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Stochastic Graph Algorithms: Clique Covering and Clustering

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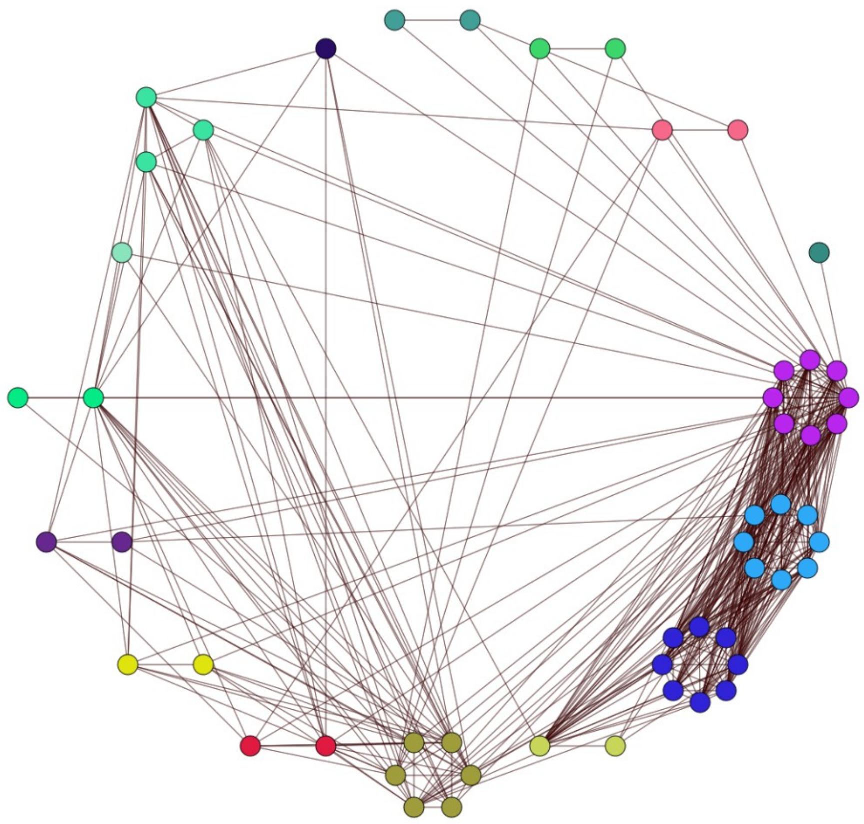
Outline of the Talk

- problems: theory and applications
- concepts of solving for the studied problems
  - algorithmic strategies for the clique covering problem (CCP) and graph clustering
  - analytical vs. experimental methodology of evaluation
- current results
  - an order-based representation for CCP and order-based algorithms: IG and RLS
  - multicriteria construction procedures (MCPs) for graph clustering
- conclusions, discussion, references

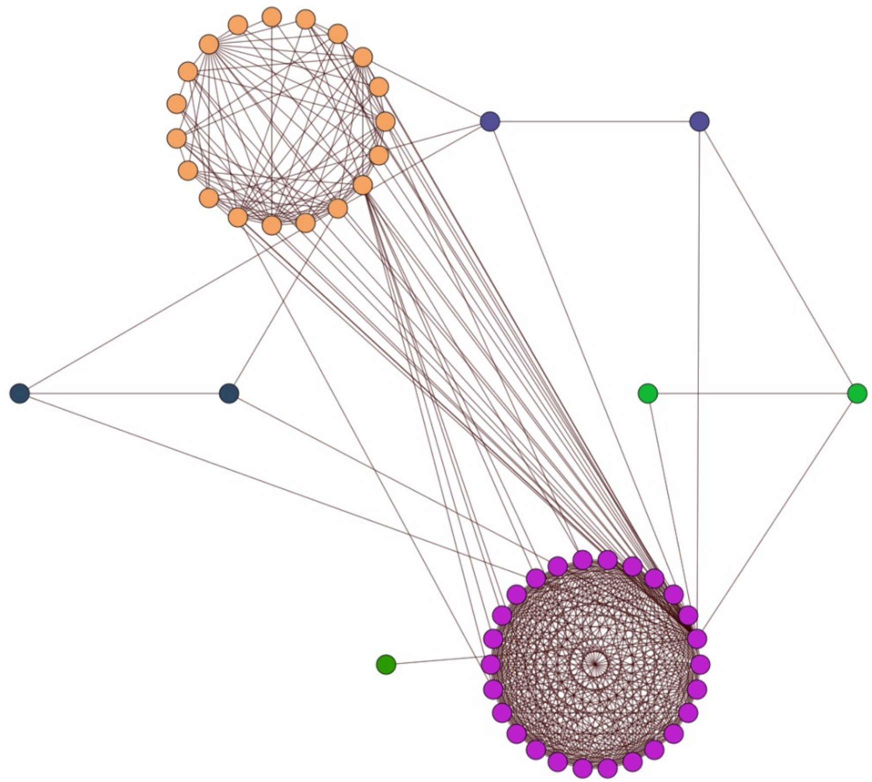
Clique Covering and Graph Clustering Problems

Problems: Clique Covering and Graph Clustering

- visual illustration on a small social network



clique covering



graph clustering

Motivation

- computational hardness
  - *clique covering* is NP-hard [Karp, 1972]
  - *graph clustering* is difficult even to define, many meaningful quality measures are NP-complete [Schaeffer, 2007]
- *real-world applications* of this type of problems
  - data mining [Sun et al., 2008] and web mining [Tang et al., 2011]
  - social network analysis [Chalupa, 2011a], social media marketing [Schaeffer, 2007]

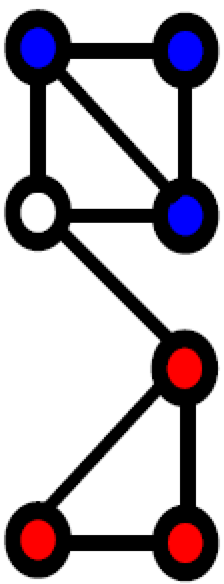
Motivation

- research citation network analysis [Sun et al., 2008]
- protein interaction in bioinformatics [Gao et al., 2009]
- gene-activation dependencies in bioinformatics [Boyer et al. 2005]
- analysis of terrorist organization networks [Patillo et al., 2012]
- infectious diseases epidemiology [Rothenberg et al., 1996]
- scheduling and timetabling [Burke et al., 2007]
- frequency assignment in mobile radio networks [Smith et al., 1998]
- and even more...

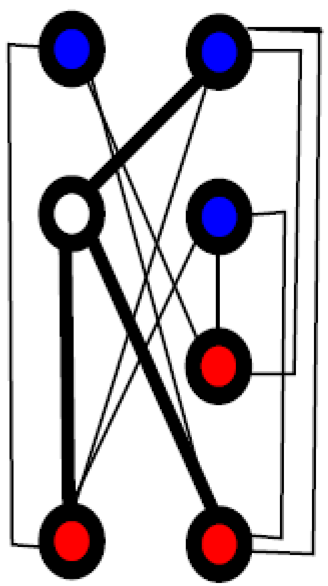
Clique Covering and Graph Coloring

- (vertex) clique covering problem (CCP)
  - „*inverse graph coloring*“
  - reduction from one problem to another [Karp, 1972]: let H = G‘ (complementary graph); then coloring of G‘ corresponds to clique covering of H and vice versa
  - *clique covering number*: $\vartheta(G)$, *chromatic number*: $\chi(G)$, $\vartheta(G) = \chi(G')$
  - coloring is *inapproximable* within $O(|V|^{1-\varepsilon})$ for any $\varepsilon > 0$ unless P = NP [Zuckerman, 2007]; the same holds probably also for the CCP
  - however, the problems are still *not the same*

Relationship Between Clique Covering and Coloring Problems



G

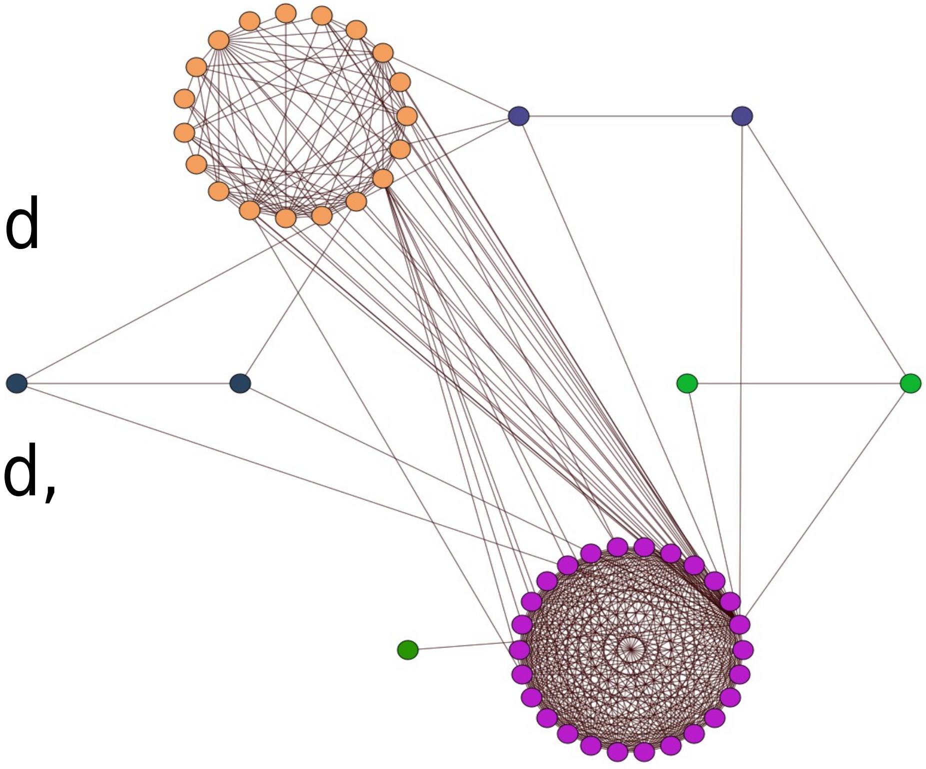


$\overline{G}$

- $\overline{G}$ – graph coloring
  - to choose a color, we have to scan the neighbors
  - we simply use a graph coloring heuristic on G
- G – clique covering
  - to choose a color, it is not enough to scan neighbors (without an additional information)

Graph Clustering

- a set of related decomposition problems
  - the aim is to decompose the graph into groups of "*similar*" vertices
  - "similarity" can be measured using *density*, *connectivity*, *centrality*, *distribution*, etc.
  - it is still not generally agreed, what is a *"good clustering"* [Schaeffer, 2007]



Concepts of Solving for Clique Covering and Graph Clustering

Concepts of Solving for Clique Covering and Graph Clustering

- clique covering (CCP)
  - *classical coloring heuristics* ([Brélaz, 1979]) - fast, quality strongly depends on the structure of the graph
  - *k-fixed local search and evolutionary algorithms* ([Galinier and Hao, 1999], [Titiloye and Crispin, 2011]) – solid quality of results, slow convergence, very inefficient if *k* is highly overestimated
  - *non-k-fixed stochastic algorithms* are less common ([Culberson and Luo, 1996])

Concepts of Solving for Clique Covering and Graph Clustering

- graph clustering
  - *hierarchical methods* ([Girvan and Newman, 2002]) – dendrogram-based, a popular metric is a betweenness of an edge
  - *centrality-based methods* ([Kaufman and Rouseeuw, 1990]) – typically *k-medoids*, using vertices as central points and optimizing their choice
  - *local search and evolutionary algorithms* ([Schaeffer, 2007])

Efficiency Issues

- analytical view
  - *classical techniques* of analysis and complexity
  - analytical techniques for *evolutionary algorithms*
- experimental view
  - *benchmarking* – quite a lot of data (DIMACS, network analysis benchmarks, real-world networks, etc.)
  - clique covering – easy evaluation and comparison, $\vartheta(G)$ is a particular number
  - graph clustering – not so straightforward, comparison to manually created solutions

Evaluation Techniques for Stochastic Graph Algorithms

- analytical techniques
  - a combination of *classical graph-theoretical approach* and *evolutionary algorithm analysis*
  - the choice of analytical method depends on the studied issue
- experimental techniques
  - optimality, success rate, statistical significance, etc.
  - *“When, we do not know, how to analyze...“*

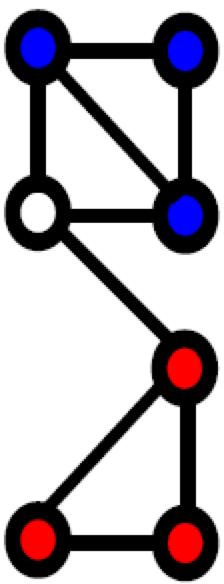
Analytical Techniques for Evolutionary Algorithms [Neumann and Witt, 2010]

- fitness-based landscape partitions
  - the search space is divided into *m* partitions, where the last one contains *only the optimum*
  - *probability of augmentation* – a lower bound on the probability that the algorithm jumps from partition *i* to *i+1* (p_i)
  - *waiting time* – the number of iterations, until the algorithm jumps to a higher partition (from geometric distribution, its expectation is $1/p_i$)
  - *expected time complexity* – the sum of waiting times, until partition *m* is reached

An Order-based Representation for CCP [Chalupa, 2012]

An Order-based Representation for CCP

- genotype-phenotype mapping based approach
  - greedy graph coloring [Welsh and Powell, 1967] can be used
  - the key issue is efficiency for real-world graphs
- $\overline{G}$ – graph coloring
  - to choose a color, we have to scan the neighbors
- G – clique covering
  - to choose a color, it is not enough to scan neighbors (without an additional information)



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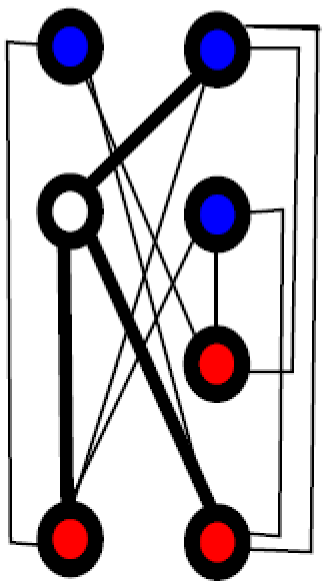


$\overline{G}$

Greedy Clique Covering (GCC)

Greedy Clique Covering

Input: graph $G = [V, E]$

permutation $P = [P_1, P_2, ..., P_{|V|}]$ of vertices in V

Output: clique covering S of G

for $c = 1..|V|$

  $sizes(c) = 0$

for $i = 1..|V|$

  $j = P_i$

  $c = find\_equal(\Gamma(v_j, c), sizes(c))$

  $V_c = V_c \cup \{v_j\}$

return $S = \{V_1, V_2, ..., V_k\}$

Optimality / Suboptimality Issues in GCC

- the basic issue in GCC – optimality
  - *Theorem:* For an arbitrary graph $G = [V,E]$, there is a permutation, for which the greedy clique covering will produce the optimal solution with $\vartheta(G)$ cliques.
  - *Proof:* Let $S = \{V_1, V_2, \ldots, V_{\vartheta(G)}\}$ be the optimal solution to the CCP. Then, the optimal permutation P can be constructed in the way that the vertices from the same classes are next to each other in P, i.e. $P = [V_{s1}, V_{s2}, \ldots, V_{s\vartheta(G)}]$, where $s_1, s_2, \ldots, s_{\vartheta(G)}$ is an arbitrary permutation of integers from 1 to $\vartheta(G)$. Since vertices of each of the subpermutations form the correct cliques, this permutation will surely lead to the optimal clique covering. QED.

Efficiency Issues in GCC

- GCC
  - computational complexity $O(|E(G)|)$
  - space complexity $O(|V|)$
- greedy graph coloring
  - computational complexity $O(|E(G')|)$
  - space complexity $O(|V|^2)$
- GCC is more efficient for sparse graphs
  - with current implementation techniques, GCC is faster than greedy coloring for graphs with density less than ca. *4/21*

Stochastic Order-based Approach to CCP: Iterated Greedy (IG) Algorithm

Block-based Mutation

- block-based properties of the representation
  - the identified cliques represent blocks of the solution
  - by reordering but (internally) preserving these blocks, the solution can be equally good or even superior to the previous one, similarly to the coloring problem [Culberson and Luo, 1996]
  - thus, although IG reminds one of random optimization, the fitness behaves similarly to local search
- reorderings of permutations
  - random order, reverse order

Iterated Greedy Algorithm with GCC

The IG heuristic for the CCP

Input: graph $G = [V, E]$
Output: clique covering S of G

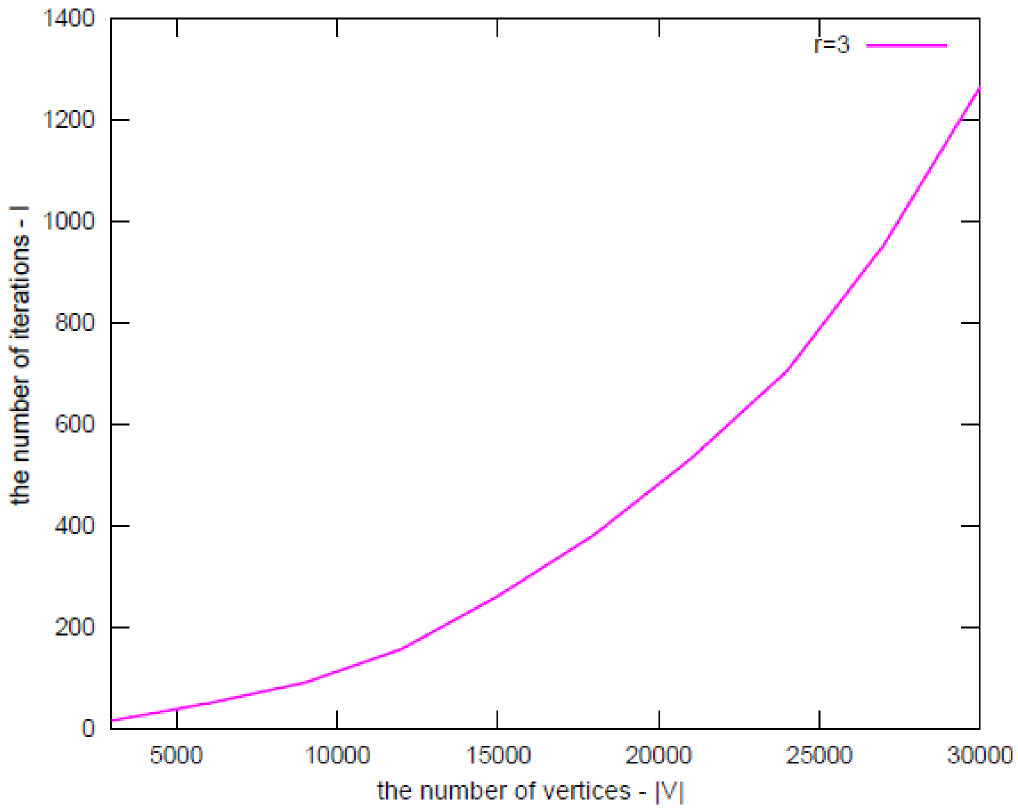
$P = random\_permutation(1, 2, ..., |V|)$
for $i = 1..I_{max}$
    $\{V_1, V_2, ..., V_k\} = greedy\_clique\_covering(G, P)$
    if $\vartheta^*(G)$ is known and $k = \vartheta^*(G)$
        return $S = \{V_1, V_2, ..., V_k\}$
    with p_{rev} probability
        $P = [V_k, V_{k-1}, ..., V_1]$
    else
        $P = random\_permutation(V_1, V_2, ..., V_k)$
return $S = \{V_1, V_2, ..., V_k\}$

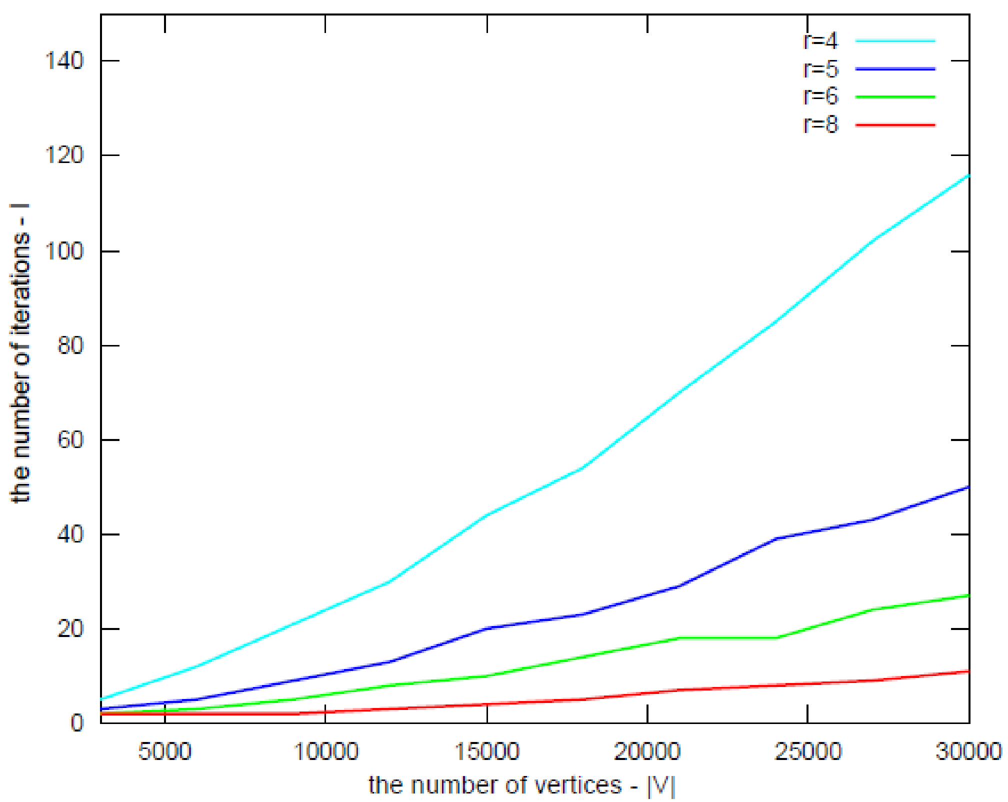
IG on Graphs with Planted Cliques

- a simple model of “clustered“ graphs
  - $\vartheta(G)$ embedded cliques of constant size r
  - probability p_{out} of generating an edge between two cliques
  - complements of k-colorable graphs in the coloring problem [Culberson and Luo, 1996]
- the key questions
  - How hard is it to find the right solution with $\vartheta(G)$ cliques?
  - How much time does IG need to find them?

Running time of IG on Sparse Graphs with Planted Cliques

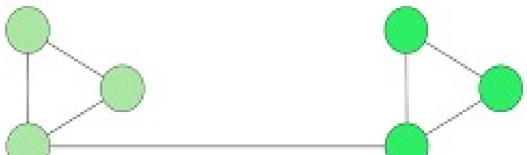
- empirical study of the performance of IG
  - $|V| = 3000 \Leftrightarrow 30000$, $r = 3 \Leftrightarrow 8$, $p_{out} = 10^{-3}$
  - p_{out} is small ➔ results indicate polynomial performance

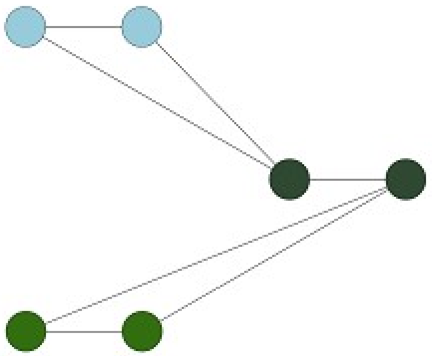


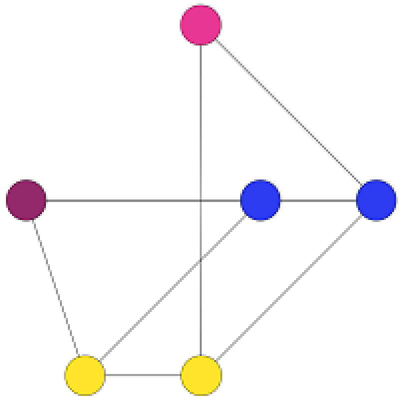


Analytical View on the Behavior of IG on Graphs with Planted Cliques

- overestimation by GCC
  - suppose that we re-represent the permutation $[v_1, v_2, \ldots, v_{|V|}]$ as $[[v_1, v_2], [v_2, v_3], \ldots, [v_{|V|-1}, v_{|V|}]]$
  - there are two ways, how GCC overestimates
    1. an inter-clique edge between two cliques precedes all intra-clique edges from the cliques it connects
    2. an inter-clique couple $[v_i, v_{i+1}]$ without an edge precedes a vertex adjacent to both v_i and v_{i+1}, which is in the same clique as v_{i+1}, but the First Fit strategy will falsely put in the same clique as v_i







Analytical View on the Behavior of IG on Graphs with Planted Cliques

- overestimation in sparse biclique graphs
  - complements of bipartite graphs
  - *Theorem:* Let G = [V,E] be a graph with planted cliques for $\vartheta = |V|/r = 2$ and $|E|_{out} < r$. Then, for each clique covering generated by GCC, a random reordering of its cliques will lead to the optimum with probability at least $1/[|V|/r+r-1]$.
  - *Proof:* By induction from small cases, evaluated exhaustively. An important implication of the property that $|E|_{out} < r$ is that there is a clique inside one of the expected ones.
  - *Consequence*: On these graphs, IG finds optimal clique covering in $O(|V|^3)$ time.

Analytical View on the Behavior of IG on Graphs with Planted Cliques

- generalization of the previous result
  - *Theorem:* Let $G = [V,E]$ be a graph with planted cliques $K_{r,1}, K_{r,2}, \ldots, K_{r,|V|/r}$. Suppose that $S_i = \{V_{1,i}, V_{2,i}, \ldots, V_{ki,i}\}$ is the current clique covering at the *i*-th iteration of IG. Furthermore, suppose that at each iteration *i*, there are *j* and *m*, such that there is a clique $G(V_{ki,j}) \in S_i$, which is a subgraph of some expected clique $K_{r,m}$ ($G(V_{ki,j}) \neq K_{r,m}$). Then, IG with GCC and random reorderings will converge to the optimal solution in $O(|V|^4)$ time.
  - *Proof:* A sketch: At each iteration, there is a clique $G(V_{ki,j})$ that is a subgraph of some of the expected cliques. This implies an $O(|V|)$ waiting time for an augmentation. The structure of the graph also implies that the number of fitness levels is $O(|V|)$. Overall, this implies an $O(|V|^4)$ upper bound.

Experimental Evaluation

- three algorithms
  - BRE - Brélaz's coloring heuristic
  - SAT-GCC – saturation-based GCC (permutation is determined greedily)
  - IG-GCC – iterated greedy with GCC (permutation is evolved)
  - best results are highlighted with bold

G	BRE	SAT-GCC	IG-GCC
Erdős-Rényi uniform random graphs			
$unif1000\_0.1$	299	310	**243**
$unif5000\_0.1$	1241	1288	**1066**
$unif10000\_0.1$	2326	2389	**2025**
$unif20000\_0.01$	7640	7817	**6387**
Leighton graphs from DIMACS instances.			
$le450\_15a$	85	89	**80**
$le450\_15b$	92	90	**82**
$le450\_15c$	68	74	**57**
$le450\_15d$	73	73	**57**
$le450\_25a$	**91**	92	**91**
$le450\_25b$	81	82	**80**
$le450\_25c$	61	59	**54**
$le450\_25d$	60	59	**51**
Social graphs			
$soc2000$	**1471**	1473	**1471**
$soc10000$	6619	6633	**6618**
$soc20000$	12770	12804	**12764**

Current Research

- analysis of order-based algorithms
  - IG – it seems that on one hand, IG is very efficient for graphs with planted cliques, as well as real world data
  - however, there are graphs, where IG performs really badly
  - RLS – another interesting algorithm, using vertex-based mutations, instead of block-based
  - seems more robust but not so efficient in practice

Multicriteria Construction Procedures (MCPs) for Graph Clustering [Chalupa and Pospíchal, 2012]

Multicriteria Construction Procedures

- constructive algorithms for graph clustering
  - a mapping of a permutation of vertices to a graph clustering

Algorithm 1: A General Framework for an MCP

A General Framework for an MCP

Input: graph $G = [V, E]$
permutation $P = [P_1, P_2, \ldots, P_{|V|}]$ of vertices
Output: a clustering S of G

for $i = 1..|V|$
    $j = P_i$
    $c = find\_cluster(v_j)$
    $V_c = V_c \cup \{v_j\}$
    $update\_auxiliary\_data(V_c)$
return $S = \{V_1, V_2, \ldots, V_k\}$

Criteria for Graph Clustering

1. Each vertex is clustered and the clusters are non overlapping.
2. The clusters are more dense than the whole graph:
   $\forall i = 1..k \; d(G(Vi)) > d(G)$, where d is the density.
3. The relative connectivity of a vertex to be newly added to the cluster must be higher than its relative connectivity to the residual, currently non-clustered subgraph:
   $w_c / |V_{c,i}| > \delta_r / [|V_r|-1]$
   where $V_{c,i}$ is the set of vertices in cluster c at the iteration i of the MCP,
   w_c is the number edges, brought into the cluster by the vertex to be newly added and
   $|V_r|$ and δ_r are the number of vertices and the degree of the newly added vertex in the subgraph containing only the currently non-clustered vertices.

Criteria for Graph Clustering

4. If there are more candidate clusters, the one with highest connectivity is taken:
$c = \arg_c \max w_c / |V_{c,i}|$
where for the cluster c, $w_c / |V_{c,i}|$ must be a feasible value, according to the previous rule.
5. The vertex to be newly added must bring at least as many edges, as is the current average intra-cluster degree in the particular cluster, while a small tolerance τ may be sometimes allowed:
$w_c + \tau \geq 2|E_{c,i}| / |V_{c,i}|$,
where $|E_{c,i}|$ is the number of edges in $G(V_{c,i})$.

Multicriteria Construction Procedure Based on Density and Connectivity (MCP-DC)

- MCP-DC implements the previous 5 criteria as follows
  - local density needed in criterion 2 is fulfilled if:
    $d(G)\,|V_{c,i}|\,(|V_{c,i}|+1) - 2|E_{c,i}| - 2w_c < 0$
  - the local connectivity in criterion 3 is fulfilled if the following holds:
    $|V_{c,i}| - w_c\,[|V_r| - 1] / \delta_r < 0$
  - the maximization of the connectivity in criterion 4, i.e. the ratio $w_c / |V_{c,i}|$, can be implemented simultaneously with criterion 3, since the necessary values are calculated in the verification of criterion 3
  - the criterion 5 yields the following condition, where $\tau \geq 0$ is a parameter of tolerance for the intra-cluster degree of the newly added vertex:
    $2|E_{c,i}| / |V_{c,i}| - \tau - w_c \leq 0$

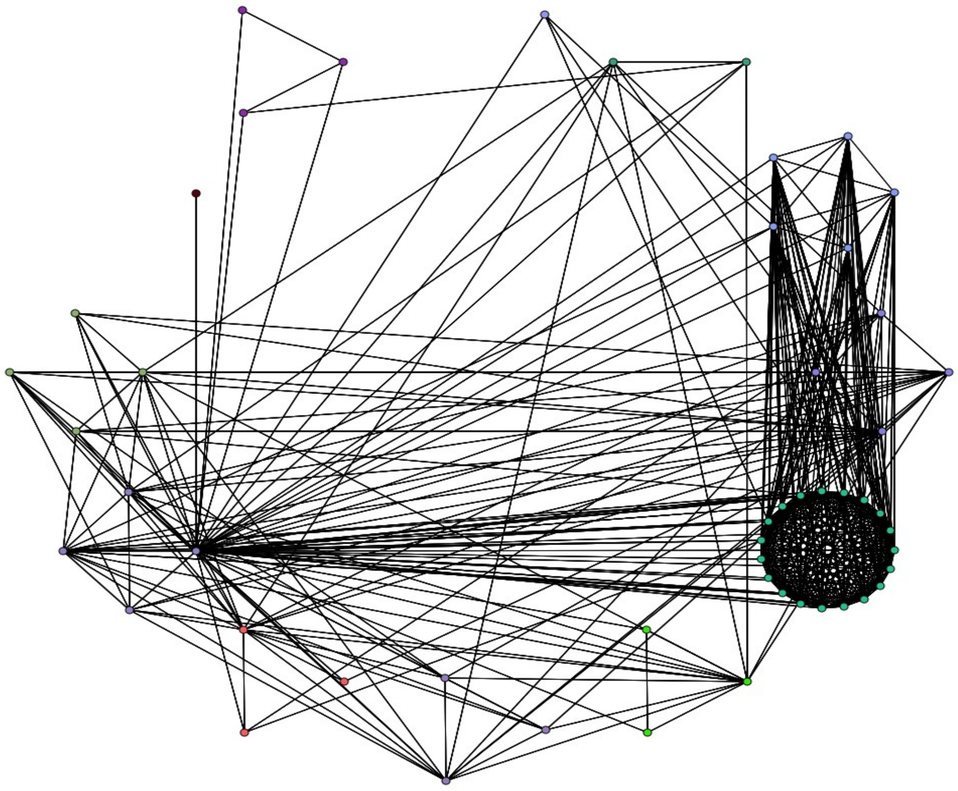
Multicriteria Construction Procedure Based on Density and Connectivity (MCP-DC)

- the advantage of this implementation of criteria in MCP-DC is that the complexity is favorable for sparse graphs
- *Theorem.* MCP-DC can be implemented to run in $O(\delta|V|) = O(|E|)$ time.
- *Proof.* $|V_{c,i}|$ and $|E_{c,i}|$ can be trivially recalculated in *O(1)* time per iteration. The previous formulations of the MCP-DC criteria can be implemented by iterative subtracting of a constant (in the cases of criteria 2 and 5) or the ratio $[|V_r| - 1] / \delta_r$ (in the case of criterion 3) from the respective values. Explicit storage of values w_c yields the same for criterion 4. Restoration of the former values after subtraction can be done by simulating the inverse process. All these operations need $O(\delta)$ average time per iteration, thus, they lead to an $O(\delta|V|) = O(|E|)$ running time of MCP-DC. QED.

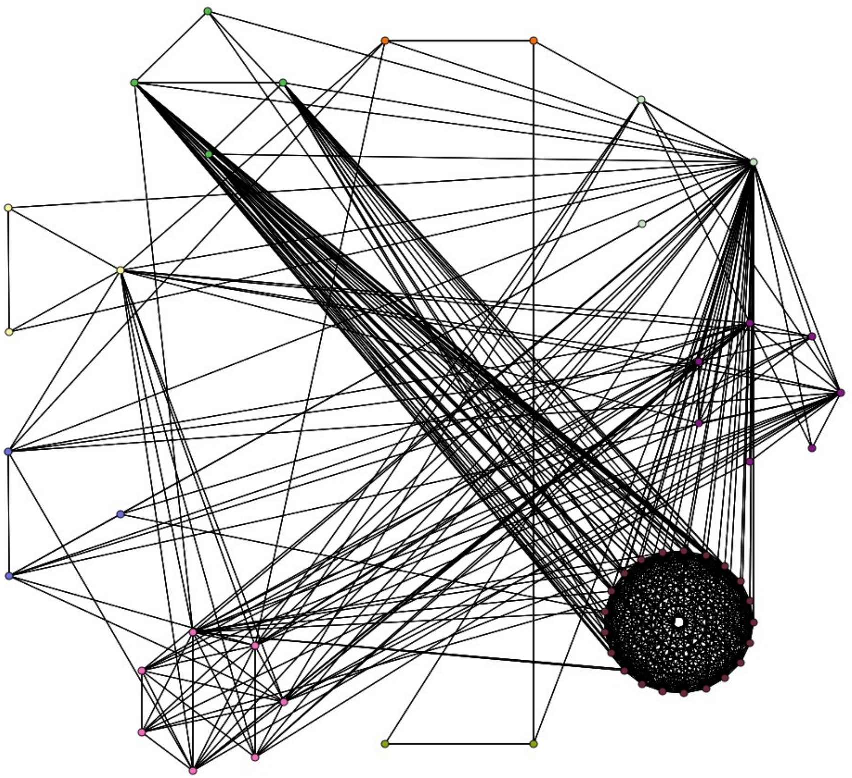
Metaheuristic Optimization for MCPs

- a simple local search algorithm
  - we begin with a random permutation of vertices and use an MCP to construct a clustering
  - *mutation:* at each iteration, we try a single random vertex exchange in the permutation and evaluate the new number of clusters using the MCP
  - *acceptance of mutation:* we accept if the new clustering has *at most as many clusters* as the current one
  - *stopping criterion:* maximum of s_{max} iterations without improvement

The Emergence of a Good Clustering

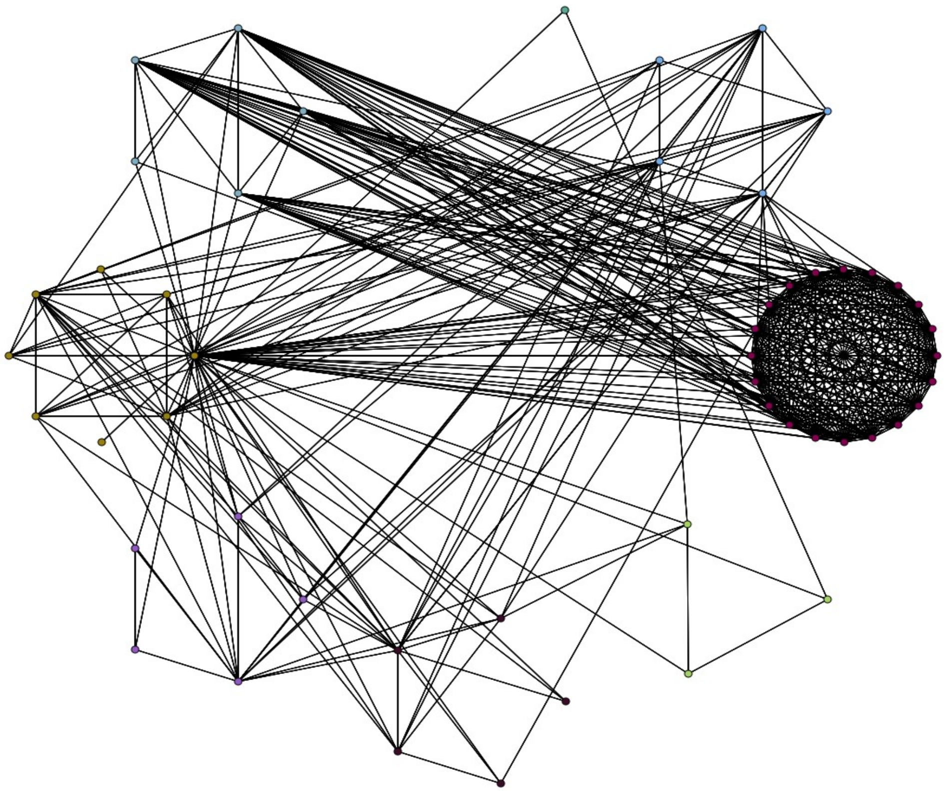


0 iterations

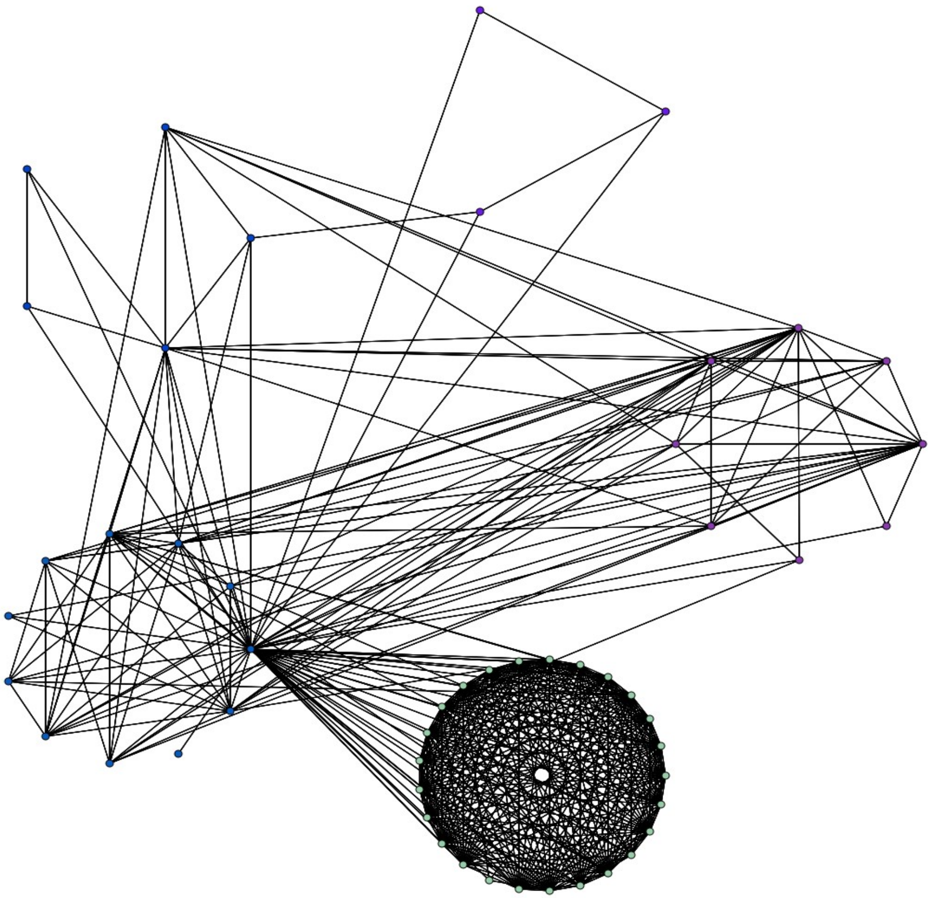


100 iterations

The Emergence of a Good Clustering



1000 iterations



10000 iterations

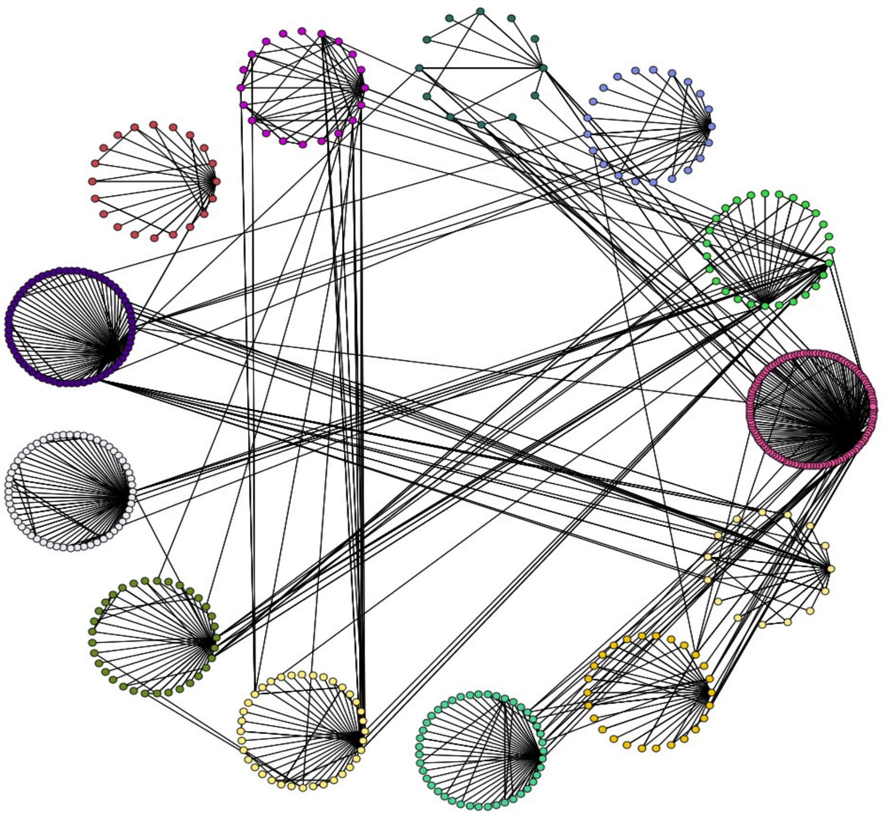
Results on Benchmark Instances

- a comparison of pure MCP-DC and MCP-DC with the metaheuristic on several graphs
  - network clustering benchmarks: *Zachary karate club* [Zachary, 1977] and *American college football network* [Girvan and Newman, 2002]
  - extracts of two different social networks
  - an artificial model from [Chalupa, 2011a]

source	$\|V\|,\|E\|$	s_{max}	τ	MCP-DC	MCP-DC+MH		
				k	k	iter.	time
Zachary karate club	$34,78$	5×10^3	1	7 - 15	2	7035	<1 s
American college football	$115,615$	10^6	0	18 - 23	10 - 12	1237965	252 s
Social network I	$52,830$	5×10^4	0	12 - 16	5 - 6	76194	9 s
Social network II	$500,924$	5×10^4	1	161 - 197	12 - 15	154964	71 s
Artificial model	$500,3536$	5×10^4	0	68 - 79	55 - 60	163449	188 s

Other Results

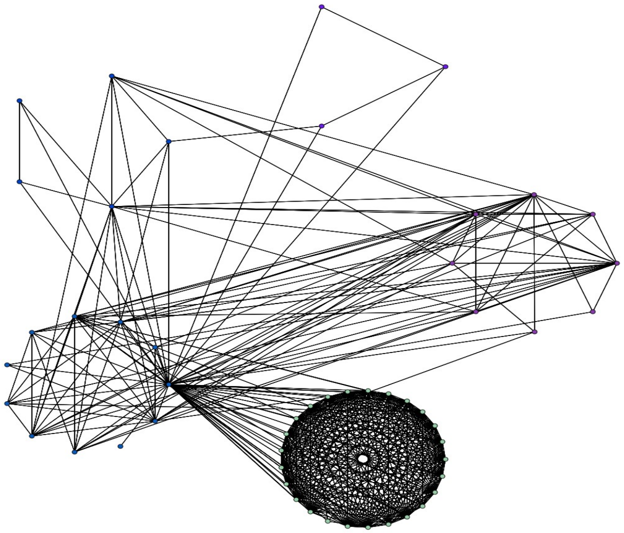
- a clustering of data obtained from a Slovak social network
  - shows a clear presence of hubs – in MCP, we preferred a centrality-based strategy



Conclusions

Conclusions

- introduction to stochastic graph algorithms
  - problems: clique covering, graph clustering
  - strategies, methodologies of evaluation
- an order-based representation for CCP
  - interesting analytical results and promising on real-world networks
- multicriteria construction procedures (MCPs) for graph clustering
  - show promise in both clustering and determining the nature of clustering problem formulation



Thank you for your attention!

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