow$ **Context freeness of a constraint**

Influence of Measures on Efficiency

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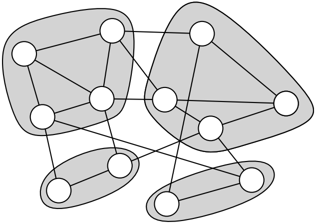

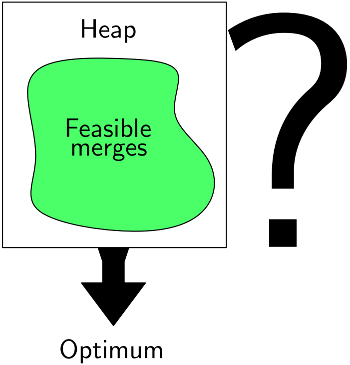

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Given *context freeness*, can the set of feasible merges be efficiently maintained in a heap?

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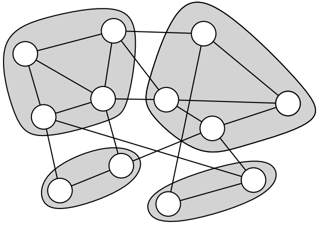

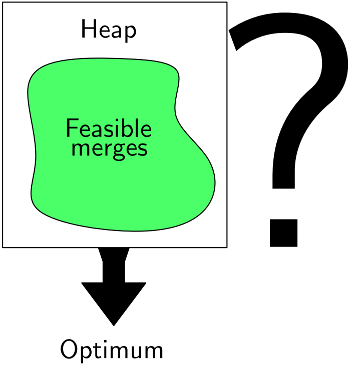

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⇒ **Locality of an objective function**

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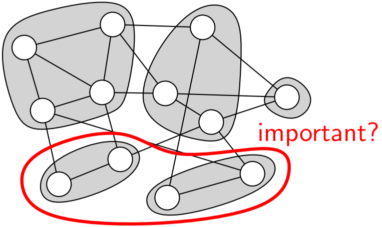

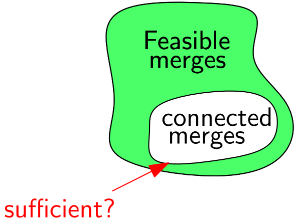

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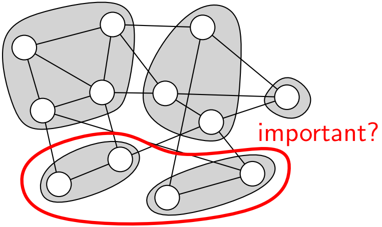

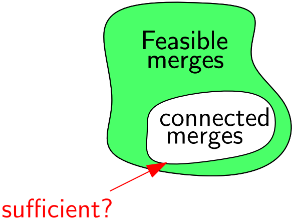

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$\Rightarrow$ **Connectedness of an objective function**

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(Given the necessary data can efficiently be maintained:)

Context insensitivity + Locality = $O(n^2 \log n)$ running time

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For more information on these topics:
[Schumm et al.: Density-constrained graph clustering, 2011]

Context Freeness

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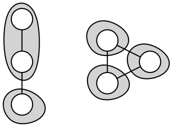

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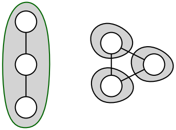

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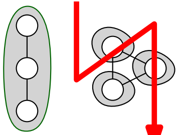

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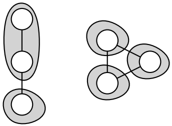

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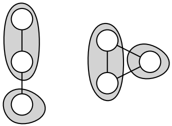

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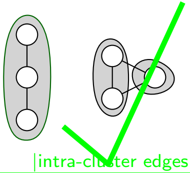

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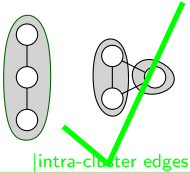

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- E.g., minimum intra-cluster density is context free

Locality: Intuition

Locality is a property of an objective functions

Example: Maximum isolated inter-cluster conductance

First approach: Use gain in inter-cluster sparsity as key

bad merges ⇦ | A, B | -0.3 | | C, D | 0 | | E, F | 0 | | C, F | 0 | | G, H | 0 | | G, I | 0.3 | ⇨ good merges

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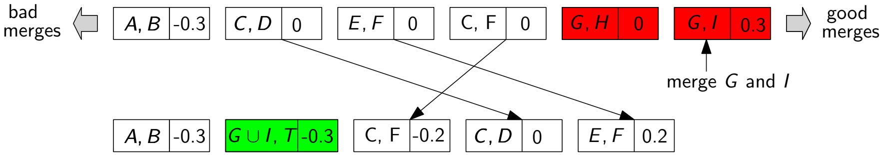

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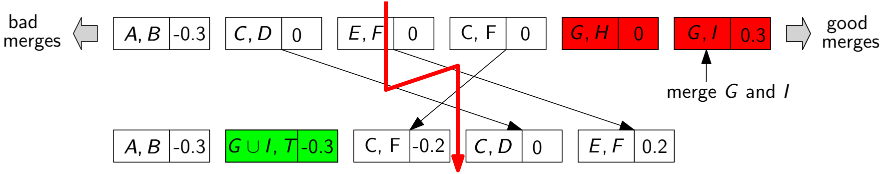

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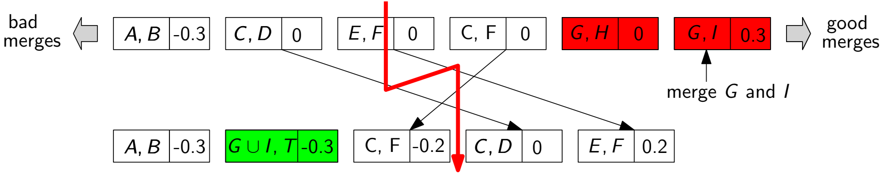

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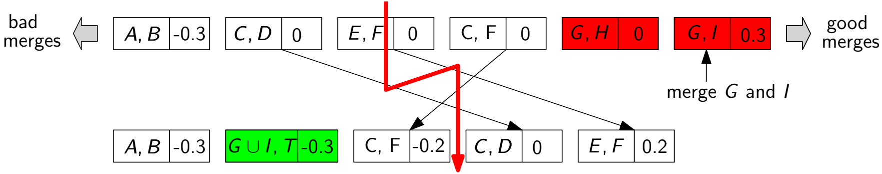

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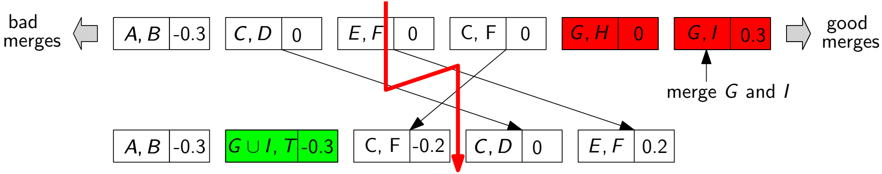

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Existence of such an order $\approx$ Locality of the inter-cluster measure

Example: Max. Isolated Inter-cluster Conductance

Current sequence of conductance of all clusters (sorted)

A	0.5	B	0.4	C	0.3	D	0.3	E	0.1

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Merging A and B is better!

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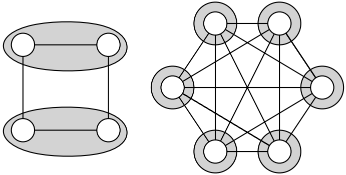
$\Rightarrow$ **Maximum isolated inter-cluster conductance is local**

Locality: Results

Does such an order exist for all objective functions?

global inter-cluster density is not local



$$\frac{|\text{inter-cluster edges}|}{|\text{possible inter-cluster edges}|} = \frac{17}{43}$$

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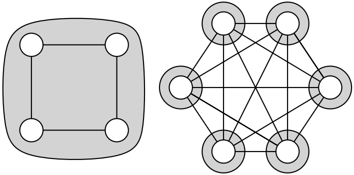

$$\frac{|\text{inter-cluster edges}|}{|\text{possible inter-cluster edges}|} = \frac{15}{39}$$

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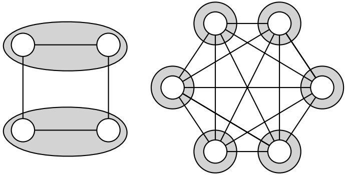

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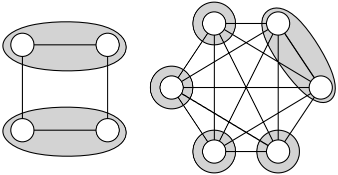

$$\frac{|\text{inter-cluster edges}|}{|\text{possible inter-cluster edges}|} = \frac{16}{42}$$

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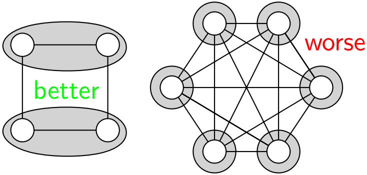

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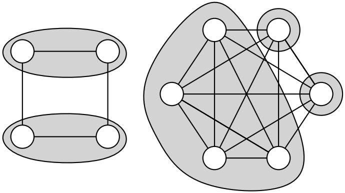

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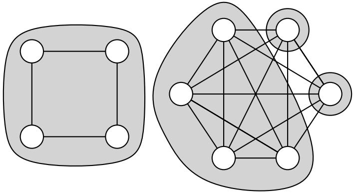

$$\frac{|\text{inter-cluster edges}|}{|\text{possible inter-cluster edges}|} = \frac{7}{33}$$

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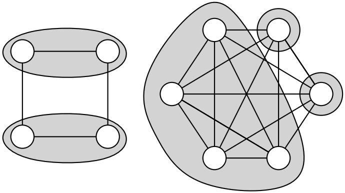

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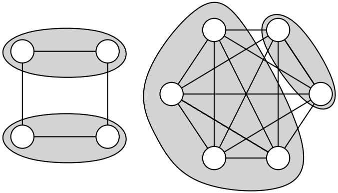

$$\frac{|\text{inter-cluster edges}|}{|\text{possible inter-cluster edges}|} = \frac{8}{36}$$

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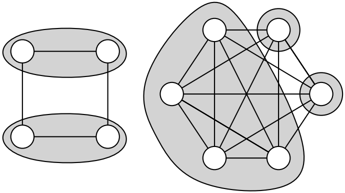

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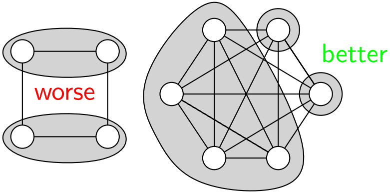

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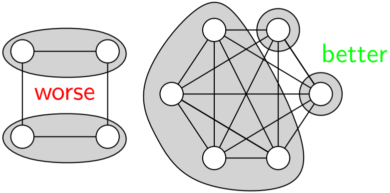

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local

- mixd
- mixc
- mixe
- aixd
- aixc
- aixe
- nxe

not local

- mpxd
- apxd
- mpxc
- mpxe
- gxd
- apxe
- apxc

Disconnectedness

Definition

An objective function *f* is *connected* if merging unconnected clusters is never the best option with respect to *f*.

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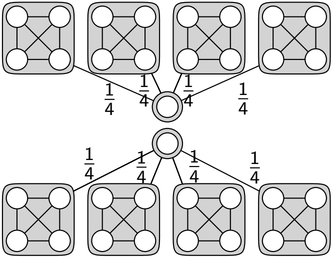

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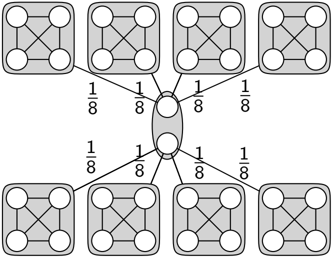

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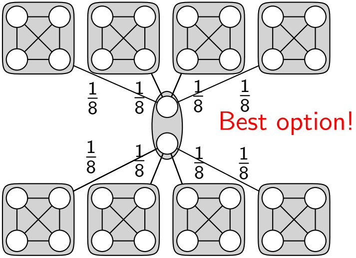

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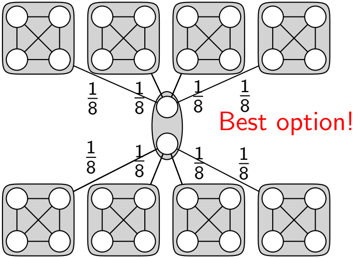

connected

- nxe

unconnected

- gxd
- mixc
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A Matrix for Maintaining Merges

Update of *merge-matrix*, when merging clusters C_i and C_j:

		j		
		$\vdots$		
i	$\cdots$	$\Delta S_{i,j}$	$\cdots$	
		$\vdots$		

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Update of *merge-matrix*, when merging clusters C_i and C_j:

- Additive update of gain, easy to handle (e.g., modularity):
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  Easy to compute,

$$
\begin{array}{c|c|c|c|c}
 & & j & & \\
\hline
 & & \vdots & & \\
\hline
i & \cdots & \Delta S_{i,j} & \cdots & \\
\hline
 & & \vdots & & \\
\hline
 & & & &
\end{array}
$$

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  Easy to compute, but **whole** matrix needs update $\Rightarrow \Omega(n^2)$

		j		
		$\vdots$		
i	$\cdots$	$\Delta S_{i,j}$	$\cdots$	
		$\vdots$		

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Key idea: geometric (2d) data structure for matrix

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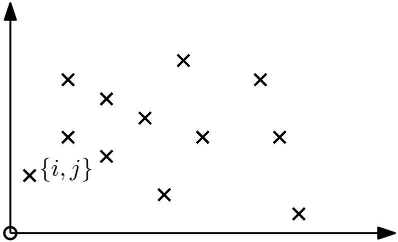

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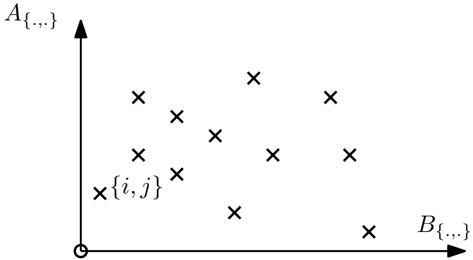

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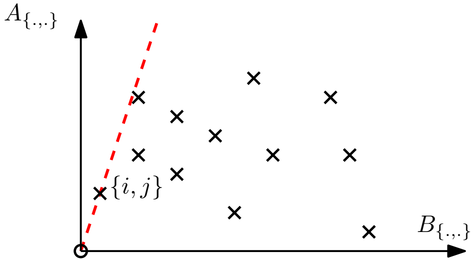

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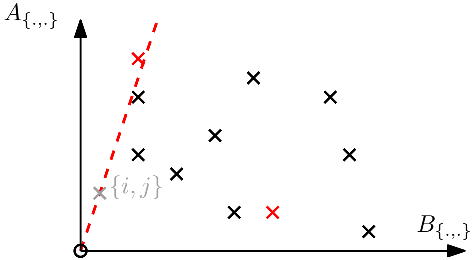

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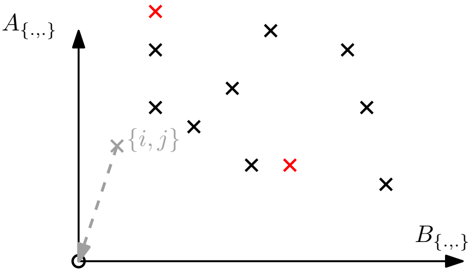
- $O(n)$ *real* updates (as in subtractive case)
- Update of nominator and denominator by *shifting origin*

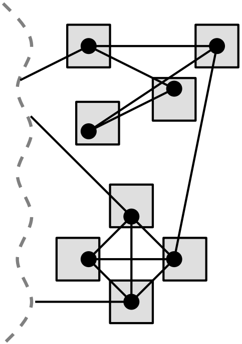


Structure

Local Movement

A common technique in graph partitioning

- locally greedy
- node shifts
- hierarchical contractions

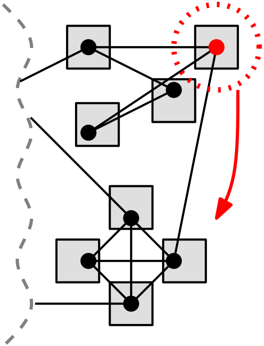


[e.g., for modularity: Blondel et al.: Fast unfolding of communities in large networks, 2008]

Local Movement

A common technique in graph partitioning

- locally greedy
- node shifts
- hierarchical contractions



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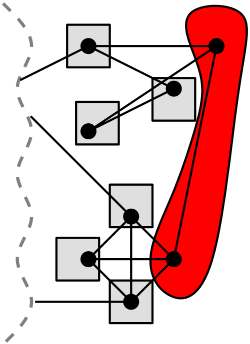

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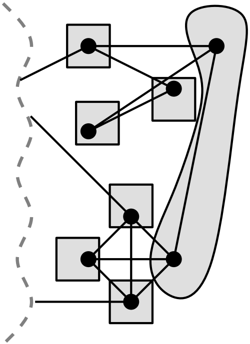

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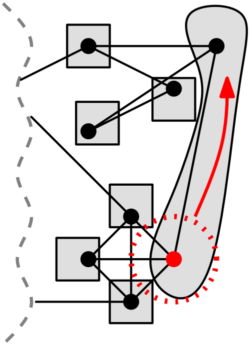

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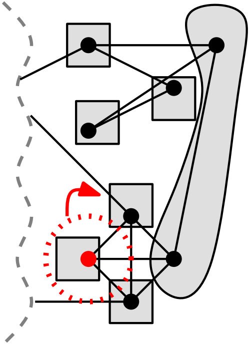

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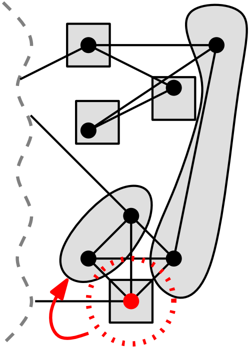

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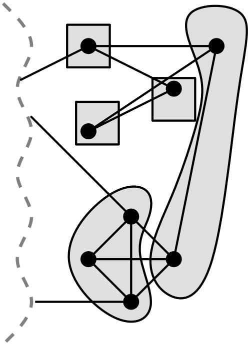

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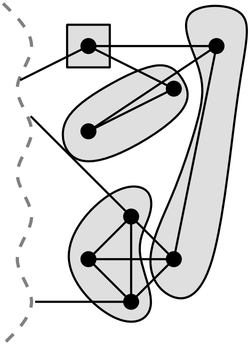

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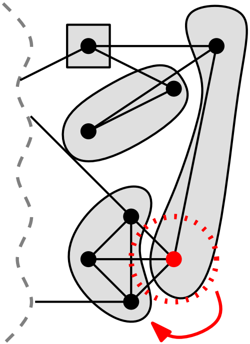

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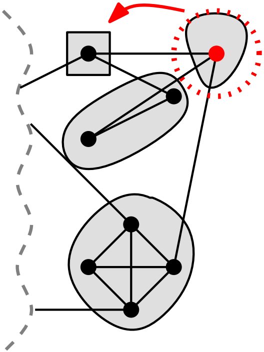

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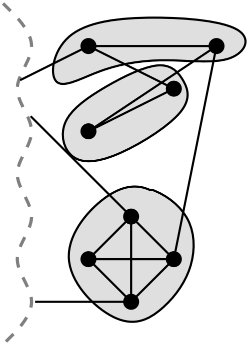

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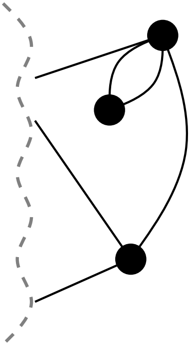

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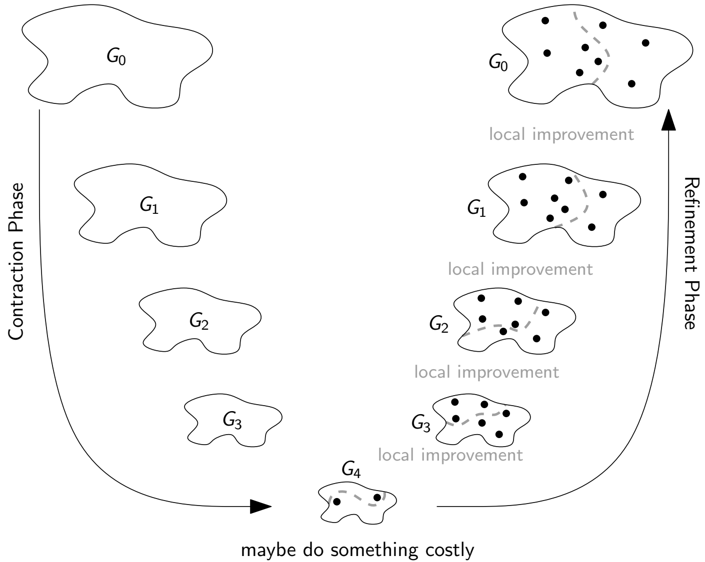
The Multilevel Approach



Local vs. Global Greedy

pro local movement

- local qualitatively superior
- local quicker in practice
- better avoidance of local minima, larger search space
- refinement adds a few more percent to quality of local approach

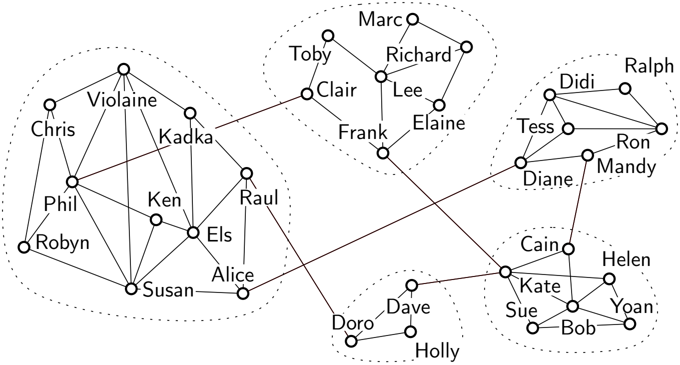
pro global agglomeration

- global easier to implement (no contraction, updates)
- runtime guarantees stronger for global
- global yields continuous hierarchy

exercise: collect edges to neighbors

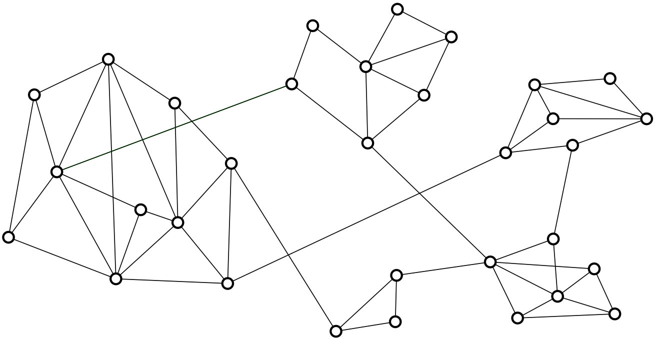
Structure

Min-Cut Tree Clustering



1. original graph

Min-Cut Tree Clustering



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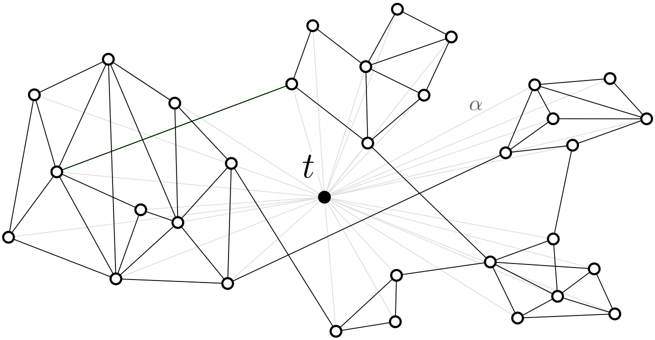

1. original graph
2. star-center t, α

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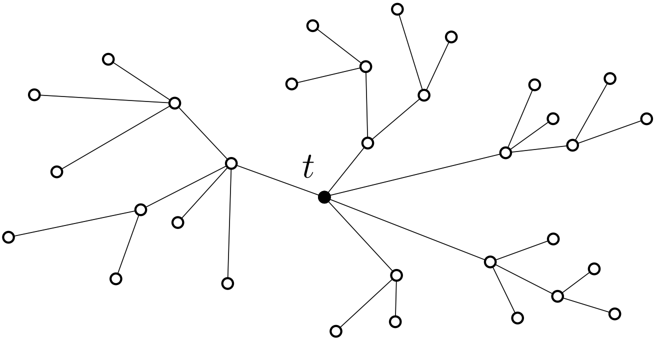
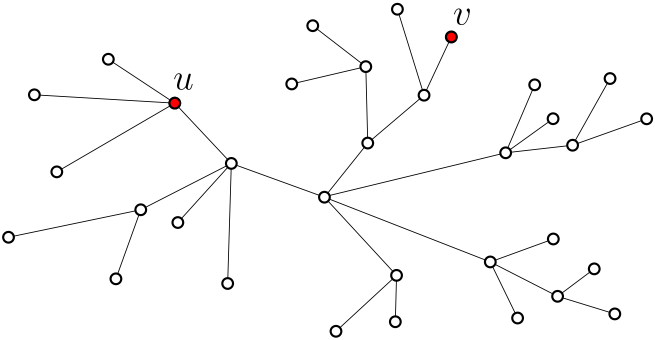


1. original graph
2. star-center t, α
3. *min-cut tree*

- coined in [Gomory and Hu '61]
- simplified in [Gusfield '90]
- construction via $(n-1)$ max-flows
  (variants e.g. $\widetilde{O}(mn)$ for unweighted)

Min-Cut Tree Clustering



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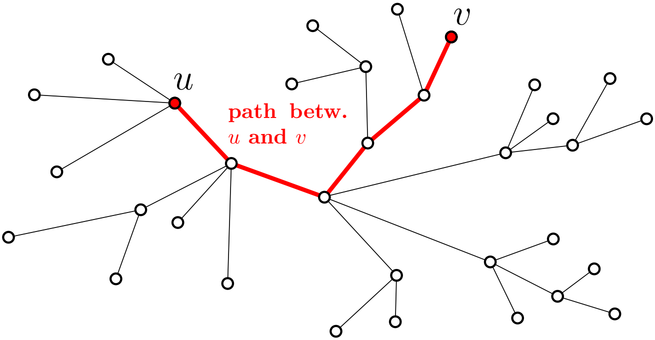

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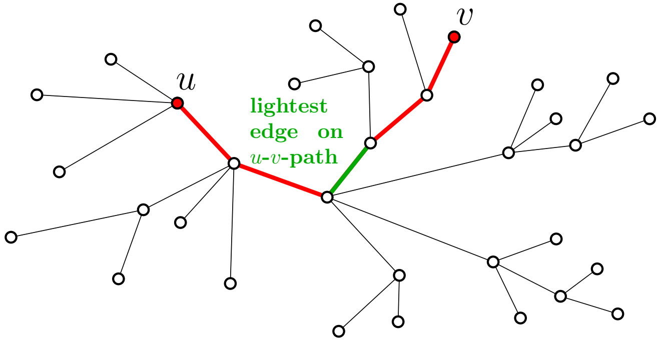

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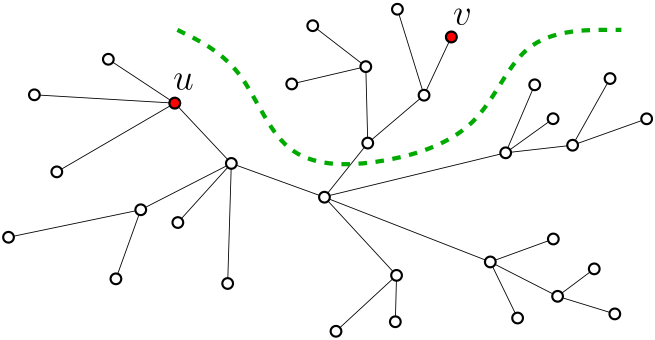

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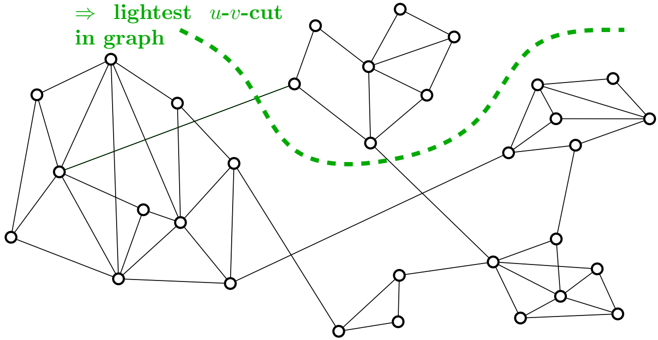

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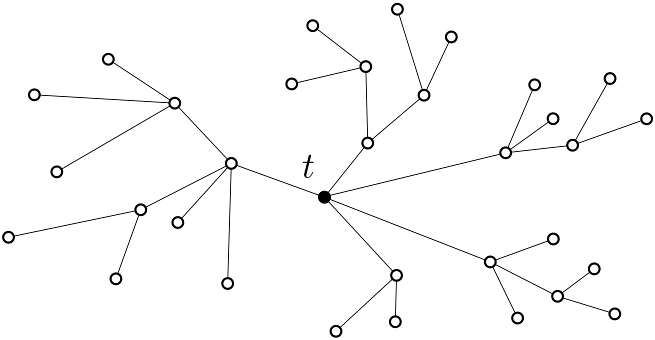

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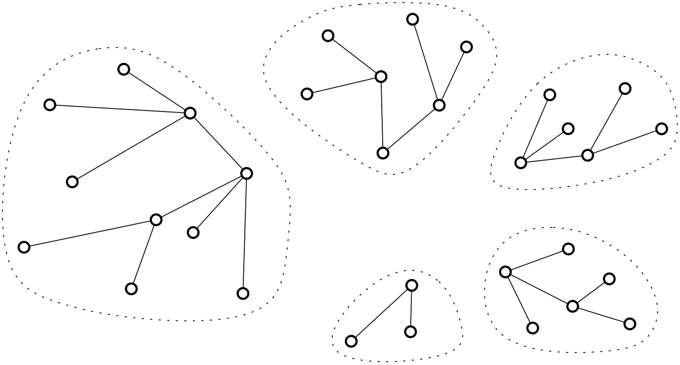

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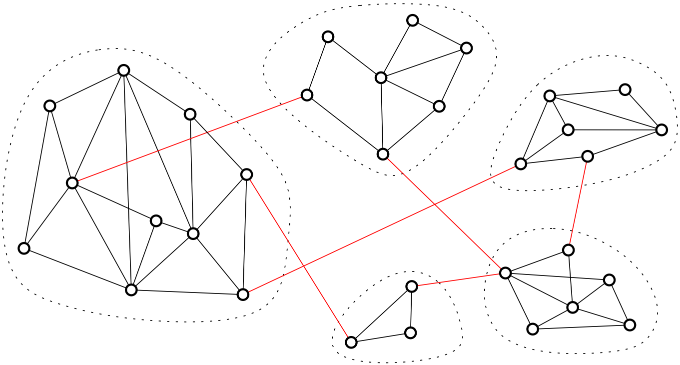
Min-Cut Tree Clustering

Karlsruher Institut für Technologie



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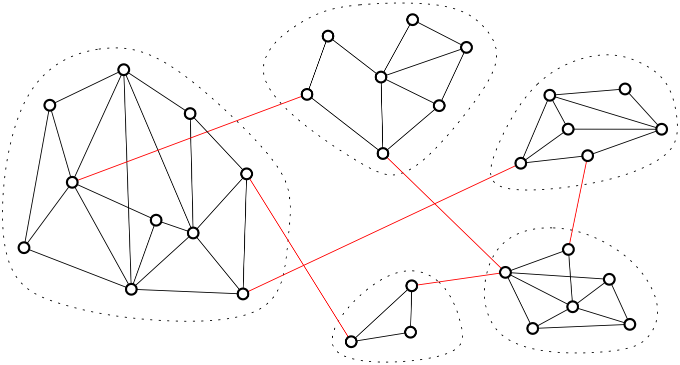
quality guarantee: [Flake et al. '04]

intra-cluster expansion $\geq \alpha \geq$ *inter-cluster expansion**

Min-Cut Tree Clustering



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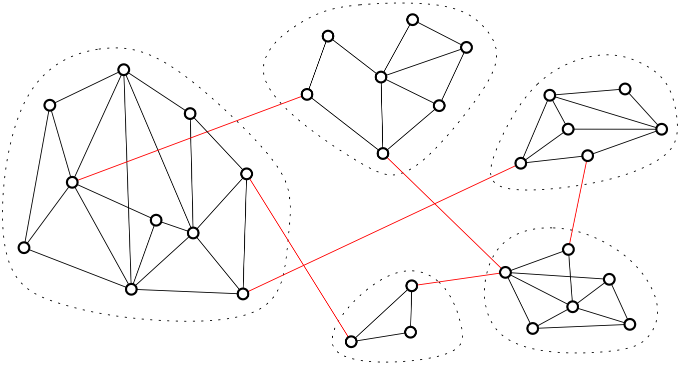
$$\frac{\omega(E(P,C\setminus P))}{\min\{|P|,|C\setminus P|\}} \geq \alpha \geq \frac{\omega(E(C,V\setminus C))}{|V\setminus C|}$$

Min-Cut Tree Clustering



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exercise: prove bounds!

Discussion: Min-Cut Tree Clustering

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- a vertex v that served to identify a cluster-defining v-t-cut is called the *representative* of the respective cluster

- scaling α yields a nested hierarchy of clusterings
- hierarchy has depth $\leq n - 1$

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- user needs to choose suitable α carefully
- high runtime: $O(n)$ max-flow computations

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- high runtime: $O(n)$ max-flow computations

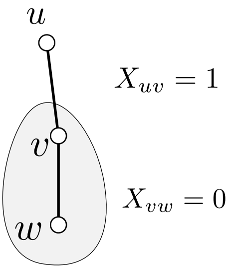
- no "minimum" in denominator of inter-cluster expansion$^* = \frac{\omega(E(C, V \setminus C))}{|V \setminus C|}$ (otherwise not always solvable)

Structure

Optimization: ILP Approach

1. introduce decision variables

$$\forall \{u, v\} \in \binom{V}{2} : X_{uv} = \begin{cases} 0 & \text{if } \mathcal{C}(u) = \mathcal{C}(v) \\ 1 & \text{otherwise} \end{cases}$$



2. ensure valid clustering with constraints (transitivity):

$$\forall \{u, v, w\} \in \binom{V}{3} : \begin{cases} X_{uv} + X_{vw} - X_{uw} \geq 0 \\ X_{uv} + X_{uw} - X_{vw} \geq 0 \\ X_{uw} + X_{vw} - X_{uv} \geq 0 \end{cases}$$

3. reflexivity and symmetry for free

Optimization: ILP Approach

4. optimize target function, e.g., modularity:

$$\mathrm{mod}_{\mathrm{ILP}}(G, \mathcal{C}_G) = \sum_{\{u,v\} \in \binom{V}{2}} \left(\omega(u,v) - \frac{\omega(u) \cdot \omega(v)}{2 \cdot \omega(E)} \right) \cdot X_{uv}$$

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Countless other constraints and objectives possible, e.g.,:

- bounded cluster sizes
- intra-/inter-expansion as constraint of objectives
- multicriteria objective functions
- maximum pairwise inter-cluster conductance (cumbersome)
- . . . **exercises**

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- …**exercises**

Example runtimes:

- modularity, 300 vertices, 1 day
- objective mpxc, constraint gid, 50 vertices, 1 day

[Görke: An algorithmic walk from static to dynamic graph clustering, 2010]
[Schumm et al.: Density-constrained graph clustering (technical report), 2011]

Structure

Clustering Huge Graphs

goals:

- fast on huge graphs
- with very good quality

algorithm: ORCA

ORCA **R**eduction-

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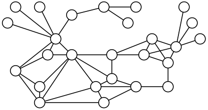

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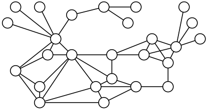

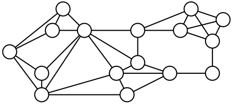

main ingredients

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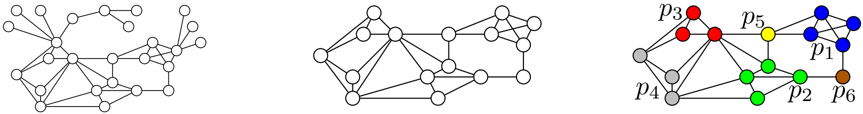

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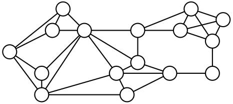

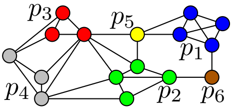

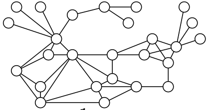

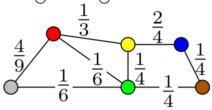

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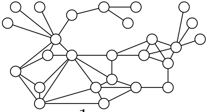

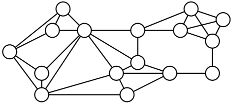

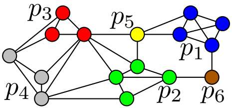

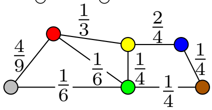

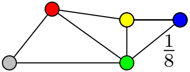

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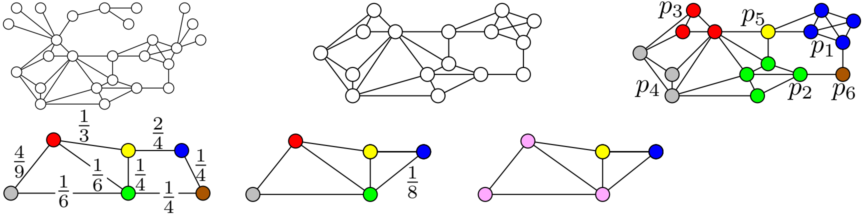

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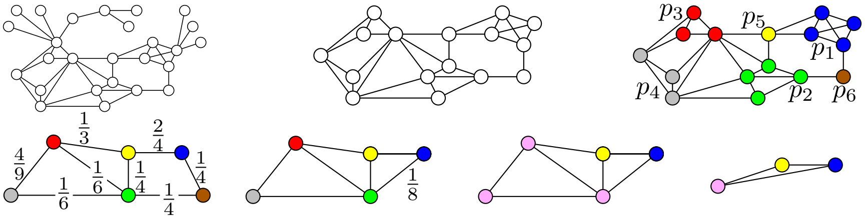

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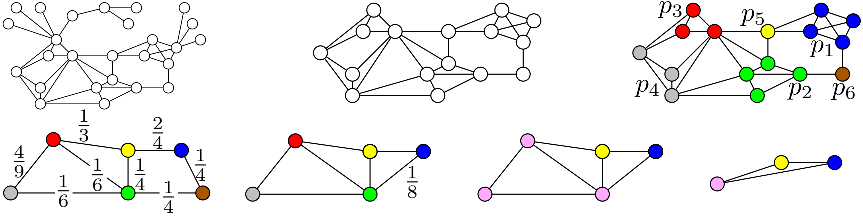

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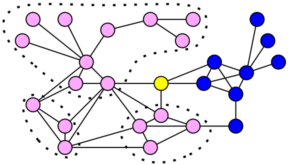

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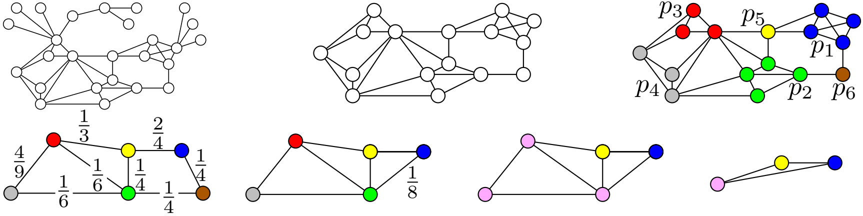

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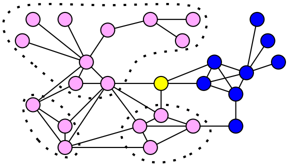


ORCA clusters

- 1M/10M in seconds
- 20M/.5B in 2h
- not “one-dimensional”
- with good quality

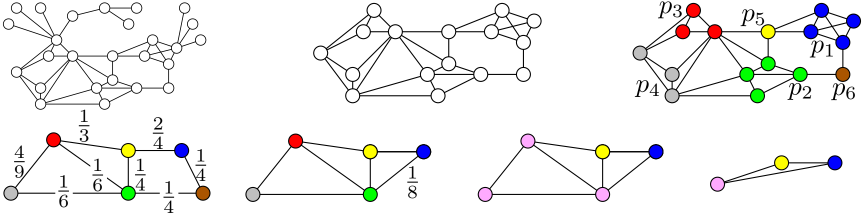
Clustering Huge Graphs

goals:

- fast on huge graphs
- with very good quality

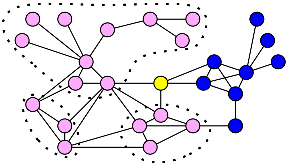
algorithm: ORCA

ORCA **R**eduction-
and **C**ontr**A**ction-based Clustering



main ingredients

- reduction: *2-core*
- local: γ*-cliques*
- contractions
- hierarchy



[Delling et al.: ORCA, '09]

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Other Approaches (I)

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Spectral Clustering

1. use adjacency matrix/Laplacian
2. project points into low (k-) dimensional space
3. assign points to closest axes (e.g. [Kannan et al. '00])
   or use k-means on embedding (e.g. [Shi and Malik '00])

- blurs the line between data- and graph clustering
- variants solve, e.g., the relaxed RATIOCUT problem

Random Walks

1. simulate long random walk through graph
2. convergence $\rightsquigarrow$ transition matrix induces clusters

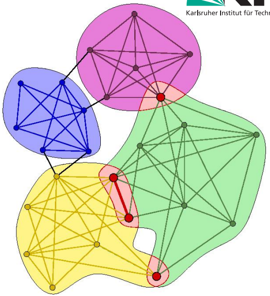
- pioneered in [van Dongen '02]
- related to spectral graph theory

Other Approaches (II)

Clique-Percolation

1. "roll" small clique-template through graph
2. reachable parts in same cluster

- resonable but sensitive to structure
- slow on large instances
- overlapping clusters!
- [Palla et al.: Uncovering the overlapping community structure of complex networks in nature and society, 2005]



(template: K_4)

Network Percolation

1. iteratively remove most central edges in graph
2. stop at threshold $\rightsquigarrow$ components induce clusters

- done, e.g., by [Girvan and Newman: Finding and evaluating community structure in networks '02]
- slow due to computation of centrality
- comp.: percolation theory from mathematics

Other Approaches (III)

- quantification of *node fitness*, migration/survival
- best clustering when using scalable parameter:
  find largest plateau in plot of $|\mathcal{C}|$
  [Santo Fortunato: Detecting the overlapping and hierarchical community structure in complex networks, 2009]
- direct translation of graph to data points $\rightsquigarrow$ k-means
  e.g.: [Gregor Stachowiak, student thesis, 2011]
- randomized rounding of linear programs
- emulating electricity: clustering by voltage potential
- ...

- overviews:
  [Brandes, Erlebach (eds.) '05, Network Analysis, Methodological Foundations]
  [Satu Elisa Schaeffer: Graph Clustering, 2007]
  [Santo Fortunato: Community Structure in Graphs, 2009]
  [Robert Görke: An algorithmic walk from static to dynamic graph clustering, 2010]

Structure

Why Experiments?

"...an experiment and emprical data are more valuable than an estimate; an estimate is more valuable than an approximate calculation; an approximate calculation is more valuable than a rigorous result."
[Dorogovtsev and Mendes: Evolution of Networks, 2003 (physicists)]

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Specifica in field of graph clustering:

- generally, "rigorous results" are always preferable, however …
- hard problems, very few results possible/probable
  (e.g. expansion via min-cut tree,
  or polylogarithmic quality via iterative. cond. cutting)
- performances of algorithms depend on graph type
  (again hard to capture, analytically)
- constants in runtimes do matter (huge networks)

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$\Rightarrow$ **graph clustering does need extensive experiments**

Real-World Networks

- hand-selected collections
- biased in origin, size, structure, . . .
- are they representative, diverse, and suitatble?
- some rather widespread, e.g.:

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source	web address
Arenas	`http://deim.urv.cat/~aarenas/data/welcome.htm`
ANoack	`http://www-sst.informatik.tu-cottbus.de/~an/GD/`
Cx-Nets	`http://cxnets.googlepages.com/`
GraphDrawing	`http://vlado.fmf.uni-lj.si/pub/networks/data/GD/GD.htm`
Newman	`http://www-personal.umich.edu/~mejn/netdata/`
pajek	`http://vlado.fmf.uni-lj.si/pub/networks/data/`
UriAlon	`http://www.weizmann.ac.il/mcb/UriAlon/`
Walshaw	`http://staffweb.cms.gre.ac.uk/~c.walshaw/partition/`
DIMACS	`http://www.cc.gatech.edu/dimacs10/`

table partially taken from and many used in:
[Noack and Rotta: Multi-level algorithms for modularity clustering, 2009]

Generated Instances

real-word networks cannot answer all questions, e.g.:

- does a measure fulfill specific desiderata on scaling?
- scaling of algorithm's runtime on specific graph family?
- quality of algorithm sensitive to graph density?
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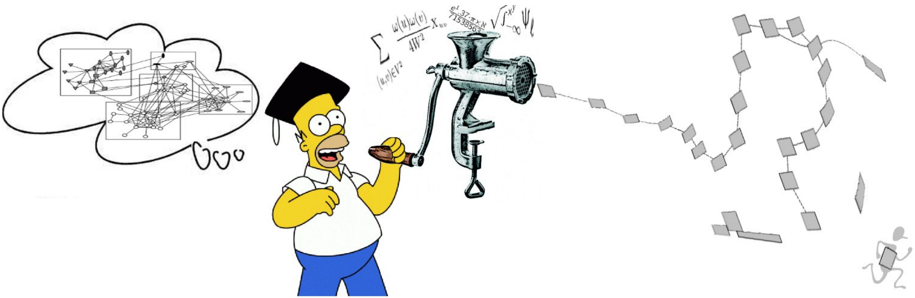
- . . .

⇒ targeted experiments using artificial instances necessary

some resources:
[Brandes et al.: Experiments on graph clustering algorithms, 2003]
[Delling et al.: Generating Significant Graph Clusterings, 2006]
[Gaertler et al.: PhD Thesis, 2007 (Unit-Test-oriented evaluations)]
[Görke and Staudt: A generator for dynamic clustered random graphs, 2009
download static & dynamic generators:
`http://i11www.iti.uni-karlsruhe.de/en/projects/spp1307/index`]
[Görke et al.: Computational aspects of lucidity-driven graph clustering, 2010]

Artificial Test Instances . . .



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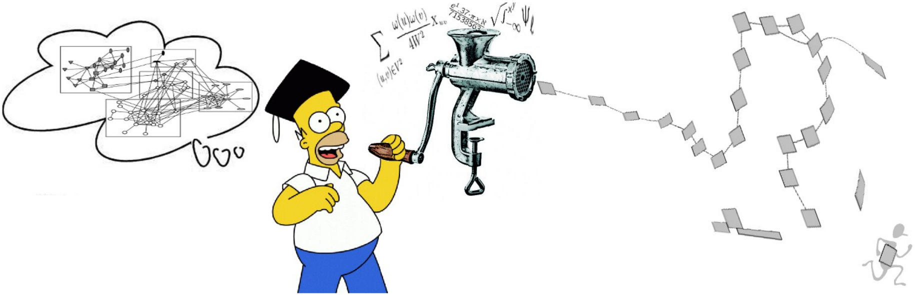
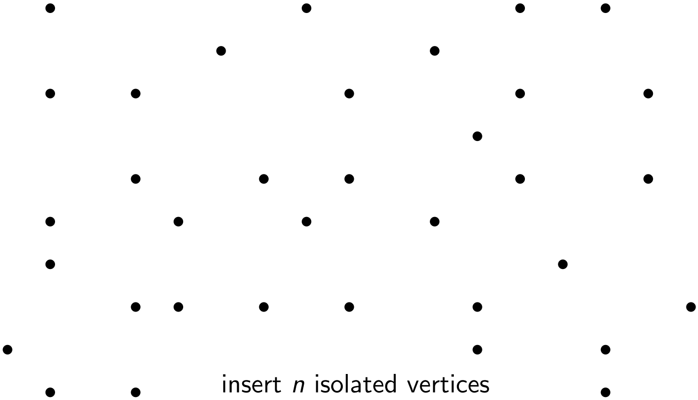


The design of artificial test instances requires care!

$G(n, p_{\text{in}}, p_{\text{out}})$

...a simple model for random preclustered graphs



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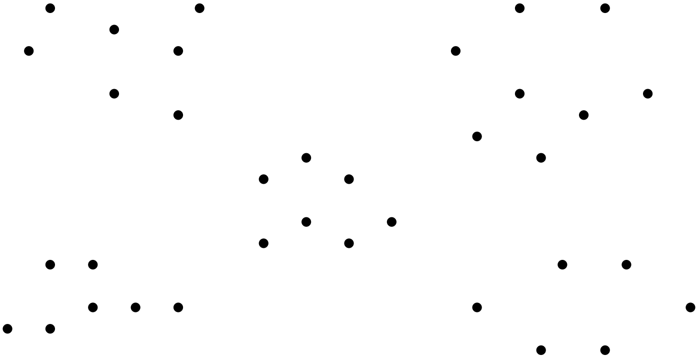

partition V into random/controlled number of blocks

$G(n, p_{\mathbf{in}}, p_{\mathbf{out}})$

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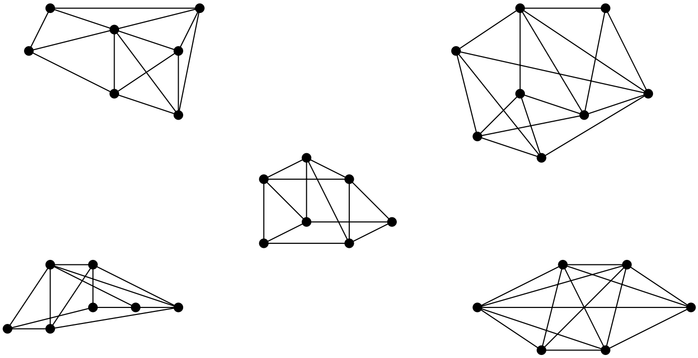

intra-edges: build a cluster $G(|C_i|, p_{\text{in},i})$ from each block i

$G(n, p_{\mathbf{in}}, p_{\mathbf{out}})$

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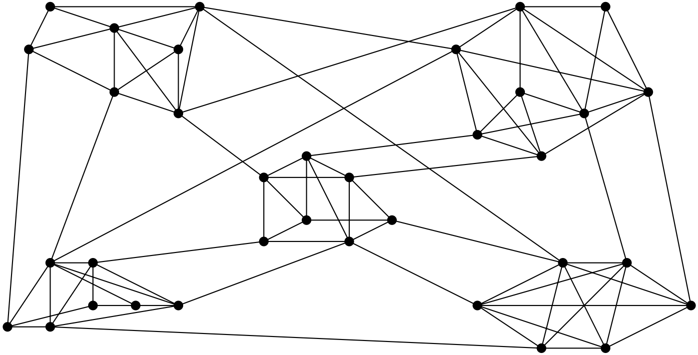
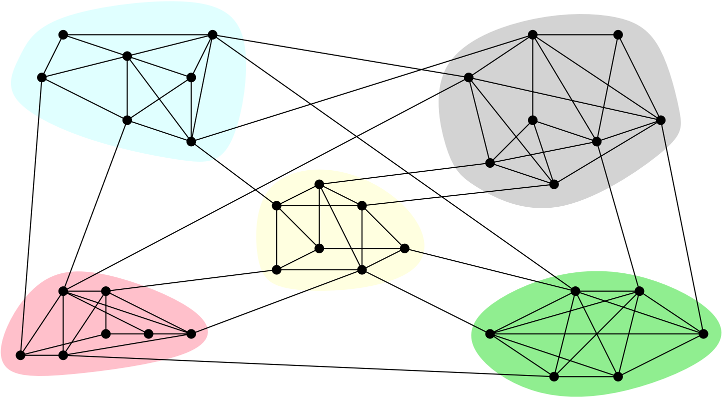


inter-edges: connect inter-cluster pairs with probability p_{out}

$G(n, p_{\mathbf{in}}, p_{\mathbf{out}})$

…a simple model for random preclustered graphs

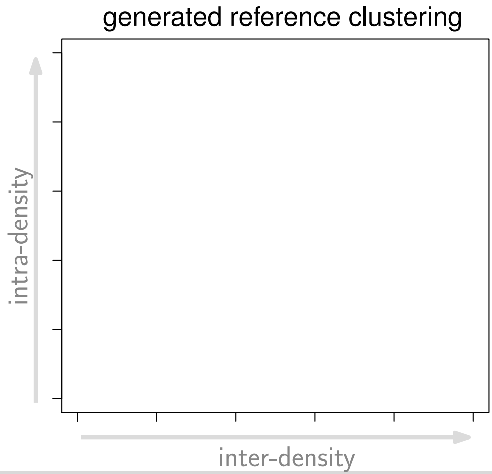


a random graph with a planted clustering

- indisputably(?) scalable intra- and inter-cluster quality
- scalable in size, generation algorithm very fast ($O(m+n)$)
- reference / ground truth to compare to

Example Experimental Setup

- systematic exp. evaluation: measure modularity vs. intuition



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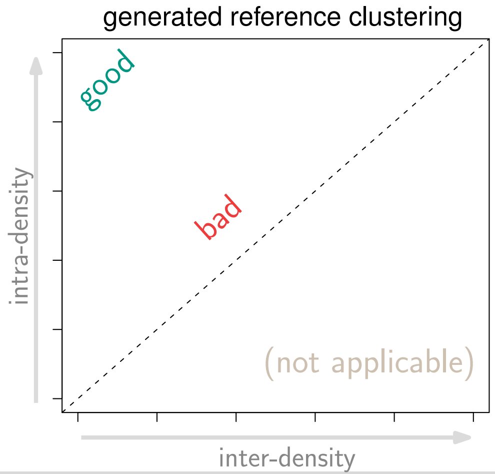

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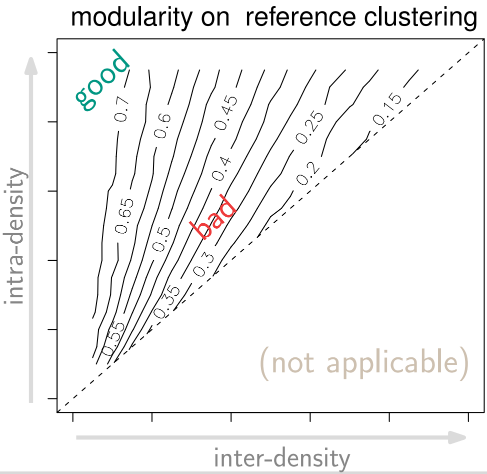

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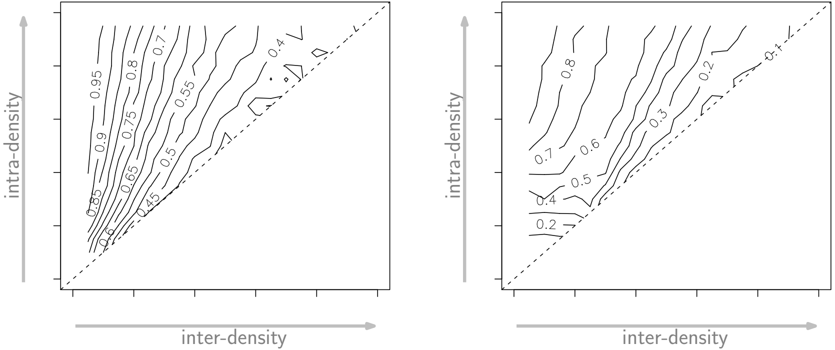
- systematic exp. evaluation: measure modularity vs. intuition $\surd$
- modularity as objective function for maximization:
  greedy maxim. vs. established algorithms wrt. established measures $\surd$

established quality measure *max. is. inter-cl. conductance* (mixc)



algo.: greedy modularity-max.

algo.: *MCL* (rand. walks, est.)

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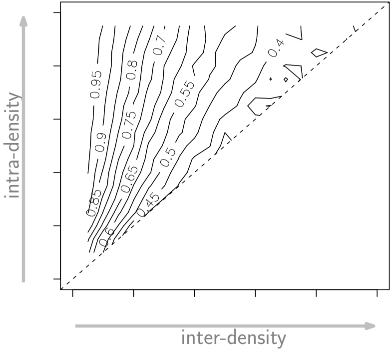

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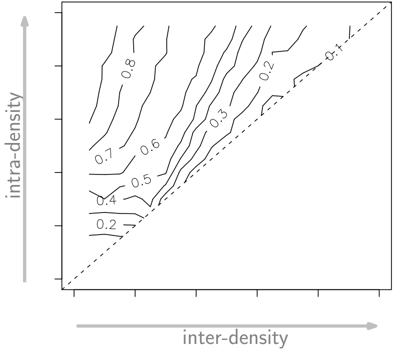

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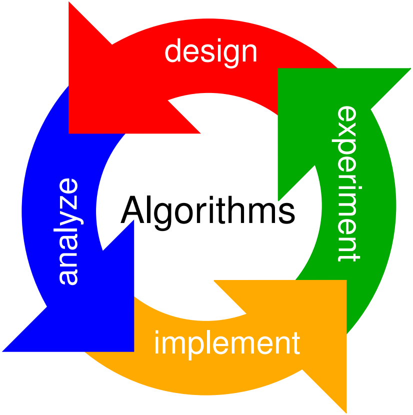
Structure

A Crucial Ingredient of AE



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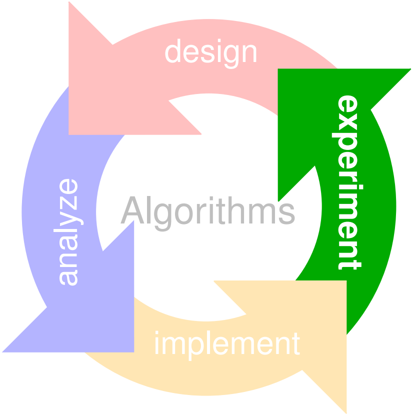

instances for experimental evaluation

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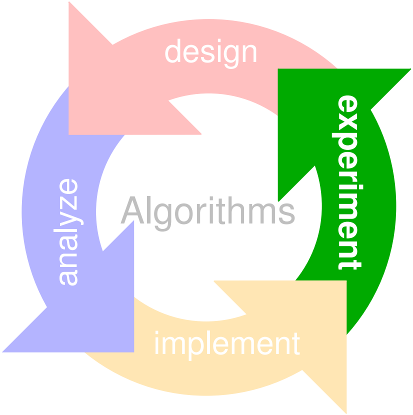

instances for experimental evaluation

“do we care enough about them?”

Meaning of Experiments in AE

State properties of algorithms via experimental evaluation

Algorithm theory:

- asymptotic runtimes: worst/average case, smoothed analysis
- quality: optimality, diverse approximation guarantees
- outcomes on special families of instances

Do experimental evaluations in AE mirror this?

Experiments in AE

Good, valuable evaluations require:

- relevant experiments
- controlled experiments
- provable properties of test instances
- behavior of algorithms on different generated instances
- outcomes on special families of graphs

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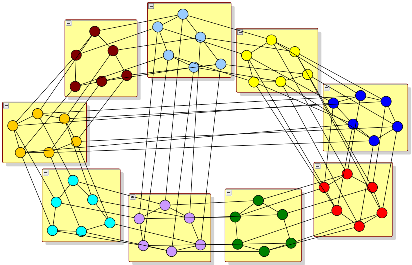
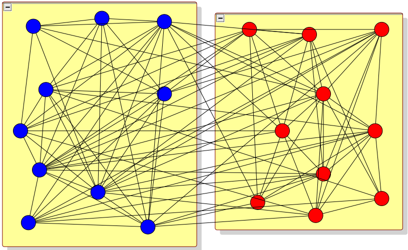
Postulation 1	more insights into characteristics of instances, characteristics that affect behavior of algorithm
Postulation 2	suitable generated instances compulsive: hard, variable outcome/properties, easy

Pitfalls of Quality Indices



meaningful clustering of six-sided tube with irregularities
coverage = 0.43



random split of a $G(20, \frac{1}{2})$ random graph
coverage = 0.66

“A Good Graph Clustering”

Widespread quality function: *modularity*

$$\text{mod}(\mathcal{C}) := \text{cov}(\mathcal{C}) - \mathbb{E}(\text{cov}(\mathcal{C}))$$

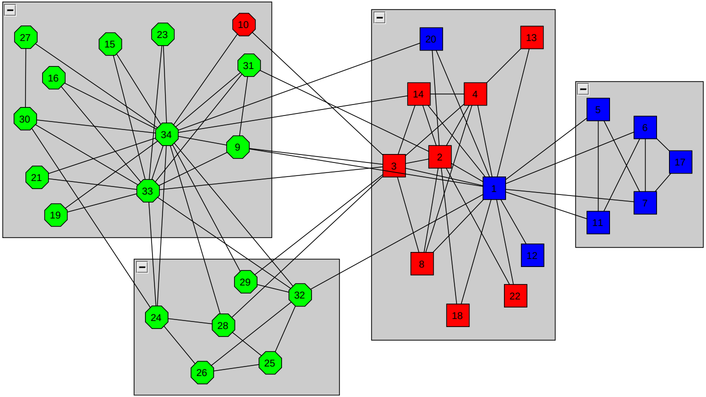
$$= \frac{\#\text{ intra-cluster edges}}{|\#edges|} - \frac{1}{4|\#edges|^2} \sum_{C \in \mathcal{C}} \left(\sum_{v \in C} \deg(v) \right)^2$$

“In practice, values [. . .] from about 0.3 to 0.7. Higher values are rare.”
[Girvan & Newman ’04]

“. . . in practice [. . .] a value above about 0.3 *is a good indicator of significant community structure . . . ”*
[Newman et al. ’04]

Archon of Benchmark Graphs

...one of roughly a dozen real-world instances:
Zachary's Karate Club



modularity:
reality (shapes) & heuristic (col.) & optimum (boxes) ≈ 0.4

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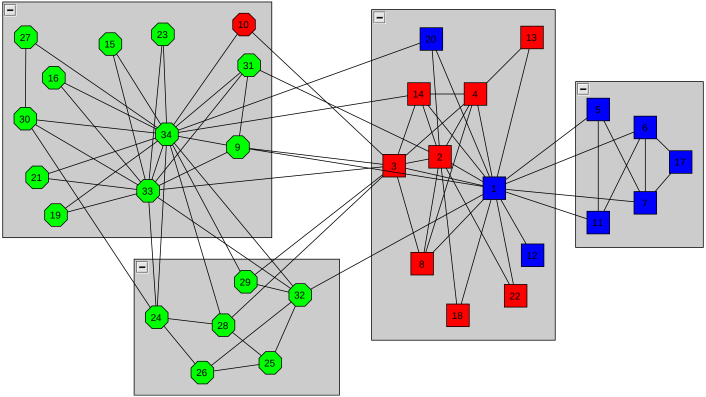

But [Reichard & Bornhold '08]: $\mathbb{E}(\text{modularity}) \approx 0.42 > 0.4$!
(in an *Erdős-Rényi* model)

Large Networks

Example results of ORCA on webgraphs
(**O**RCA **R**eduction and **C**ontr**A**ction-based Clustering
[Delling et al.: ORCA Reduction and ContrAction Graph Clustering, 2009]

Instance	n/m	Algorithm	clusters	icc	perf.	cov.	mod.
cnr-2000	325 556	local greedy	242	0.8571	0.9799	0.9971	0.9130
	5 565 376	ORCA	110	0.0002	0.9632	0.9427	0.8567
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"Modularity tends to 1 for practical instances" [Good et al. 09]

Graph Partitioning

Established benchmark library: “Walshaw’s test set”
(Walshaw gathered instances from existing evaluations)

Good, since:

- well known, accepted
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- easy access, immediate usability

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Own experience:
- traditional network analysis
  $\Rightarrow$ no good characterization
- social networks $\Rightarrow$ bad runtime & cuts

Sensor Networks

Topics:

- minimum energy communication
- localization (without gps)
- interference minimization
- efficient data collection at sink node
- . . .

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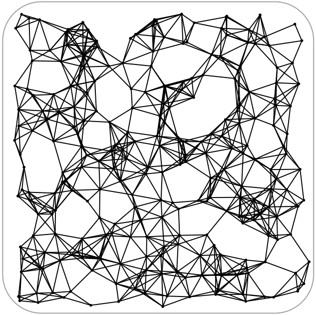
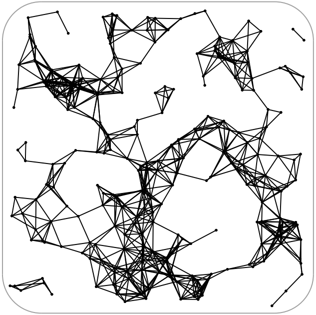
random instances: distribution of sensor nodes in plane
parameters: $|V|$, transmission radius $\Rightarrow$ average degree

Sensor Network Simulations

Bad: *"real randomness not nice":* smaller holes ⇒ better results!





1. place nodes on grid
2. slightly perturb

⇒ no big holes
⇒ method works

1. place nodes uniformly at random

⇒ harder challenges for method

Other researchers copy to compete . . .

Random Planar Graphs

Some generators in the literature:

- *CHT*[3] from LEDA
- *Delaunay* from LEDA
- *Node insertion* from LEDA
- *Node expansion* [Krug 08]
- *Edge-on-off* Markov chain [Denise et al. 07]
- *Boltzmann sampler* [Fusy 07]

[3] Convex Hull Triangulation

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Equivalent? Biased?
"Does the choice impact my experiments?"

[3] Convex Hull Triangulation

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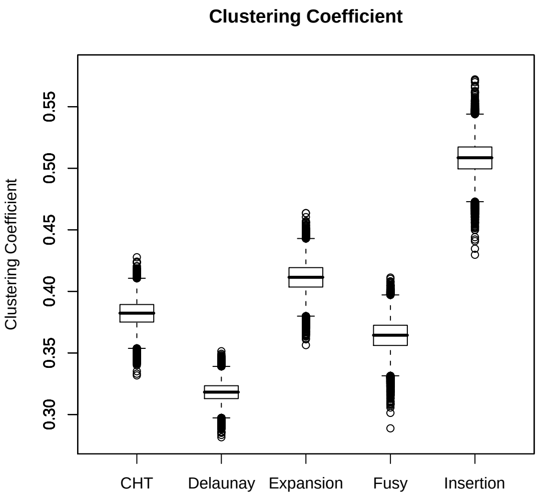
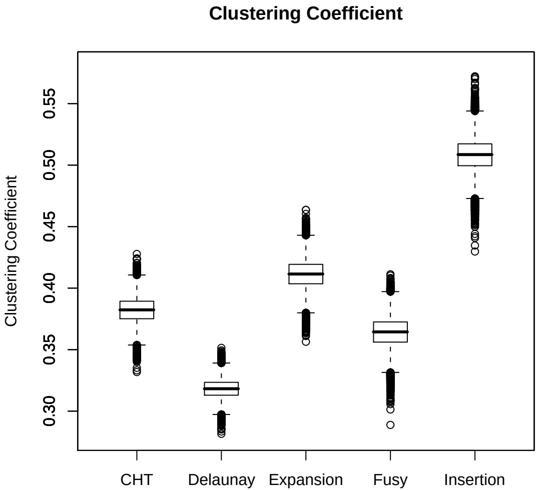


Fixed $|V|$

stat. sign.

different behavior!

Random Planar Graphs



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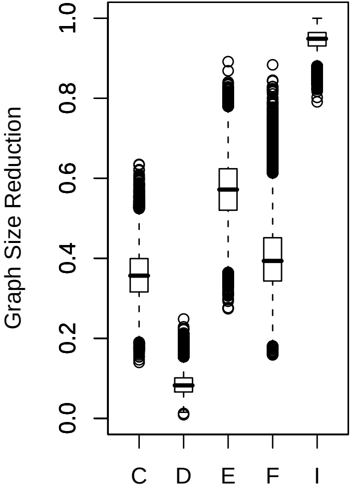
Does it matter?

Random Planar Graphs



Yes, it matters!

algorithm:
k-VertexCover FPT

measure:
reduction by 0,1,2-kernelization

Concluding Claim

In algorithm engineering we need more

- test instances with provable properties,
  (hard, variable outcome/properties, easy, etc.)
  leading to...
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  leading to...
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- insights into characteristics of instances, characteristics that affect behavior of algorithm

Structure

Three Paradigms

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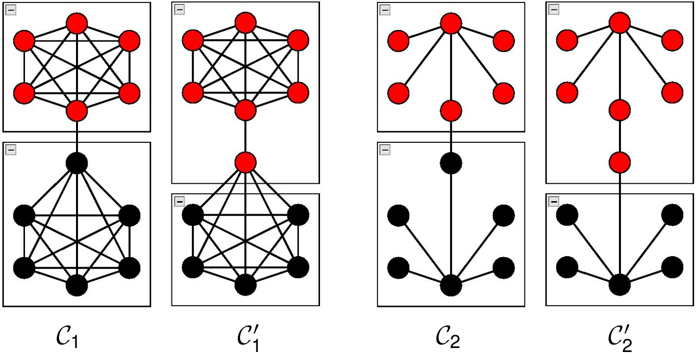
3. **Graph-based:** distance depends on partitioning of nodes and structure of graph

Comparing Graph Clusterings

. . . how set-based measures fail intuition



"Are the two left-hand clusterings less similar than those on the right?"

Augmenting Set-based Measurements 1/3

Counting Pairs:

- compare co-classification of all pairs of nodes
- example: *Rand ('71)* index

Augmenting Set-based Measurements 1/3

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$$\mathcal{R}(\mathcal{C},\mathcal{C}') := 1 - \frac{n_{\text{tog,tog}} + n_{\text{sep,sep}}}{\frac{1}{2}|N|(|N|-1)} \quad \leadsto \quad 1 - \frac{e_{\text{tog,tog}} + e_{\text{sep,sep}}}{|E|}$$

$n_{\text{tog,tog}} =$ number of pairs of nodes that are together in $\mathcal{C}$ and together in $\mathcal{C}'$,
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(will be used later when clustering dynamic graphs)

Augmenting Set-based Measurements 2/3

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Maximum Overlap:

- match clusters
- example: *normalized van Dongen ('00)* index

Augmenting Set-based Measurements 2/3

Maximum Overlap:

- match clusters
- example: *normalized van Dongen ('00)* index
- $\Rightarrow$ weight nodes by their degrees

$$\mathcal{NVD}(\mathcal{C},\mathcal{C}') := 1 \quad - \frac{1}{2n}\sum_{C_i\in\mathcal{C}} \max_{C'_j\in\mathcal{C}'} \underbrace{m_{ij}}_{\rightsquigarrow m^d_{ij}} \quad - \frac{1}{2n}\sum_{C'_j\in\mathcal{C}'} \max_{C_i\in\mathcal{C}} \underbrace{m_{ij}}_{\rightsquigarrow m^d_{ij}}$$

with $m_{ij} = |C_i \cap C'_j|$, where $C_i \in \mathcal{C}$ and $C'_j \in \mathcal{C}'$ (so-called *confusion matrix*)

Augmenting Set-based Measurements 3/3

Information Theory:

- ”what do you know about $\mathcal{C}'$ if $\mathcal{C}$ is given?”
- example: *Fred and Jain ('03)* index

Augmenting Set-based Measurements 3/3

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$$\mathcal{F}\mathcal{J}(\mathcal{C},\mathcal{C}') := \frac{2\mathcal{I}(\mathcal{C},\mathcal{C}')}{\mathcal{H}(\mathcal{C}) + \mathcal{H}(\mathcal{C}')}$$

Node-Entropy $\rightsquigarrow$ Edge-Entropy

Augmenting Set-based Measurements 3/3

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Node-Entropy $\rightsquigarrow$ Edge-Entropy

for all augmentations:
G regular $\Rightarrow$ graph-based $\cong$ set-based

(see [Delling at al.: Engineering comparators for graph clusterings, 2008] for definitions)

Editing Set Difference: Def.

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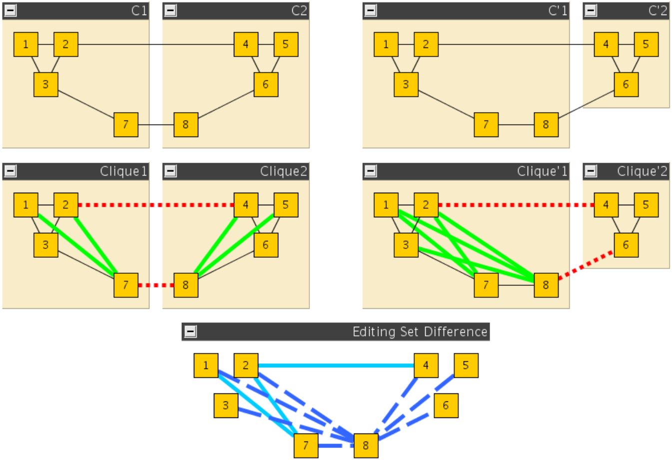
Definition (Editing Set Difference)

Let the Editing Sets of $G, \mathcal{C}$ and of $G, \mathcal{C}'$ be $F_{\mathcal{C}}, F_{\mathcal{C}'}$

$$\mathcal{ESD}(\mathcal{C}, \mathcal{C}') := \frac{|F_{\mathcal{C}} \triangle F_{\mathcal{C}'}|}{|F_{\mathcal{C}} \cup F_{\mathcal{C}'}|} = 1 - \frac{|F_{\mathcal{C}} \cap F_{\mathcal{C}'}|}{|F_{\mathcal{C}} \cup F_{\mathcal{C}'}|}$$

where $\triangle$ denotes the geometric difference between two sets

Editing Set Difference: Example

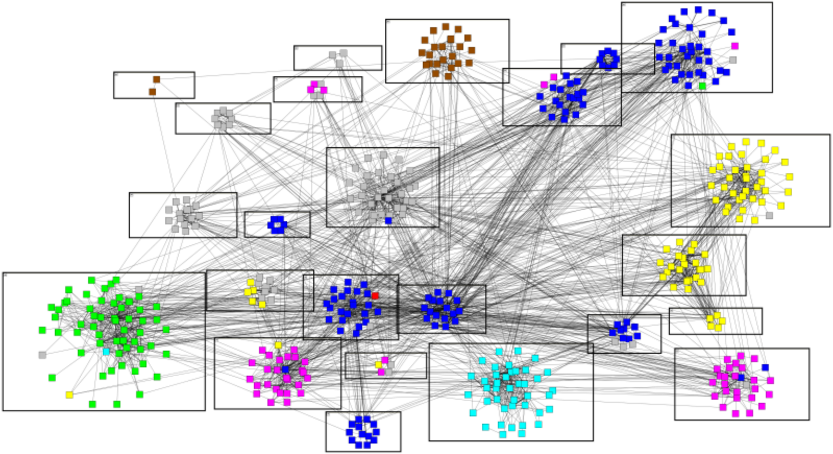


two clusterings

their editing sets

difference:
$1 - \frac{3}{10} = 0.7$

Real-World Graphs



. . . nice and necessary, but what about systematic insights?

Apparent Behavior

- High-degree nodes have more influence
- Cutting many edges $\leadsto$ higher difference

. . . average / practical / large-scale behavior?

Formalizing Postulations

The measure shall be *sensitive to the graph structure:*

Good vs. Random Clustering:

- $\textsc{dist}$(good cl., random cl.) $\approx$ big

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Formalizing Postulations

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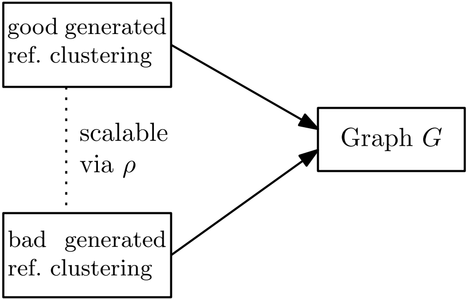
Perturbation:

- DIST(good cl., Δgood cl.) $>$ DIST(Δgood cl., $\Delta\Delta$good cl.)

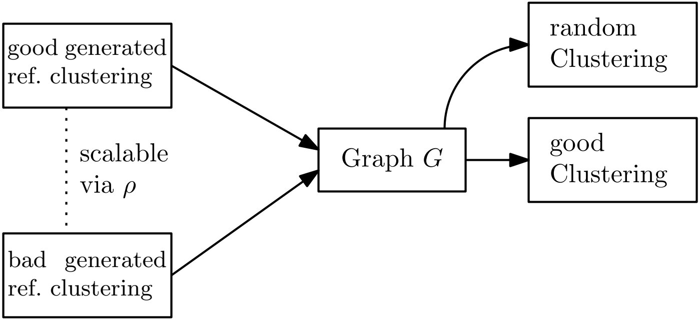
Experimental Setup



Systematic evaluation with *random preclustered graphs*:

- random graphs of parameterized structure
- *implanted* community structure with tunable significance ρ

Experimental Setup



testing *Good vs. Random Clustering* by:

- $\mathcal{C}$: implanted (good) clustering
- $\mathcal{C}_R$: random clustering, same graph amd parameters

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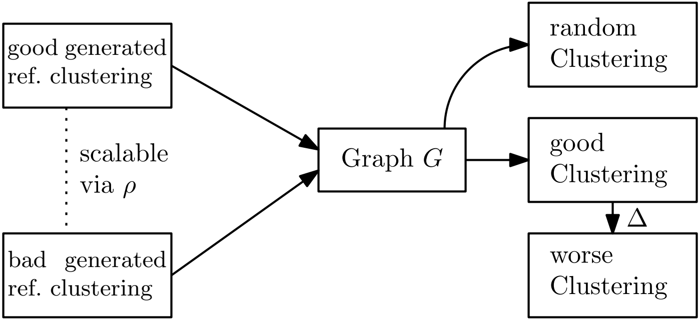

testing *Perturbation* by:

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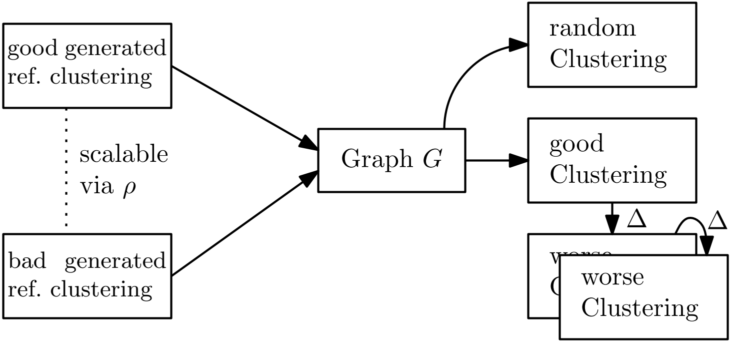

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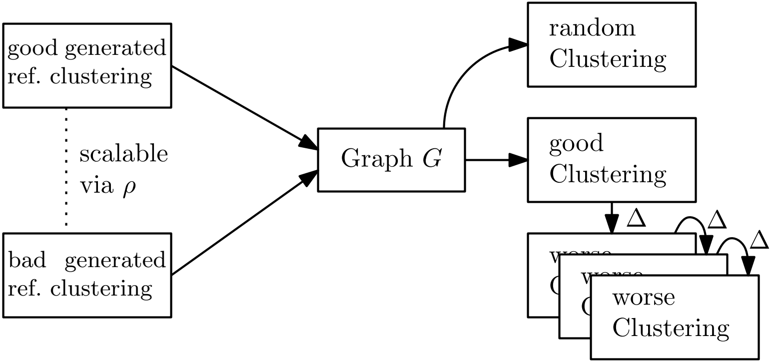

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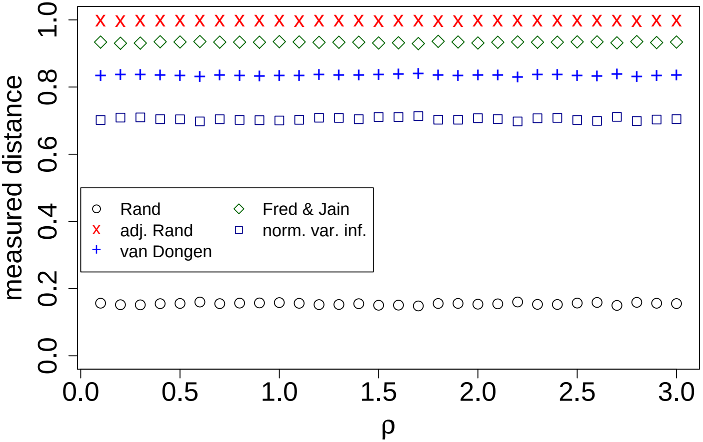
Good vs. Rand. Clustering, $\mathcal{C}$ vs. $\mathcal{C}_R$

set-based measures fail postulations



ρ tunes clarity of implanted clustering (high $\rho \Rightarrow$ bad clust.)

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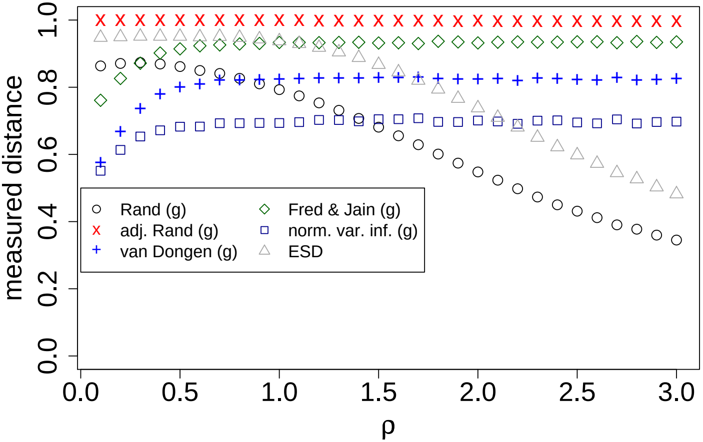
some graph-based measures comply



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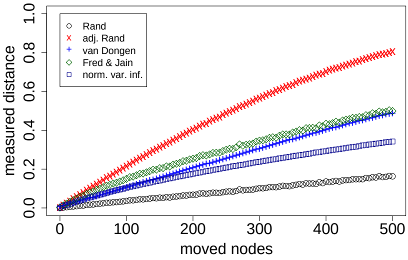
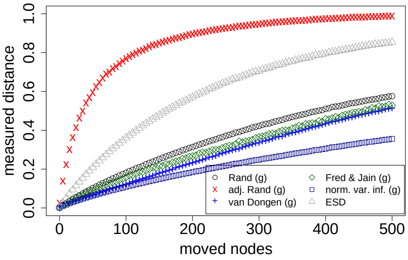
Perturbation of Good Clustering

set-based vs. graph-based



set-based
almost linear

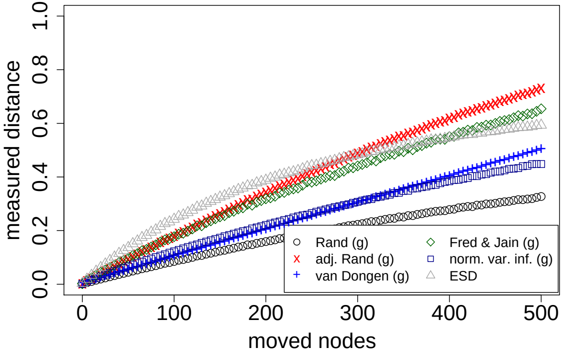


graph-based *ESD* and *adj. Rand*
non-linear

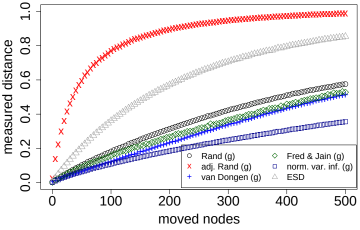
distance from implanted clustering after node migrations

Perturbation of Decent Clustering

set-based vs. graph-based



graph-based
less clear community structure



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Summary on Comparators

- many well known measures for comparing set partitions
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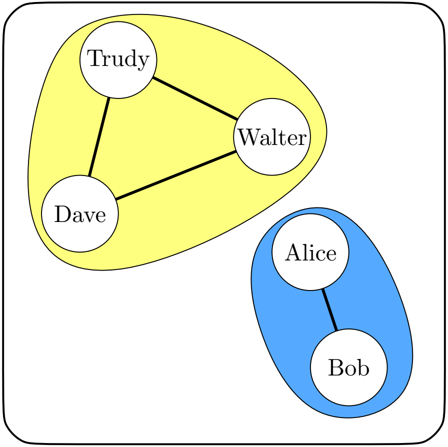
[Delling at al.: Engineering comparators for graph clusterings, 2008]

Structure

A Dynamic Network



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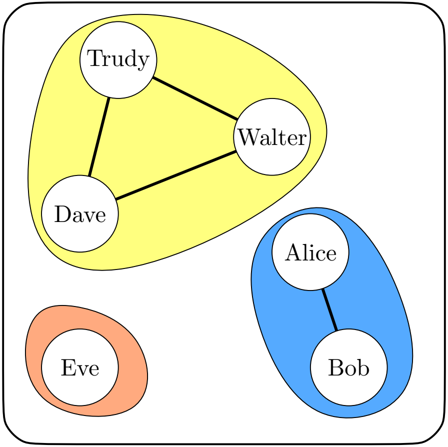

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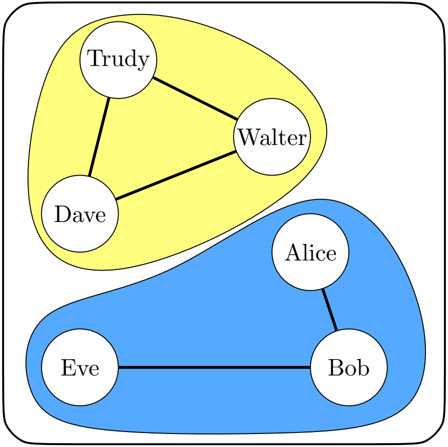

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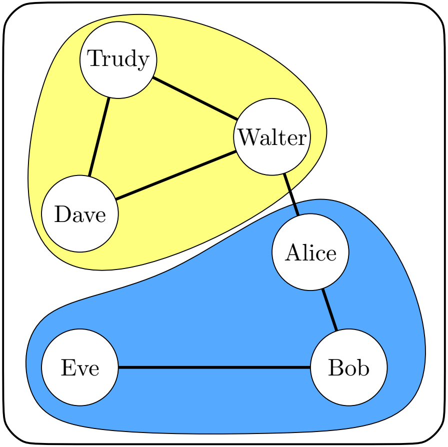

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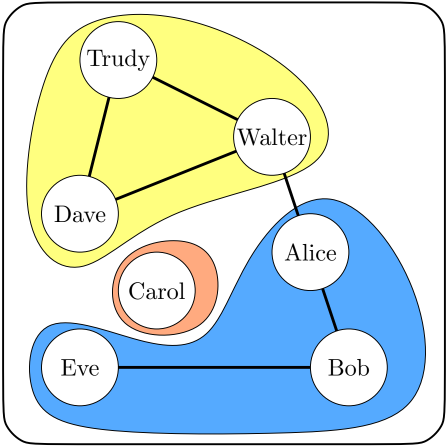

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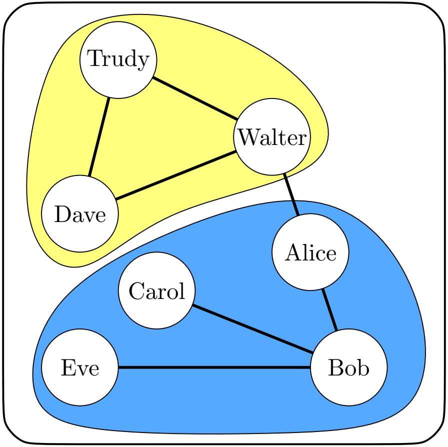

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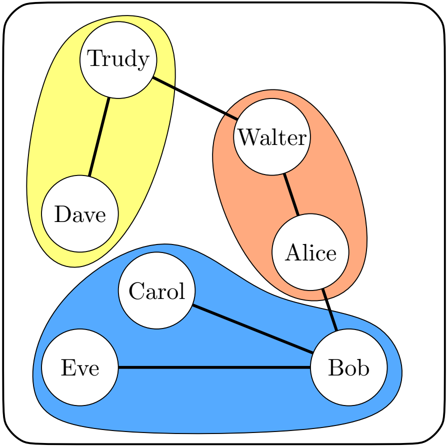

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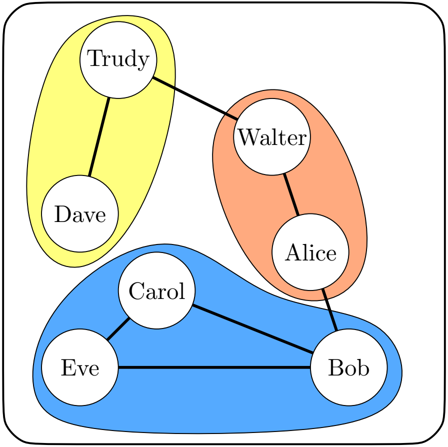

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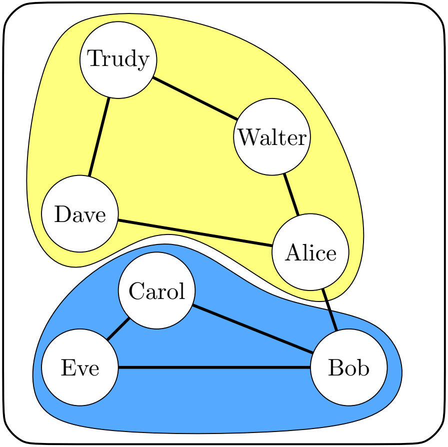
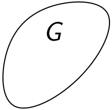


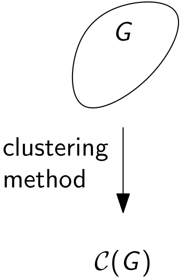
Structure

The Update Problem



Given: graph G,

The Update Problem



Given: graph G, technique $\mathcal{T}$, $\Rightarrow$ clustering $\mathcal{C}$

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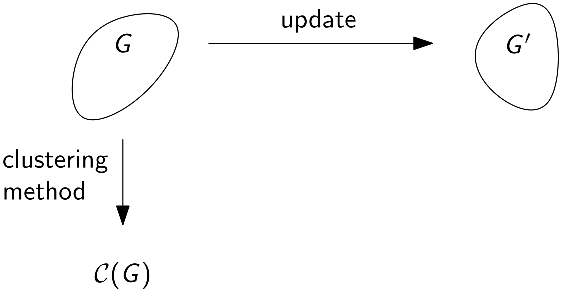

Given: graph G, technique $\mathcal{T}$, $\Rightarrow$ clustering $\mathcal{C}$
Then: modification Δ, $\Rightarrow$ graph G',

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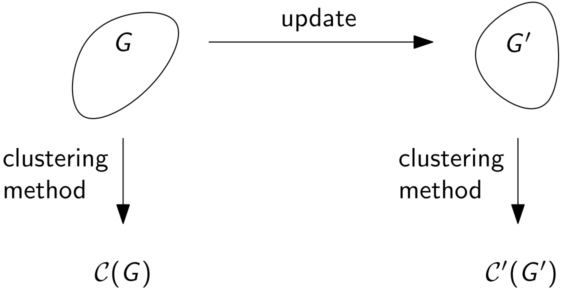

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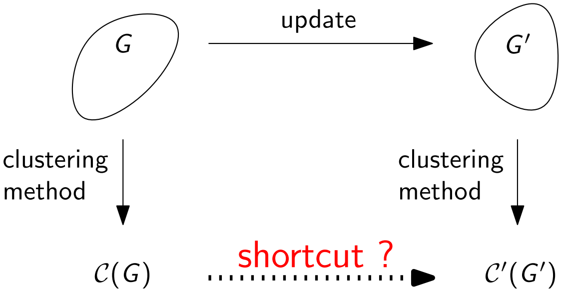


Given: graph G, technique $\mathcal{T}$, $\Rightarrow$ clustering $\mathcal{C}$
Then: modification Δ, $\Rightarrow$ graph G', $\mathcal{T} \Rightarrow$ clustering $\mathcal{C}'(G')$
Question: Is there a shortcut ?

Online Dynamic Graph Clustering

Dynamic Instances

changing networks with evolving group structure

$$\Downarrow$$

Dynamic Approach

update previous clustering reacting to changes in the graph

$$\begin{tikzcd} G \arrow[rr, "\Delta"] \arrow[d, "\mathcal{T}"'] & & G' \arrow[d, "\mathcal{T}"] \\ \mathcal{C}(G) \arrow[rr, dashed, "\mathcal{A}"] & & \mathcal{C}'(G') \end{tikzcd}$$

Clustering update problem

Criteria

- speed
- quality
- smooth transitions

Complexity of Optimization

Generally NP-hard if static problem is hard
$\Rightarrow$ generally NP-hard.

e.g., modularity:

Theorem

MODOPT is NP-hard [Brandes et al. 2008]

$$\Downarrow$$

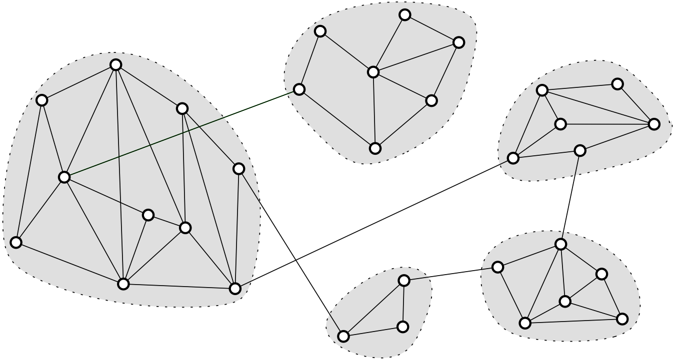
Corollary

DYNMODOPT is NP-hard [Görke et al. 2010]

idea for reduction: incrementally find static optimum with an efficient dynamic algorithm

Heuristics Based on Locality

Dynamic *modularity*-maximization *without provable* quality



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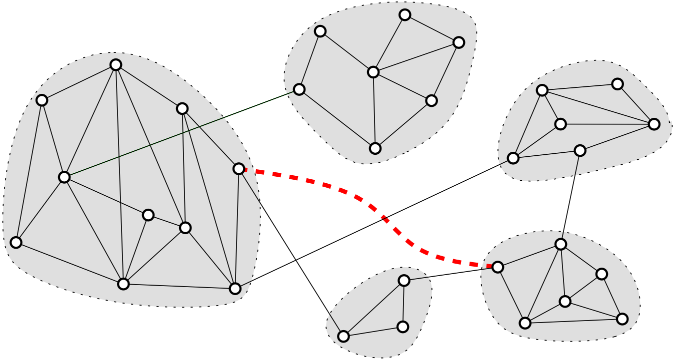

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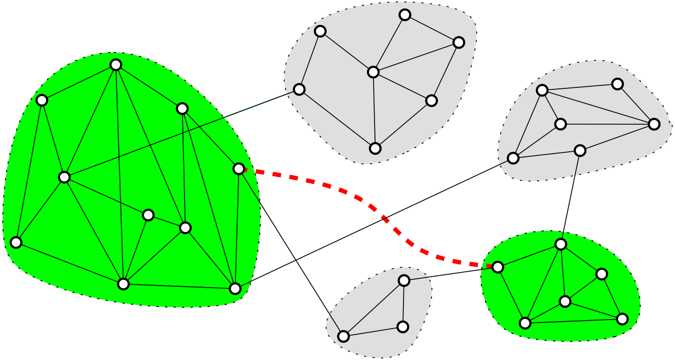

Changes in the graph invalidate:
affected clusters

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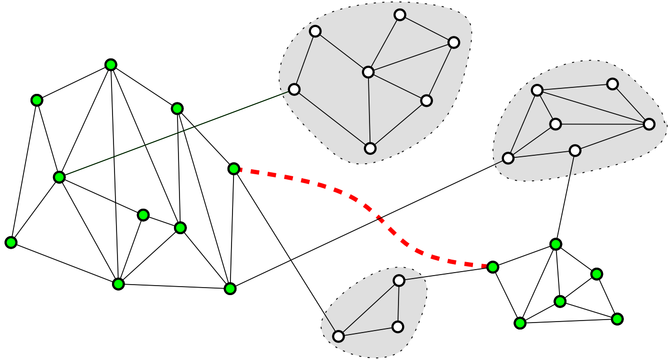

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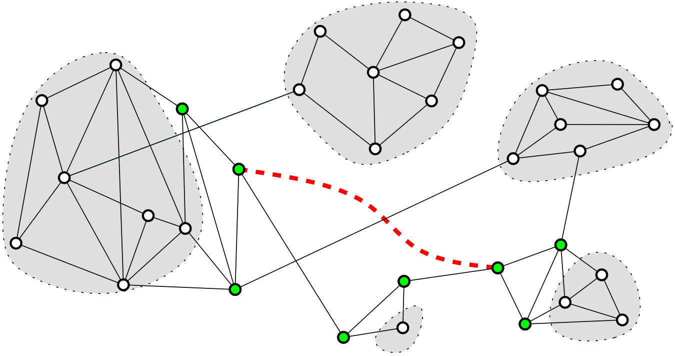

Changes in the graph invalidate:

local area: 1-hop neighborhood

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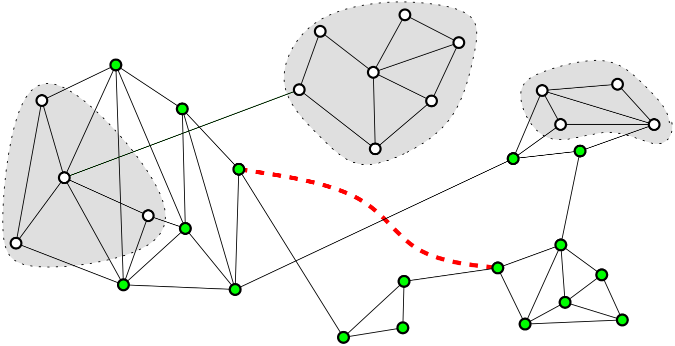

Changes in the graph invalidate:
local area: 2-hop neighborhood

Heuristics Based on Locality

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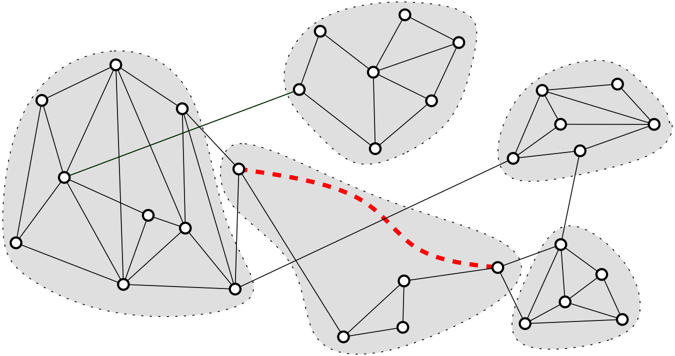
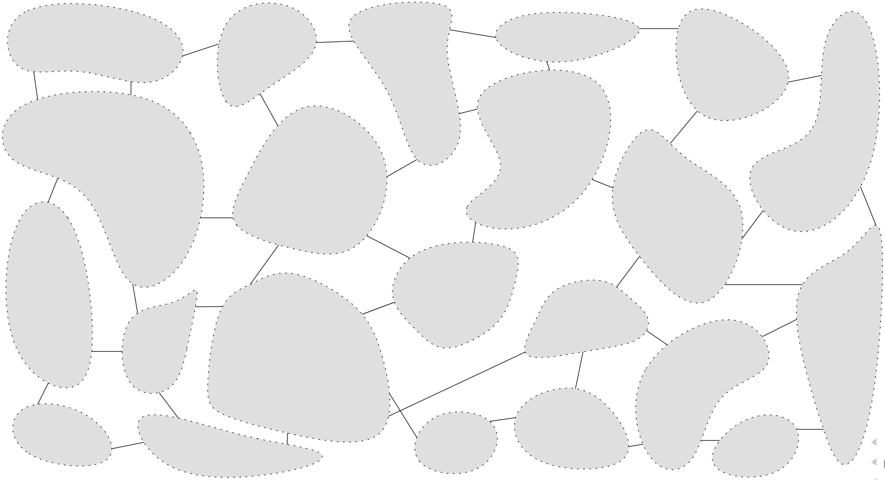


Changes in the graph invalidate:

local area: 2-hop neighborhood

⇒ **update of clustering**

Prep Strategies



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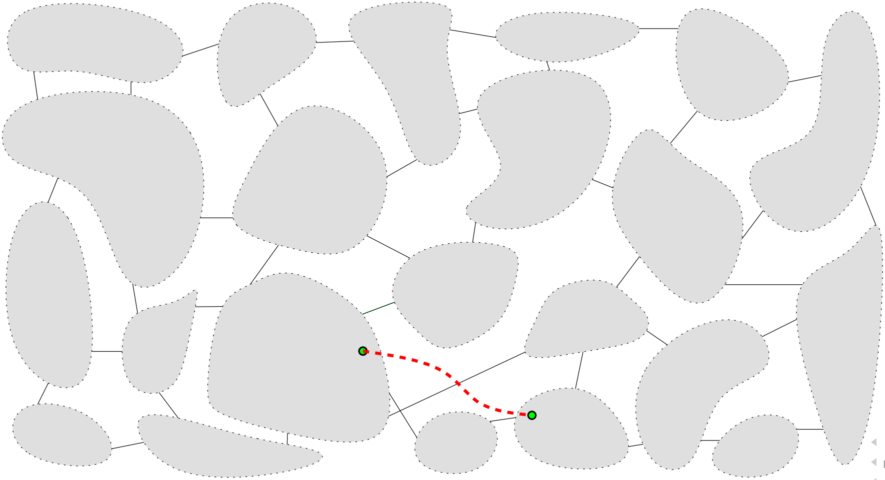

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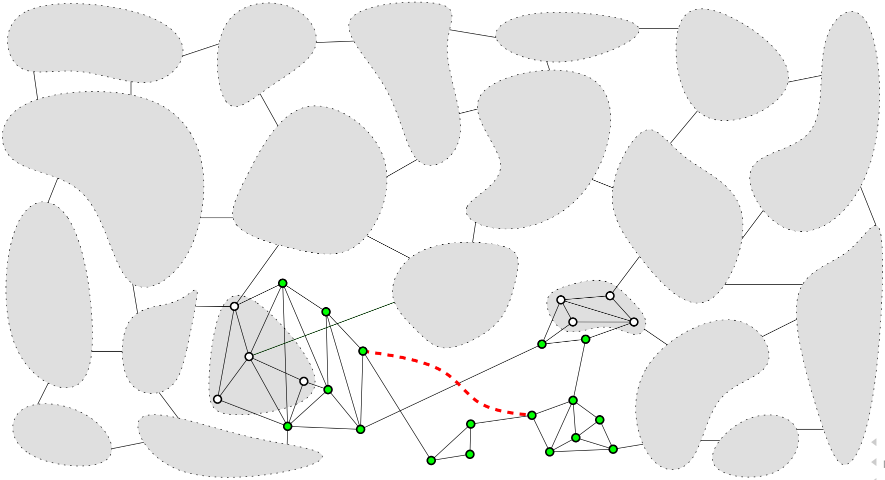

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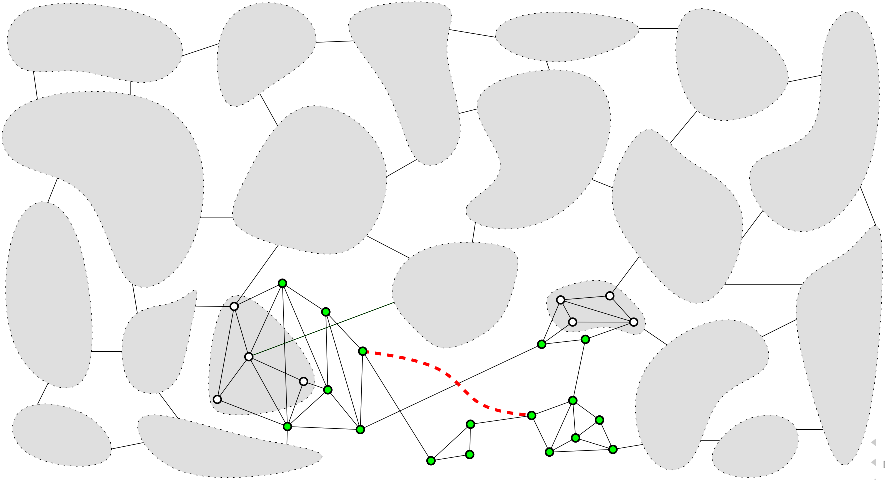
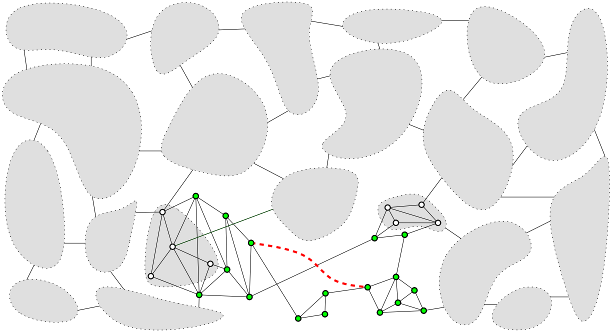


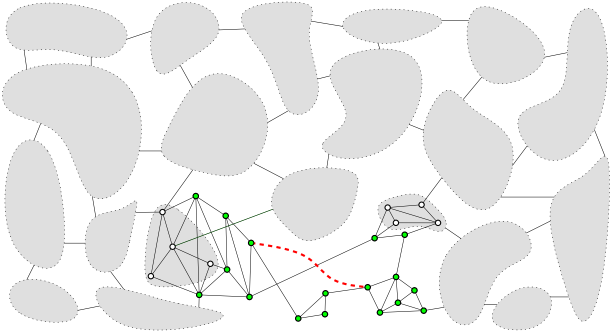
locality assumption

Local Heuristic in Bigger Context



motivation: local changes ⇒ local consequences,
„revolutions“ rare in practice

Local Heuristic in Bigger Context



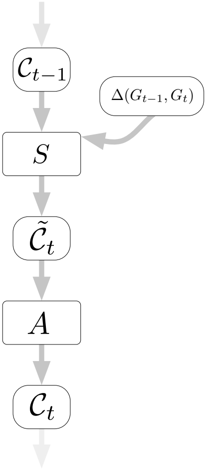
motivation: local changes ⇒ local consequences, „revolutions" rare in practice

hope: small changes ⇒ smooth transitions
small search space ⇒ fast
local optimization ⇒ quality ?

Prep Strategies: Concept

prep strategy S

- reacts to changes
- prepares half-finished *preclustering* $\tilde{\mathcal{C}}$
- passes $\tilde{\mathcal{C}}$ on to algorithm



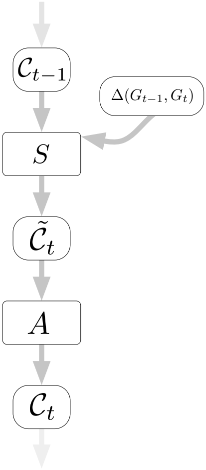
Prep Strategies: Concept

prep strategy S

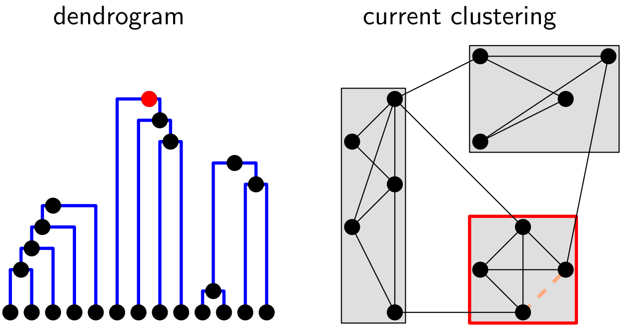
- reacts to changes
- prepares half-finished *preclustering* $\tilde{\mathcal{C}}$
- passes $\tilde{\mathcal{C}}$ on to algorithm

strategies based, e.g., on

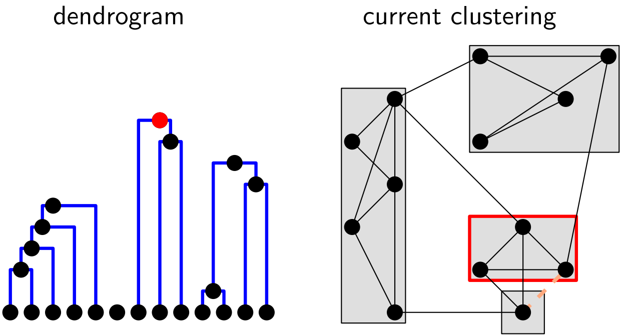
- limited local search
- backtracking the dendrogram



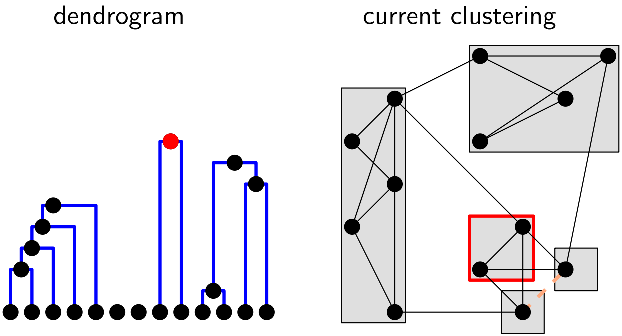
Prep Strategy BT: Illustration



Prep Strategy BT: Illustration



Prep Strategy BT: Illustration



Prep Strategy Backtrack

Backtrack Global's merges according to heuristic rules

Measuring Smoothness

Distance measures based on:

- counting pairs
- maximum overlap
- information theory

[3] [Delling et al.: Engineering comparators for graph clustering, 2008]

Measuring Smoothness

Distance measures based on:

- **counting pairs**
- maximum overlap
- information theory

Example: *Rand*-distance

[3] [Delling et al.: Engineering comparators for graph clustering, 2008]

Measuring Smoothness

Distance measures based on:

- **counting pairs**
- maximum overlap
- information theory

Example: *Rand*-distance

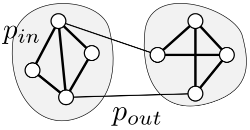
"compare co-classification of all pairs of nodes"

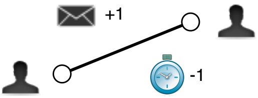
$$\mathcal{R}(\mathcal{C},\mathcal{C}') := \underbrace{1 - \frac{n_{\text{tog,tog}} + n_{\text{sep,sep}}}{\frac{1}{2}|N|(|N|-1)}}_{(\textit{Rand}\text{, set-based})} \rightsquigarrow \underbrace{1 - \frac{e_{\text{tog,tog}} + e_{\text{sep,sep}}}{|E|}}_{(\text{graph-based } \textit{Rand}^{3})}$$

[3] [Delling et al.: Engineering comparators for graph clustering, 2008]

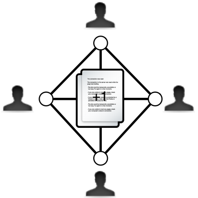
Dynamic Graph Instances

- generator for dynamic clustered random graphs
  [Görke and Staudt: A generator for dynamic clustered random graphs, 2009]



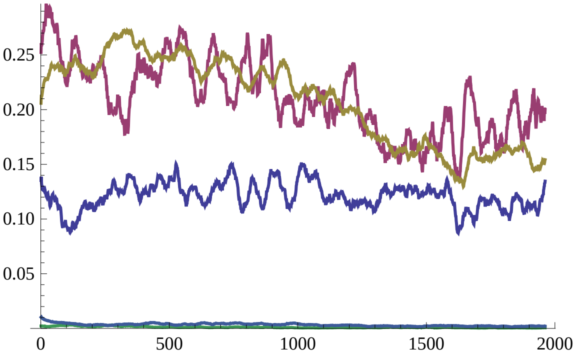


- e-mail graph of KIT CompSci



- arXiv collaboration graph

Dynamic *Modularity*-Clustering: Smooth Transitions



distances between time steps
(graph-based *Rand*-distance)

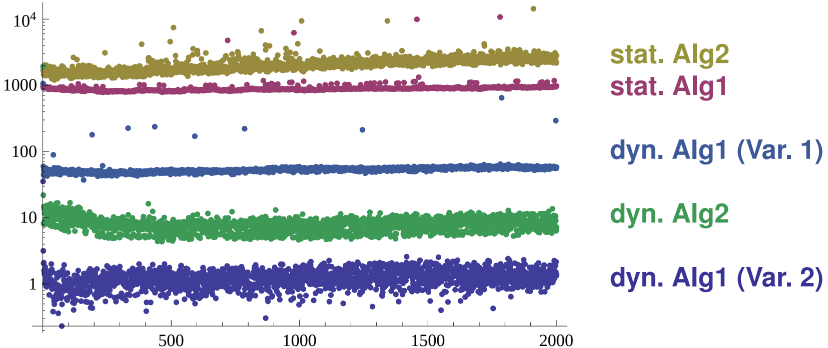
stat. Alg1
stat. Alg2
dyn. Alg1 (Var. 2)

dyn. Alg2 and
dyn. Alg1 (Var. 1)

$\Rightarrow$ Dynamics yield smoother transitions

[Görke et al.: Modularity-driven clustering of dynamic graphs 2010]

Dynamic *Modularity*-Clustering: Runtime

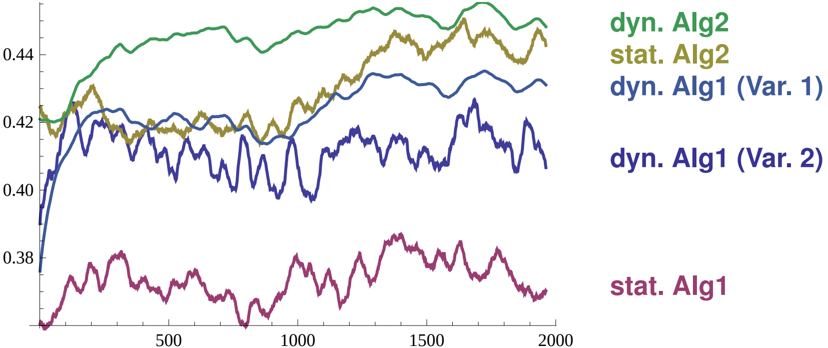


runtime per time step
(milliseconds, logarithmic *y*-axis)

⇒ dynamics yield lower runtimes

[Görke et al.: Modularity-driven clustering of dynamic graphs 2010]

Dynamic *Modularity*-Clustering: Quality

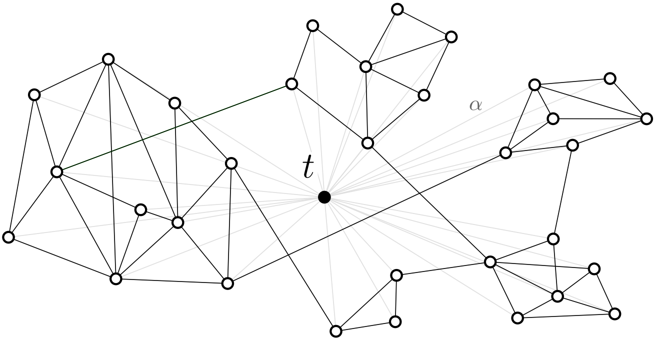


quality over time
(modularity)

⇒ dynamics yield higher quality

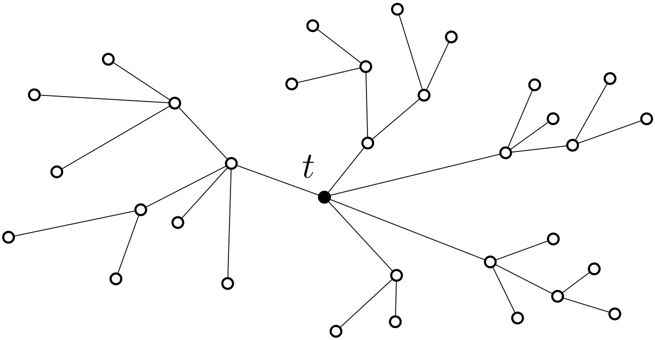
[Görke et al.: Modularity-driven clustering of dynamic graphs 2010]

Min-Cut Tree Clustering (Rep.)



1. original graph
2. star-center *t*, α

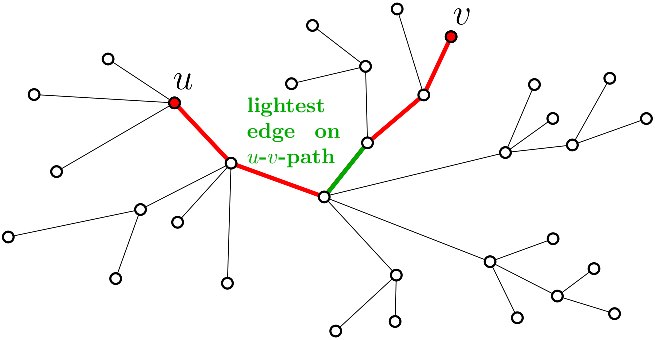
Min-Cut Tree Clustering (Rep.)



1. original graph
2. star-center t, α
3. *min-cut tree*

- coined in [Gomory and Hu '61]
- simplified in [Gusfield '90]
- construction via $(n-1)$ max-flows
  (variants e.g. $\widetilde{O}(mn)$ for unweighted)

Min-Cut Tree Clustering (Rep.)



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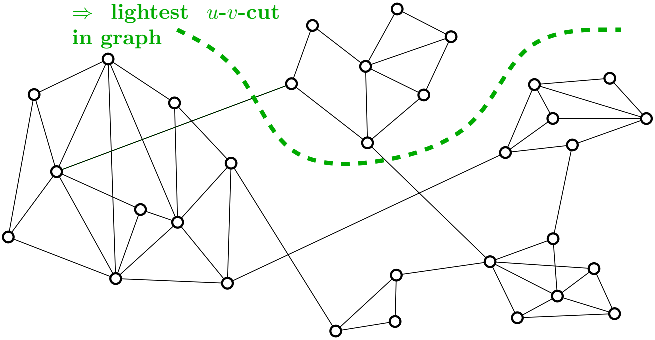

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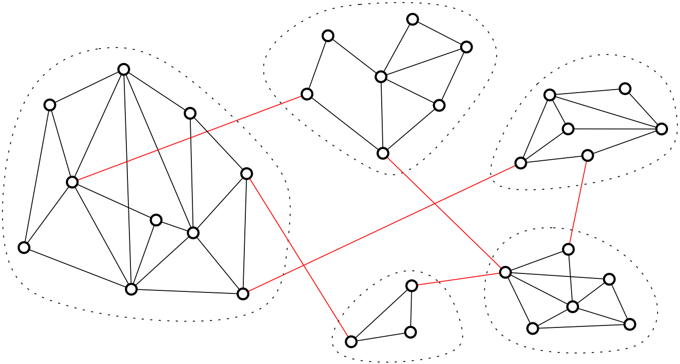
Min-Cut Tree Clustering (Rep.)



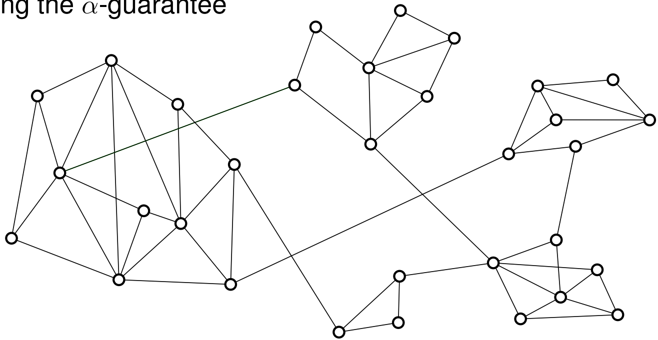
1. original graph
2. star-center t, α
3. *min-cut tree*
4. delete center $\Rightarrow$ clustering

quality guarantee: [Flake et al. '04]

intra-cluster expansion $\geq \alpha \geq$ *inter-cluster expansion**

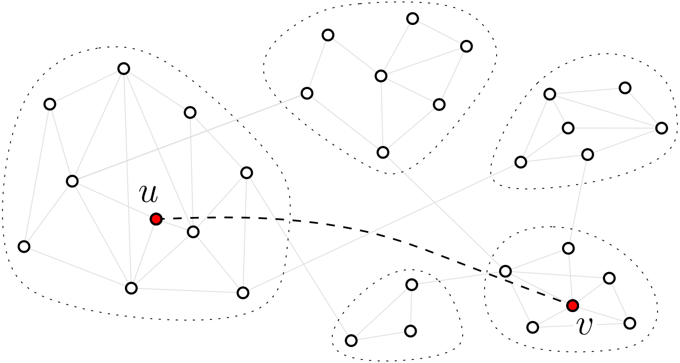
Dynamizing the Clustering

maintaining the α-guarantee



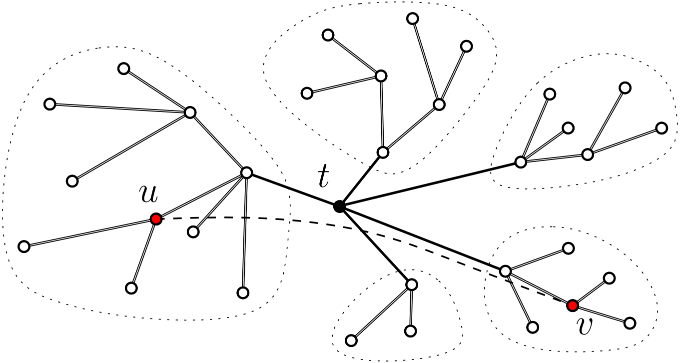
- new edge in graph affects *u*-*v*-path in tree

Dynamizing the Clustering



- new edge in graph affects *u-v-path* in tree

Dynamizing the Clustering



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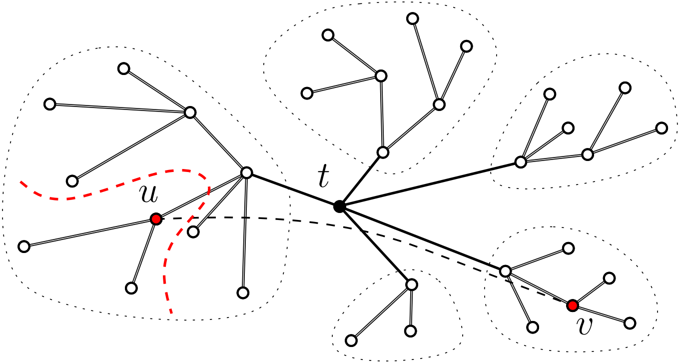
Dynamizing the Clustering



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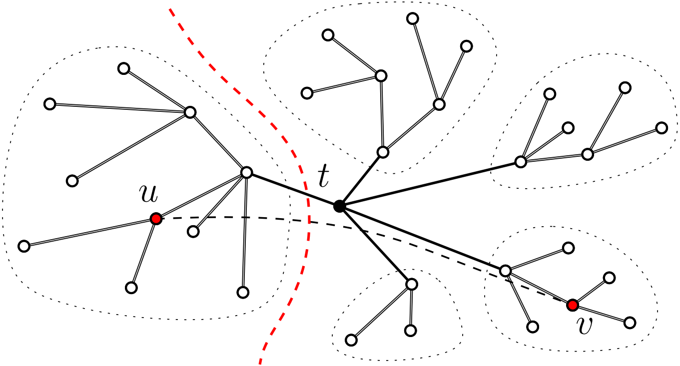

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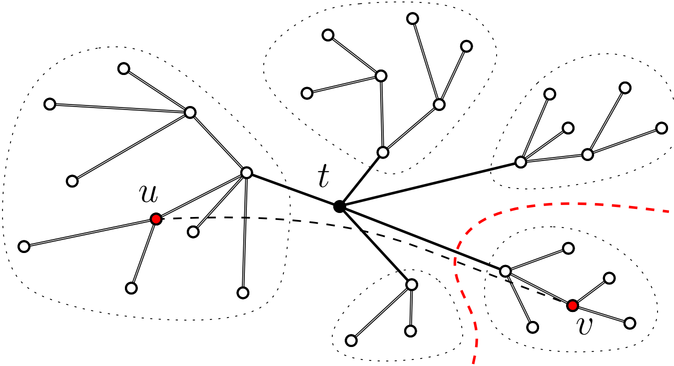
Dynamizing the Clustering



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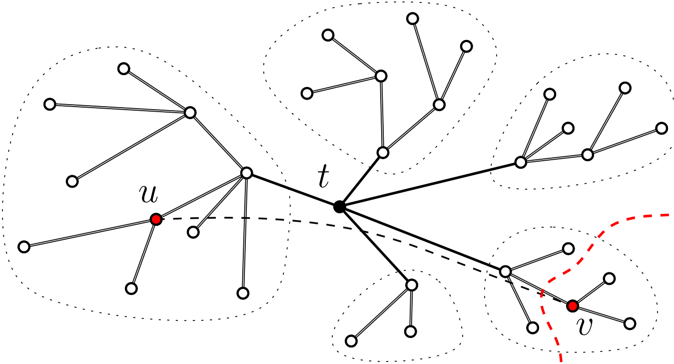
Dynamizing the Clustering



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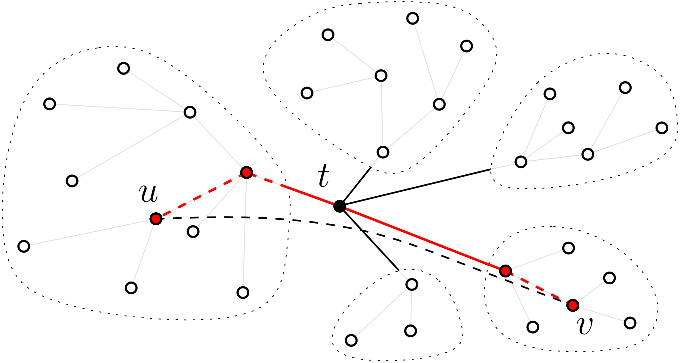
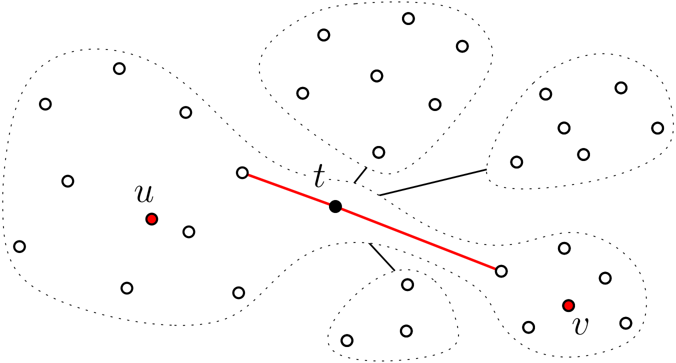
Dynamizing the Clustering



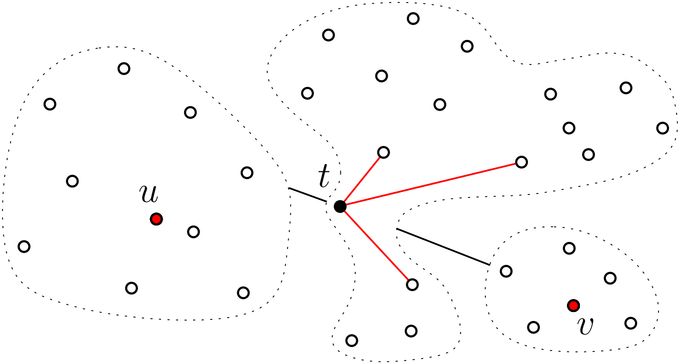
- new edge in graph affects *u*-*v*-path in tree
- safe parts of the clustering reusable

Dynamizing the Clustering



- new edge in graph affects *u*-*v*-path in tree
- safe parts of the clustering reusable
- *Theorem:* “starting here is feasible”

Dynamizing the Clustering



- new edge in graph affects *u*-*v*-path in tree
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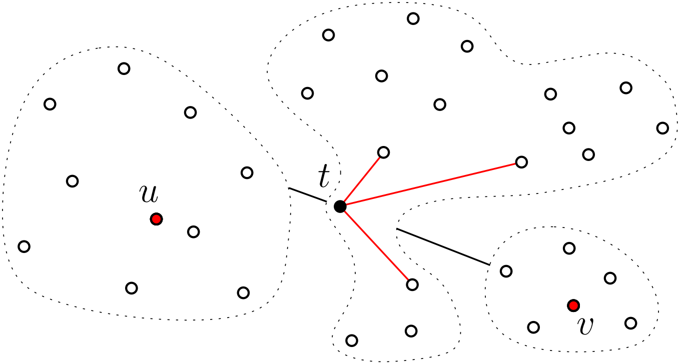
- *Theorem:* “starting here is feasible”
- edge deletion affects off-path cuts analogously

Dynamizing the Clustering



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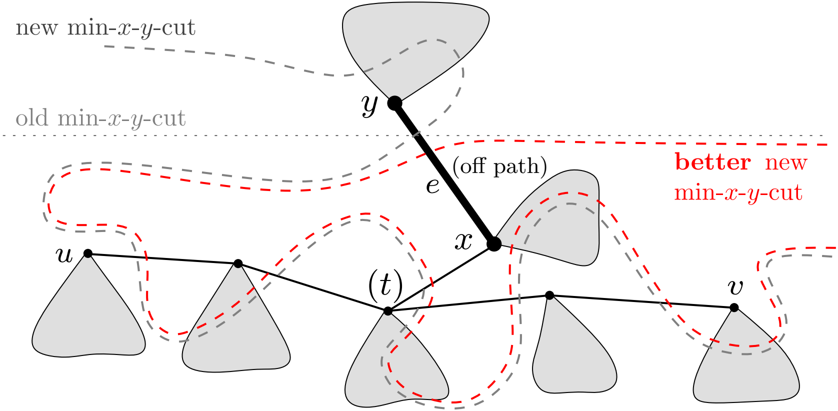
- safe parts of the clustering reusable
- *Theorem:* “starting here is feasible”
- edge deletion affects off-path cuts analogously

[Hartmann et al.: Dynamic Graph Clustering Using Minimum-Cut Trees, 2009]

Dynamizing the Clustering

a glimpse into retaining clusters and saving more effort
example: *inter-cluster edge deletion* $\rightsquigarrow$ check/correct old $\mathcal{C}$



Dynamizing the Clustering

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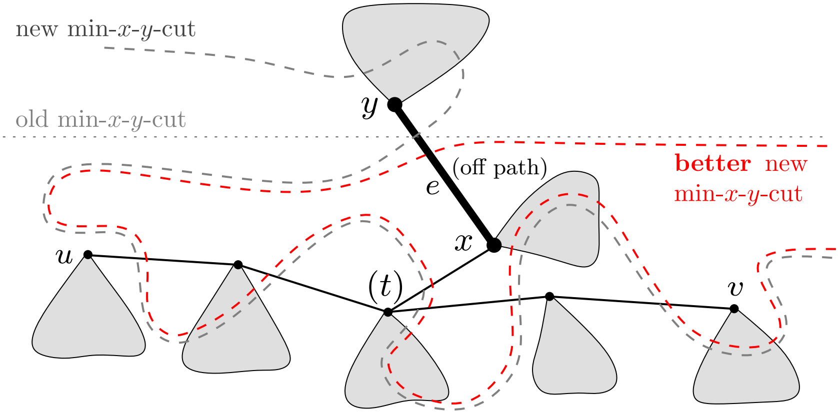
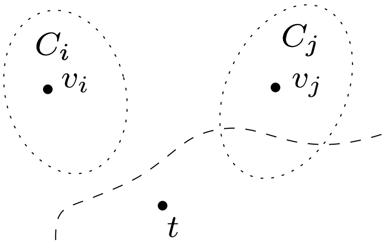


Lemma $\Rightarrow$ cut (gray) can be reshaped, retaining old cluster (red)

Dynamizing the Clustering: Case 1

adjustments for all pairs of clusters:

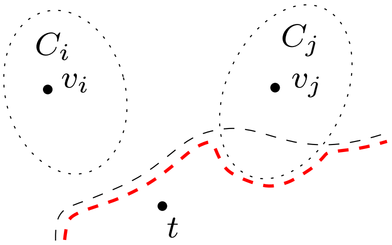


v_i is tree-reference vertex of C_i

check old cluster C_i in new graph $\rightsquigarrow$ new v_i-t-cut separates v_j, t
Lemma (last slide) $\Rightarrow$ cut can be reshaped, retaining C_i (black)

Dynamizing the Clustering: Case 1

adjustments for all pairs of clusters:

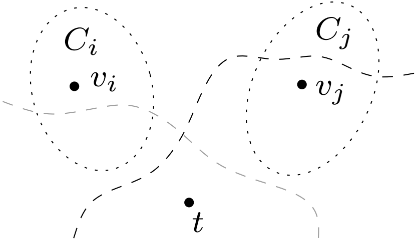


v_i is tree-reference vertex of C_i

check old cluster C_i in new graph $\leadsto$ new v_i-t-cut separates v_j, t
- *Lemma* (last slide) $\Rightarrow$ cut can be reshaped, retaining C_i (black)
- *Lemma* $\Rightarrow$ cut can be re-reshaped, swallowing C_j (red)

Dynamizing the Clustering: Case 2

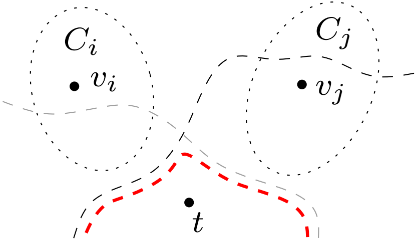
adjustments for all pairs of clusters:



symmetric case: new v_j-t-cut (gray) separates v_i from t, **after** new v_i-t-cut (black) does not separate v_j from t

Dynamizing the Clustering: Case 2

adjustments for all pairs of clusters:

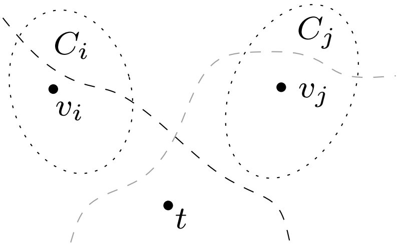


symmetric case: new v_j-t-cut (gray) separates v_i from t, **after** new v_i-t-cut (black) does not separate v_j from t

Lemma $\Rightarrow$ reshape cut (red)

Dynamizing the Clustering: Case 3

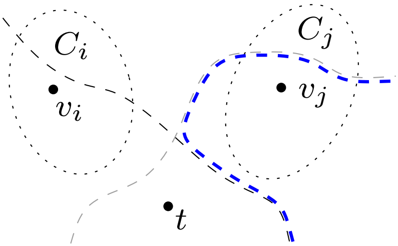
adjustments for all pairs of clusters:



both new cuts do not separate other vertex from t

Dynamizing the Clustering: Case 3

adjustments for all pairs of clusters:

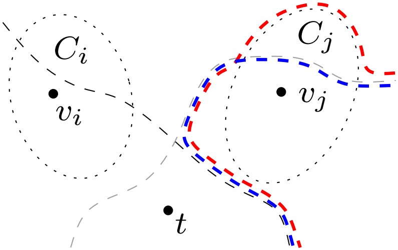


both new cuts do not separate other vertex from t

folklore $\Rightarrow$ crossing min-cuts $\rightsquigarrow$ non-crossing (blue for v_j's cut)

Dynamizing the Clustering: Case 3

adjustments for all pairs of clusters:



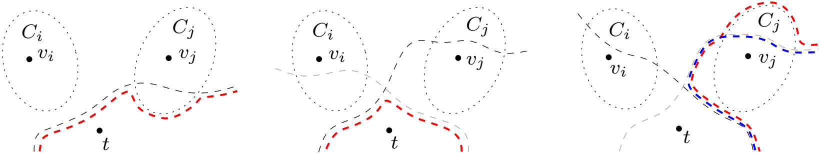
both new cuts do not separate other vertex from t

folklore $\Rightarrow$ crossing min-cuts $\rightsquigarrow$ non-crossing (blue for v_j's cut)

Lemma $\Rightarrow$ reshape to retain old cluster (red for v_j's cut)

Dynamizing the Clustering

adjustments for all pairs of clusters:



- adjust cuts to all other clusters C_j
- old cuts retained or swallowed
- order affects speed, but lemmata hold for all orders
- similar arguments for intra-/inter-cluster addition/deletion

$\Rightarrow$ **smoothness + speed**

Results of the Dynamization

instance: email network, 12 000 time steps
measurement: number of s-t-cut calculations (vs. static)

runtime saved $> 90\%$

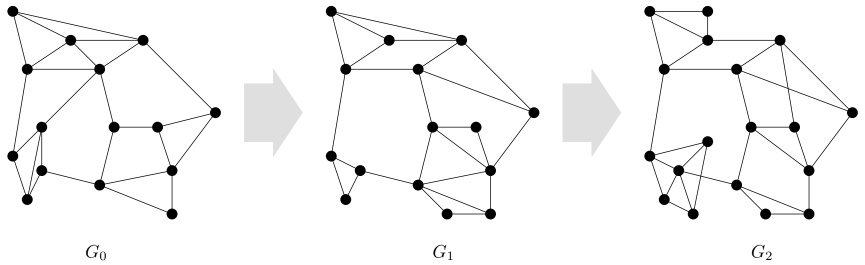
smooth transitions: minimal changes per step (max. 2 cluster split)

continuity: old clustering valid? $\Rightarrow$ confirmed via only 2 s-t-cuts

quality: $\surd$

Structure

Clustering Graph Sequences

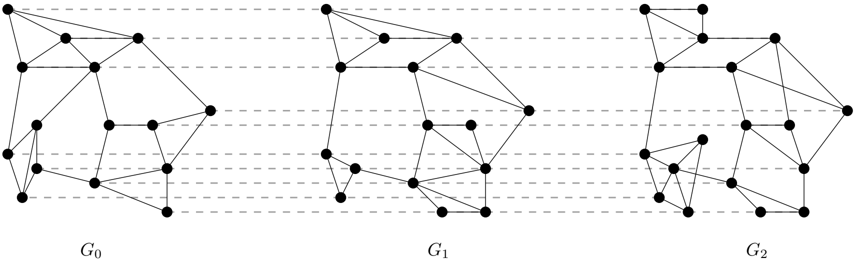


Goals:
1. a clustering of each step
2. tracking clusters
3. smooth transitions
4. find critical changes

naïve approach: comparison of unrelated, static clusterings

[4] [Gaertler et al.: How to cluster an evolving graph, 2006]

Clustering Graph Sequences



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time-expanded clustering[4]: stack snapshots

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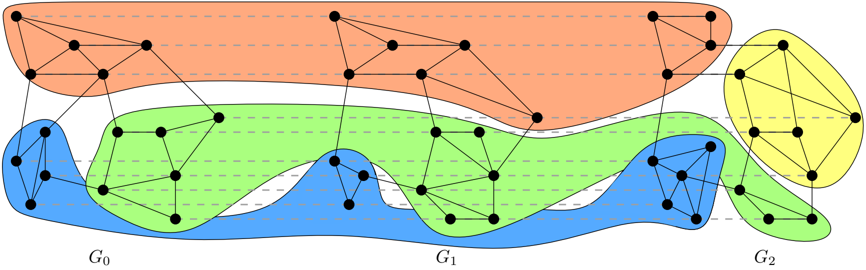

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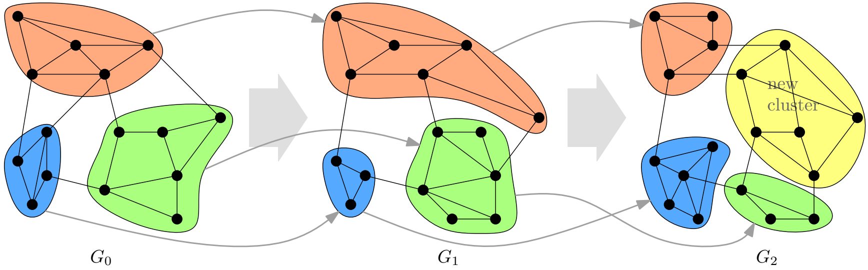
Clustering Graph Sequences



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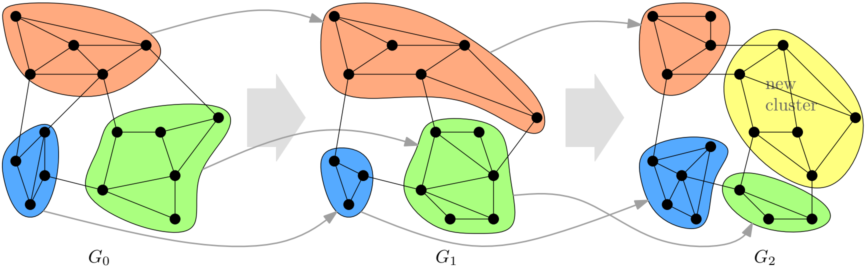
Clustering Graph Sequences



Goals:
1. a clustering of each step
2. tracking clusters
3. smooth transitions
4. find critical changes

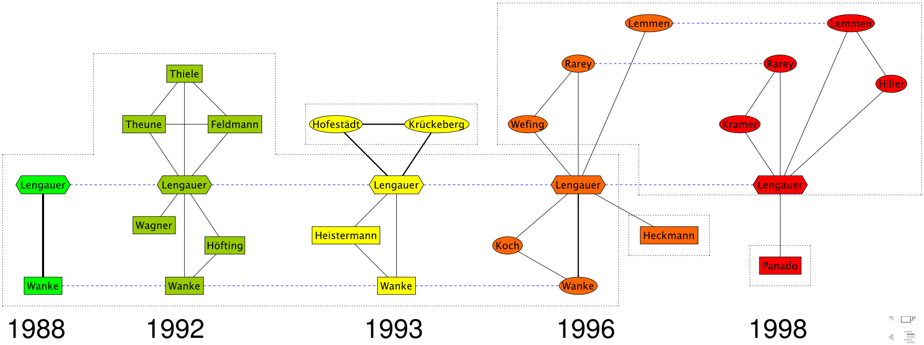
applications:
- email-network
- customer profiles
- technological trends

naïve approach: comparison of unrelated, static clusterings
time-expanded clustering[4]: stack snapshots ⇒ cluster ⇒ evolution visible

[4] [Gaertler et al.: How to cluster an evolving graph, 2006]

Time-Expanded Graph Clustering

- **Thomas Lengauer** started career as a *computer scientist* (rectangles)
- cooperations with *biologists* (ellipses)
- . . . today a renown bioinformatician



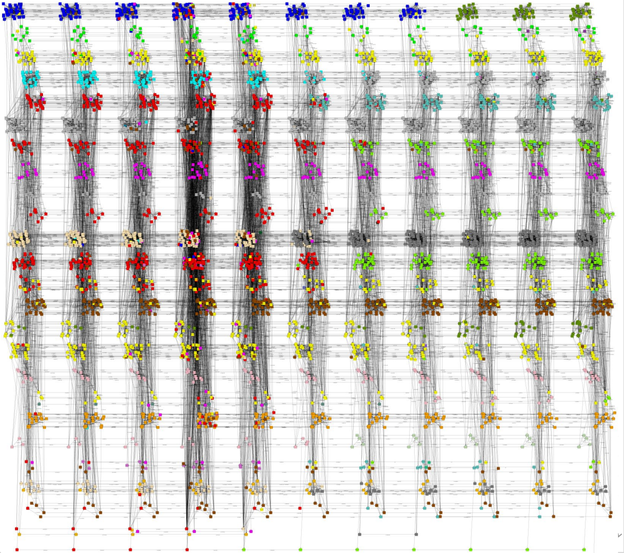
Application: Email-Network [Görke: Diss. 2010]

email data (KIT's CompSci)

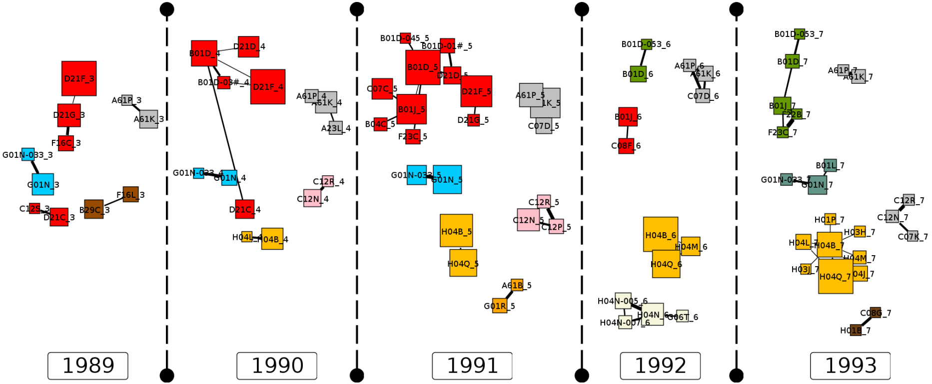
- nodes = employee
- edge = emails
- 36 months collected

- vertical str. = month
- horiz. str. = chair
- color = clustering

⇒ colors in vertical strip = current cooperations



Application: Technological Trends



Patent Categories, Finland, interconnected via multi-category patents

break: from 1992 on telecommunications dominate
before: paper, pharmaceuticals, material sciences
later: paper forms new cluster

Explicitly Bicriterial Formulations

1. Among all sequences $\zeta = (\mathcal{C}_0, \ldots, \mathcal{C}_{t_{\max}})$ of clusterings of $\mathcal{G}$ with $\mathcal{C}_i(G_i)$ optimal regarding quality, find the sequence ζ_{smooth} that minimizes $\sum_{i=1}^{t_{\max}} \text{distance}(\mathcal{C}_{i-1}, \mathcal{C}_i)$.

2. Among all sequences $\zeta = (\mathcal{C}_0, \ldots, \mathcal{C}_{t_{\max}})$ of clusterings of $\mathcal{G}$ with $\sum_{i=1}^{t_{\max}} \text{distance}(\mathcal{C}_{i-1}, \mathcal{C}_i) \leq D$, find the sequence ζ_{good} that maximizes $\sum_{i=0}^{t_{\max}} \text{quality}(\mathcal{C}_i)$.

3. Is there a sequence $\zeta = (\mathcal{C}_0, \ldots, \mathcal{C}_{t_{\max}})$ of clusterings of $\mathcal{G}$ such that $\forall i : \text{quality}(\mathcal{C}_i) \geq \alpha(\mathcal{C}_i^{\text{optimal}})$ and $\forall i \geq 1 : \text{distance}(\mathcal{C}_{i-1}, \mathcal{C}_i) \leq \beta$?

4. Among all sequences $\zeta = (\mathcal{C}_0, \ldots, \mathcal{C}_{t_{\max}})$ of clusterings of $\mathcal{G}$ find the sequence ζ_{best} which optimizes $\alpha \sum_{i=0}^{t_{\max}} \text{quality}(\mathcal{C}_i) + \beta \sum_{i=1}^{t_{\max}} \text{distance}(\mathcal{C}_{i-1}, \mathcal{C}_i)$.

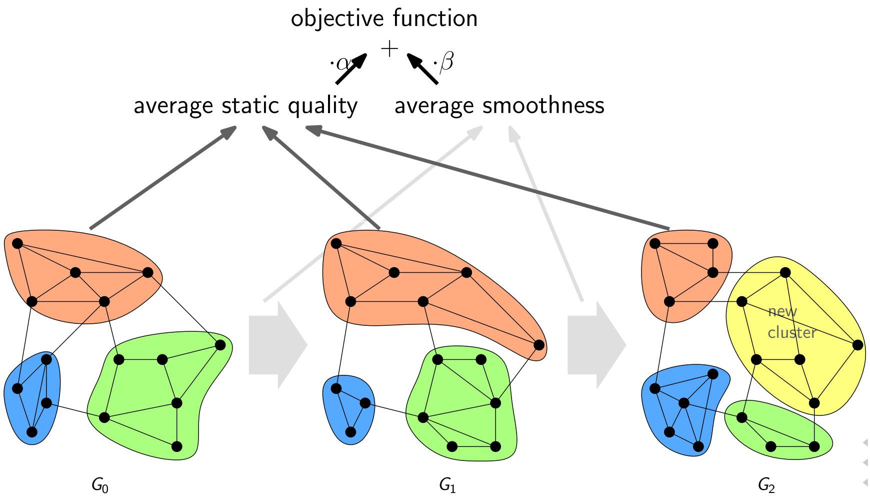
5. ...

[Görke: An algorithmic walk from static to dynamic graph clustering, 2010]

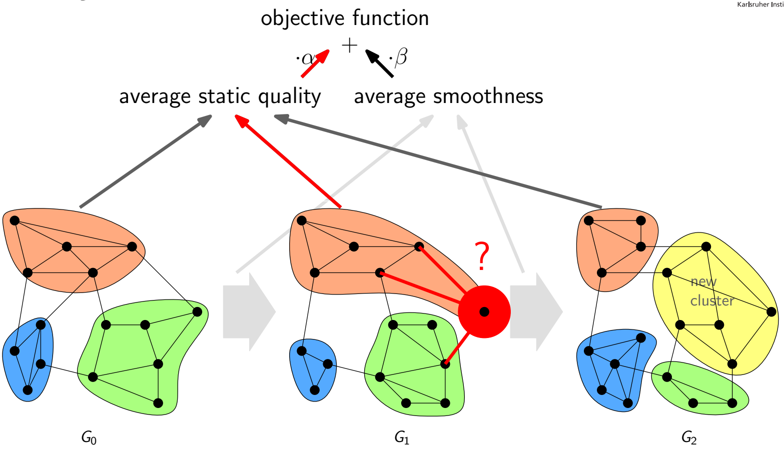
Explicitly Bicriterial ILP (generic)

- set up a static ILP for each time step
- link "neighboring" variables $X^t_{u,v}$ and $X^{t+1}_{u,v}$,
  e.g., $Z^t_{u,v} = X^t_{u,v}$ XOR $X^{t+1}_{u,v}$
- formulate smoothness by Z-variables
  e.g., Rand index: $\mathrm{dist}(\mathcal{C}_t, \mathcal{C}_{t+1}) := 1 - \frac{\sum_{u<v}(1-Z_{uv}(t))}{\frac{1}{2}n(n-1)}$
- use quality / smoothness as constraint / objective
  (some formulations do need quite some thought)
- overview of many variables, constraints and objectives:
  [Schumm et al.: Density-Constrained Graph Clustering, 2010, full technical report version]

Sum of Quality and Smoothness



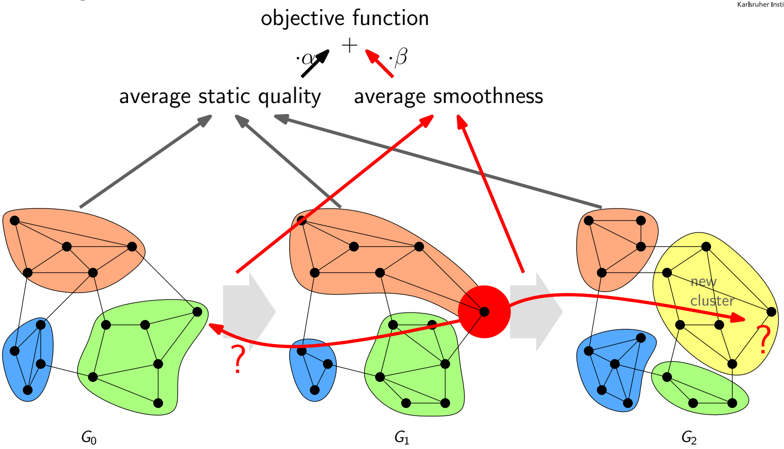
Explicitly Bicriterial Heuristic



Using, e.g., a local greedy heuristic, for each vertex move:

- calculate gain in snapshot quality

Explicitly Bicriterial Heuristic



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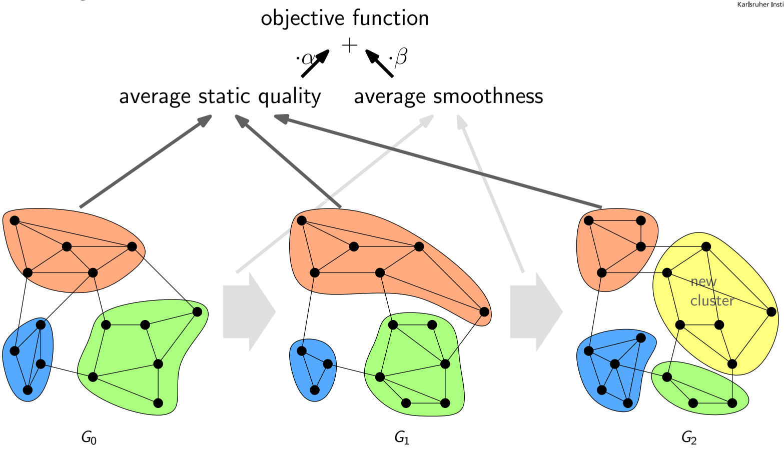

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complications: (non-)sequential, contraction, refinement, being efficient

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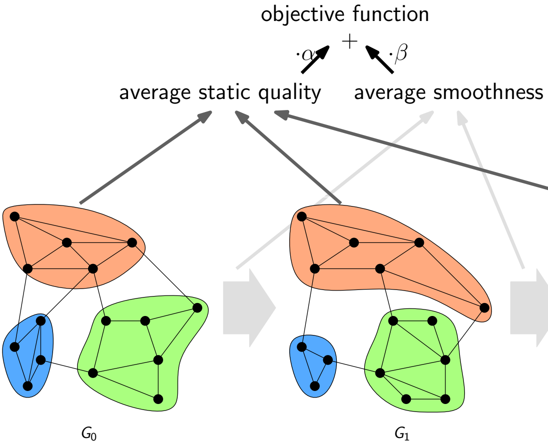

[Lisowski: Modularity-basiertes Clustern von dynamischen Graphen im Offline-Fall, 2011]

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Selected Summary of Lecture

Objective Functions

a formal foundation for the informal paradigm of *intra-cluster density and inter-cluster sparsity*

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- crucial topic in clustering
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Dynamic Clustering

- formalization of aims
- online and offline methods

Structure

Core-Decomposition: Algorithm

Karlsruher Institut für Technologie

Given: graph G
Wanted: *coreness* of each vertex

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Algorithm: `Core-Decomposition`

compute degrees of all vertices
bin-sort vertices into bins $B_0 \ldots B_{\text{max deg}}$
foreach $v \in V$ *in sorted order* **do**
    core(v) $\leftarrow$ deg(v)
    foreach $u \in N(v)$ **do**
        if deg(u) $>$ deg(v) **then**
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Complexity: $O(\max\{m, n\})$

see, e.g., [Batagelj, Zaveršnik '02, *An O(m) Algorithm for Cores Decomposition of Networks]*
or [Brandes, Erlebach (eds.) '05, Network Analysis, Methodological Foundations]