Evaluation of separation routines for some classes of inequalities of the Clique Partitioning polytope Colloquium "Großer Beleg"

Maximilian Moeller

21.11.2023



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Agenda

- 1. Introduction to Clique Partitioning
- 2. Separating Inequalities
- 3. Data
- 4. Empirical Results
- 5. Conclusion



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└-Agenda

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- . Introduction to Clique Partitioni
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 Separating Inequalities
- Empirical Resu
 Conclusion

Introduction



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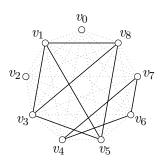
Evaluation of separation routines for some classes of inequalities of the Clique Partitioning polytope

Evaluation of separation routines for some classes of inequalities of the Clique Partitioning polytope \sqsubseteq Introduction

Introduction

Clique Partitioning

- clustering based on pairwise similarities
- framework for aggregation of binary relations
- useful in biology, medicine





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Evaluation of separation routines for some classes of inequalities of the Clique Partitioning polytope -Introduction



Clique Partitioning

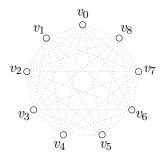
- 1. biology: taxonomy of animals (e.g., whales and dolphins)
- 2. medicine: clustering of organoids in light microscopy images
- 3. probably also operations research

Clique Partitioning

Definition

Given a graph G = (V, E), a subset of edges $A \subseteq E$ is called a clique partitioning of G if there exists a partition $\Gamma = \{ W_1, W_2, \dots, W_k \} \text{ of } V$ such that

$$A = \bigcup_{i=1}^{k} \{(u, v) \in E \mid u, v \in W_i\}.$$





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Clique Partitioning



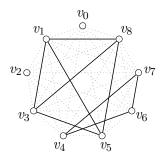
- 1. show which partition is induced
- 2. typically only complete graphs considered (indicates for every pair of nodes)
- 3. then one-to-one corresponds to an equivalence relation
- 4. induces complete subgraphs clique partitioning

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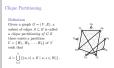


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-Clique Partitioning



- 1. show which partition is induced
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Input: complete graph $K_n = (V_n, E_n)$ and edge costs $w \in \mathbb{R}^{E_n}$

Compute: a clique partitioning of minimum weight

$$\min \qquad \sum_{e \in E_n} w_e x_e$$

 $\forall e \in E_n : x_e \in \{0, 1\}$ s.t. x characterizes a clique partitioning



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The Clique Partitioning Problem

sut: complete graph $K_n = (V_n, E_n)$ and edge costs $w \in \mathbb{R}^{K_n}$

- 1. characterize clique partitionings by binary vectors
- 2. 1 means it is in the clique partitioning and 0 means it is not in it
- 3. exactly opposite to multicut (equivalent problem)

NP-complete

 $\begin{array}{c} {\rm Introduction} \\ {\rm 0000}{\bullet}{\rm 00} \end{array}$



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The Clique Partitioning Problem

The Clique Partitioning Problem

- 1. blue drawn are edges with negative weights, all others non-negative
- 2. interesting instances need to have 'conflicts'

- NP-complete
- Trivial cases:



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The Clique Partitioning Problem

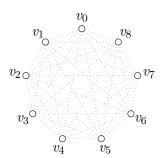
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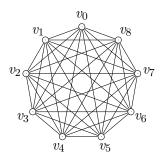
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 - w ≤ 0





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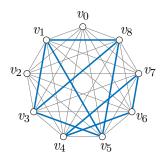
—Introduction

The Clique Partitioning Problem $\begin{array}{c} \bullet \text{ NP-samplete} \\ \bullet \text{ NP-samplete} \\ \bullet \text{ Tr} \\ \bullet \circ \circ \circ \\ \bullet \circ \circ \circ \circ \end{array}$

The Clique Partitioning Problem

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- NP-complete
- Trivial cases:
 - w > 0
 - w ≤ 0
 - w induces cliques





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The Clique Partitioning Problem

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An ILP-formulation of Clique Partitioning

characteristic vectors x



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An ILP-formulation of Clique Partitioning characteristic vectors x

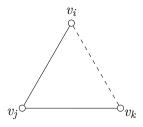
—An ILP-formulation of Clique Partitioning

- 1. we want to make use of (I)LP techniques: linear inequalities
- 2. explain support graph: left hand side can be drawn as graph, dotted negative, solid positive
- 3. triangle inequalities ensure transitivity
- 4. for the same i, j, k there are actually three triangles (show)

An ILP-formulation of Clique Partitioning

characteristic vectors x need to satisfy triangle inequalities $(i, j, k \in V_n, \text{ pairwise distinct})$

$$x_{ij} + x_{jk} - x_{ik} \le 1$$





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An ILP-formulation of Clique Partitioning characteristic vectors x need to satisfy triangle $(i, j, k \in V_a$, pairwise distinct)



An ILP-formulation of Clique Partitioning

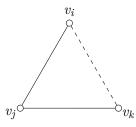
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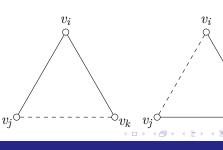
An ILP-formulation of Clique Partitioning

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 $x_{ij} - x_{jk} + x_{ik} \le 1$
 $-x_{ij} + x_{jk} + x_{ik} \le 1$





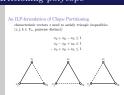
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Introduction

An ILP-formulation of Clique Partitioning



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Introduction



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_Introduction

The Tas

└─The Task

- 1. original task: branch-and-cut algorithm, i.e., solving the ILP
- 2. consists of multiple parts: **cutting planes for bounds**, finding good solutions and branch management
- 3. explain overall iteration procedure
- 4. even if not integral, a few percent off might be good for practical use
- 5. however, no guarantee to arrive at integral or within a constant factor

focus on cutting plane procedure:

• solve LP relaxation of the problem



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—Introduction

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- hopefully arrive at integral solution



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focus on cutting plane procedure:

- solve LP relaxation of the problem
- tighten the solution iteratively
- hopefully arrive at integral solution
- ???
- profit



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L—The Task

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focus on cutting plane procedure:

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Evaluation of separation routines for some classes of inequalities of the Clique Partitioning polytope

Evaluation of separation routines for some classes of inequalities of the Clique Partitioning polytope Separating Inequalities

• classes of facet-defining linear inequalities



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Evaluation of separation routines for some classes of inequalities of the Clique Partitioning polytope

—Separating Inequalities

Ingredients

└─Ingredients

- 1. explain: what is separation (check (and produce))
- 2. explain: facet-defining

Ingredients

- classes of facet-defining linear inequalities
- algorithms for separating them



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- classes of facet-defining linear inequalities
- algorithms for separating them
- data to test on (next section)



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classes of facet-defining linear inequalities
 algorithms for separating them
 data to test on (next section)

- 1. explain: what is separation (check (and produce))
- 2. explain: facet-defining

Triangle Inequalities (Δ)

Using complete enumeration $\mathcal{O}(n^3)$

Four variations



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—Separating Inequalities

Triangle Inequalities (Δ)

Using complete enumeration $O(n^2)$ Four variations

└─Triangle Inequalities (Δ)

- 1. Separation algorithms: separators
- 2. separators get abbreviations
- 3. maxcut is for limiting lp size
- 4. var_once is for solving the graph evenly

Triangle Inequalities (Δ)

Using complete enumeration $\mathcal{O}(n^3)$

Four variations

abbreviation	maxcut	var_once
Δ	400	_
Δ_{∞}	∞	_
Δ_{∞} $\Delta^{\leq 1}$	400	\checkmark
$\Delta_{\infty}^{\leq 1}$	∞	\checkmark



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—Separating Inequalities

separating inequalities

_Triangle Inequalities (Δ)



- 1. Separation algorithms: separators
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2-Partition Inequalities (st)

Let $S, T \subseteq V_n$ disjoint.

2-partition inequality ([S, T]-inequality)

$$\sum_{s \in S} \sum_{t \in T} x_{st} - \sum_{\substack{s,s' \in S \\ s \neq s'}} x_{ss'} - \sum_{\substack{t,t' \in T \\ t \neq t'}} x_{tt'} \le \min(|S|, |T|)$$



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—Separating Inequalities

2-Partition Inequalities (st)

Let S, T ⊆ V_a disjoint.

2-partition inequality ([S, T]-inequality)

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_2-Partition Inequalities (st)

1. Generalization of triangle inequalities

2-Partition Inequalities (st)

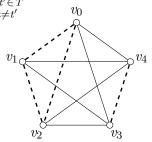
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2-partition inequality ([S, T]-inequality)

Separating Inequalities

$$\sum_{s \in S} \sum_{t \in T} x_{st} - \sum_{\substack{s,s' \in S \\ s \neq s'}} x_{ss'} - \sum_{\substack{t,t' \in T \\ t \neq t'}} x_{tt'} \le \min(|S|, |T|)$$

facet defining for $|S| \neq |T|$





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Evaluation of separation routines for some classes of inequalities of the Clique Partitioning polytope -Separating Inequalities

-2-Partition Inequalities (st)



1. Generalization of triangle inequalities

• already NP-hard for any fixed |S|



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—Separating Inequalities

Separation of 2-Partition Inequalities (s

already NP-hard for any fixed

Separation of 2-Partition Inequalities (st)

- 1. no use in using approximation if it is np-hard again
- 2. not explaining details, involve random choosing of an order of some nodes. Thus re-run three times.

Separation of 2-Partition Inequalities (st)

- already NP-hard for any fixed |S|
- using two heuristics: st¹ and st²



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—Separating Inequalities

Separation of 2-Partition Inequalities (st

- already NP-hard for any fixed |S|
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- 1. no use in using approximation if it is np-hard again
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Separation of 2-Partition Inequalities (st)

- already NP-hard for any fixed |S|
- using two heuristics: st¹ and st²
- only search for constraints with |S| = 1



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—Separating Inequalities

Separation of 2-Partition Inequalities (st)

- already NP-hard for any fixed |S|
 using two heuristics: gt¹ and gt²
 only search for constraints with |S| = 1
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Data



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Dat

Natural instances

- cetacea (30)
- cetacea (36)



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Natural instances

• cetacea (30)

• cetacea (35)

└─Natural instances

Natural instances

- cetacea (30)
- cetacea (36)
- football (115)
- adjnoun (112)
- polbooks (105)
- lesmis (77)
- dolphins (62)
- karate (34)



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- organoid_[size]_[difficulty] (160, 100, 80, 40)



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- organoid_[size]_[difficulty] (160, 100, 80, 40)

Random instances

• Binary r_binary_[size] size $\in \{25, 50\}$



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Data

• Binsey r_binary_[size] size $\in \{25,50\}$

Random instances

Random instances

- Binary r_binary_[size] $size \in \{25, 50\}$
- Uniform r_uniform_[size]_[lb]_[ub] $size \in \{25, 50\}$ $(lb, ub) \in \{(-10, 10), (-100, 100), (-10, 100)\}$



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Evaluation of separation routines for some classes of inequalities of the Clique Partitioning polytope -Data

-Random instances

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- Uniform r_uniform_[size]_[lb]_[ub] $size \in \{25, 50\}$ $(lb, ub) \in \{(-10, 10), (-100, 100), (-10, 100)\}$
- Normal r_normal_[size]_[mu]_[sigma] $size \in \{25, 50\}$ $(mu, sigma) \in \{0, 0.5, 2\} \times \{0.5, 1, 2\}$



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Empirical Results



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Empirical Results

Empirical Results

Conclusion



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Evaluation of separation routines for some classes of inequalities of the Clique Partitioning polytope \sqsubseteq Conclusion

Conclusion