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

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Agenda
Introduction
Separating Inequalities
Data
Empirical Results
Conclusion

Introduction

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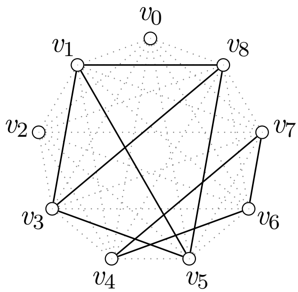
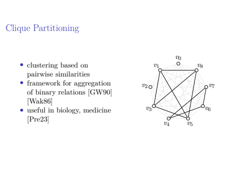
Evaluation of separation routines for some classes of inequalities of the Clique Partitioning polytope
└─Introduction

Introduction

Clique Partitioning

- clustering based on pairwise similarities
- framework for aggregation of binary relations [GW90] [Wak86]
- useful in biology, medicine [Pre23]





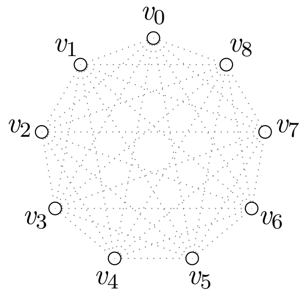
1. biology: taxonomy of animals (*e.g.*, whales and dolphins)
2. medicine: clustering of organoids in light microscopy images
3. probably also operations research

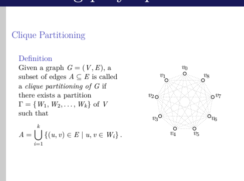
Clique Partitioning

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 $\Gamma = \{W_1, W_2, \ldots, W_k\}$ of V such that

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





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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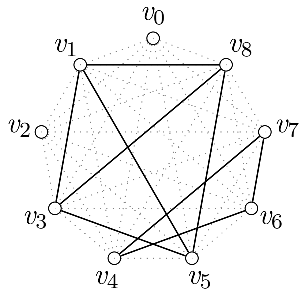

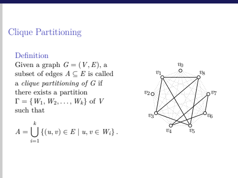
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The Clique Partitioning Problem

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

$$\begin{aligned} \min \quad & \sum_{e \in E_n} w_e x_e \\ \text{s.t.} \quad & \forall e \in E_n \colon x_e \in \{0,1\} \\ & x \text{ characterizes a clique partitioning} \end{aligned}$$

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

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)

The Clique Partitioning Problem

- NP-complete [Wak86]

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

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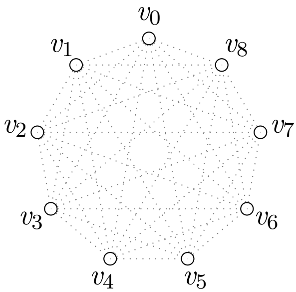

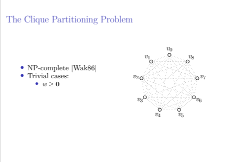

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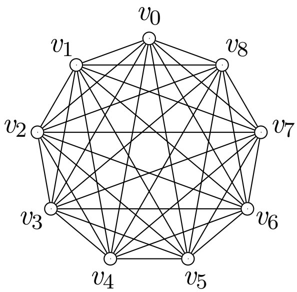

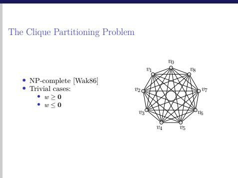

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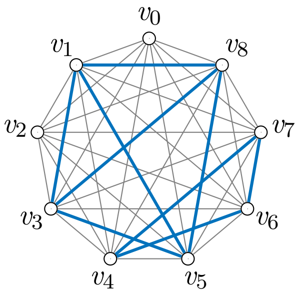
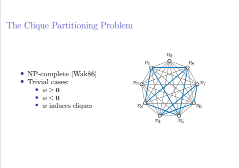
  - w induces cliques





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An ILP-formulation of Clique Partitioning

characteristic vectors x

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2. explain support graph: left hand side can be drawn as graph, dotted negative, solid positive
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4. for the same i, j, k there are actually three triangles (show)

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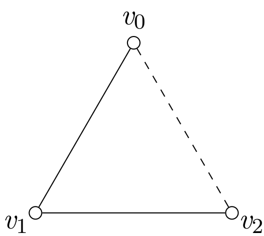
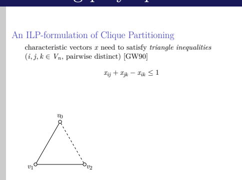
characteristic vectors x need to satisfy *triangle inequalities* ($i, j, k \in V_n$, pairwise distinct) [GW90]

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

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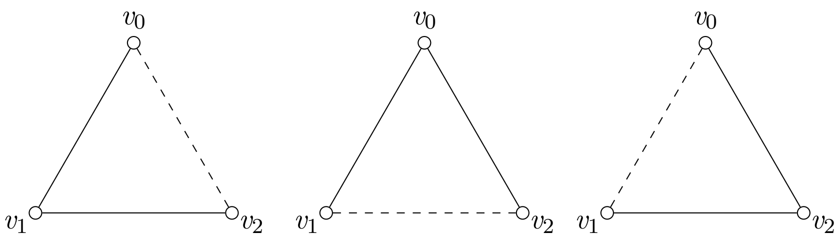
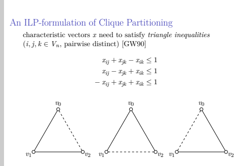
$$\begin{aligned} x_{ij} + x_{jk} - x_{ik} &\leq 1 \\ x_{ij} - x_{jk} + x_{ik} &\leq 1 \\ -x_{ij} + x_{jk} + x_{ik} &\leq 1 \end{aligned}$$





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The Task

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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

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Separating Inequalities

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└─Separating Inequalities

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

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abbreviation	`maxcut`	`var_once`
Δ	400	–
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2-Partition Inequalities

Let $S, T \subseteq V_n$ disjoint.

2-*partition inequality* ([S, T]-inequality) [GW90]

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

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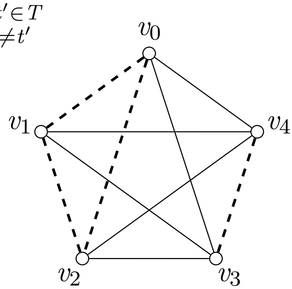
facet defining for $|S| \neq |T|$



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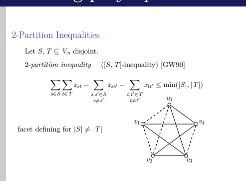

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Let $5 \leq k \leq n$ and $v : \mathbb{Z}_k \to \mathbb{Z}_n$ injective

two-chorded odd cycle inequality [GW90]

$$\sum_{i \in \mathbb{Z}_k} x_{v_i v_{i+1}} - x_{v_i v_{i+2}} \leq \left\lfloor \frac{1}{2} k \right\rfloor$$

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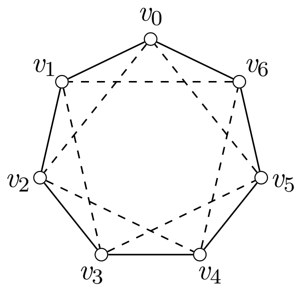
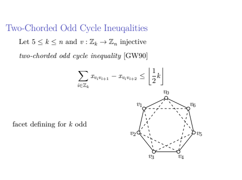
facet defining for k odd





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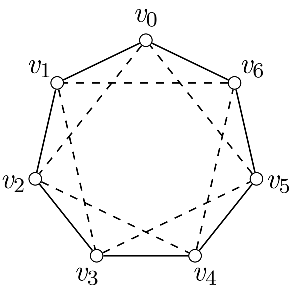
Separating Two-Chorded Odd Cycle Inequalities (`two`)



[Mül96]

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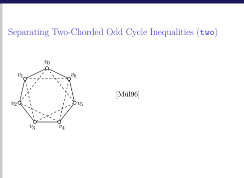

1. following an odd cycle and summing edges by +- 1 gives left hand side
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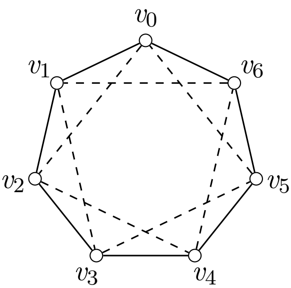

$$\overbrace{v_0\, v_1\, v_2\, v_3\, v_4\, v_5\, v_6\, v_0}^{\text{cycle}}\underbrace{v_2\, v_4\, v_6\, v_1\, v_3\, v_5\, v_0}_{\text{two-chords}}$$

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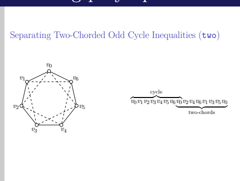

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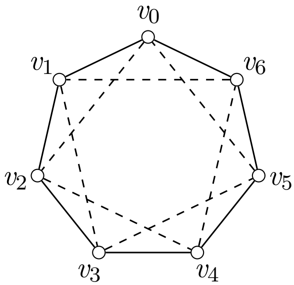


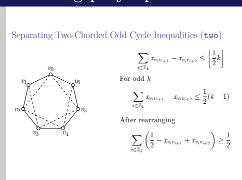
$$\sum_{i\in\mathbb{Z}_k} x_{v_iv_{i+1}} - x_{v_iv_{i+2}} \leq \left\lfloor \frac{1}{2}k \right\rfloor$$

For odd k

$$\sum_{i\in\mathbb{Z}_k} x_{v_iv_{i+1}} - x_{v_iv_{i+2}} \leq \frac{1}{2}(k-1)$$

After rearranging

$$\sum_{i\in\mathbb{Z}_k} \left(\frac{1}{2} - x_{v_iv_{i+1}} + x_{v_iv_{i+2}}\right) \geq \frac{1}{2}$$



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For every pair $(i, j) \in V_n^2$ with
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1. bipartide graph can distinguish between odd and even walks
2.

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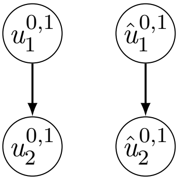
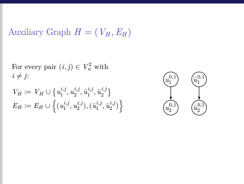
For every pair $(i, j) \in V_n^2$ with $i \neq j$:

$$V_H := V_H \cup \left\{ u_1^{i,j}, u_2^{i,j}, \hat{u}_1^{i,j}, \hat{u}_2^{i,j} \right\}$$

$$E_H := E_H \cup \left\{ (u_1^{i,j}, u_2^{i,j}), (\hat{u}_1^{i,j}, \hat{u}_2^{i,j}) \right\}$$





1. bipartide graph can distinguish between odd and even walks
2.

Auxiliary Graph $H = (V_H, E_H)$

For every triple $(i, j, k) \in V_n^3$
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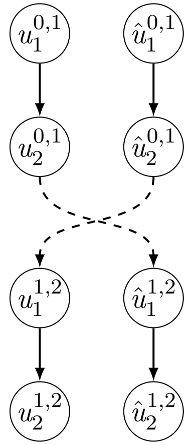
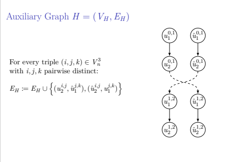


2023-11-21

Evaluation of separation routines for some classes of inequalities of the Clique Partitioning polytope
└─Separating Inequalities
└─Auxiliary Graph $H = (V_H, E_H)$



1. bipartide graph can distinguish between odd and even walks
2.

Weights for the auxiliary graph

$$\sum_{i \in \mathbb{Z}_k} \Bigg(\underbrace{\frac{1}{2} - x_{v_i v_{i+1}}}_{\text{inner-gadget weights}} + \underbrace{x_{v_i v_{i+2}}}_{\text{inter-gadget weights}} \Bigg) \geq \frac{1}{2}$$

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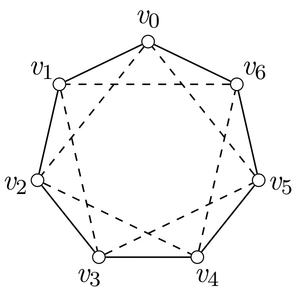
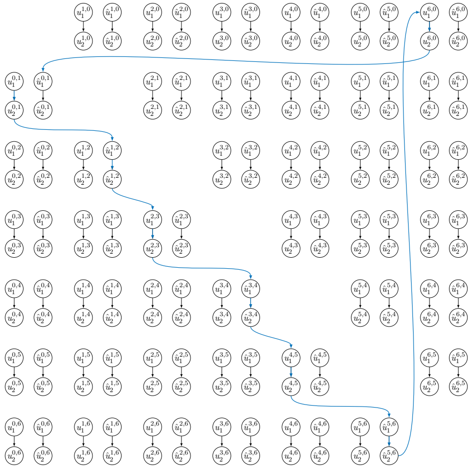
1. no negative cycles as long as triangle inequalities are satisfied! (müller)





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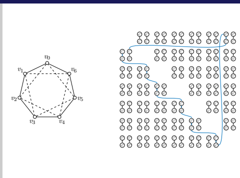

1. each violated odd-cycle inequality corresponds to a u,uhat walk (same gadget)

Dimensions of H

$$|V_H| = 4n(n-1) = 4n^2 - 4n$$

$$|E_H| = \underbrace{2n(n-1)}_{\text{inner-gadget edges}} + \underbrace{2n(n-1)(n-2)}_{\text{inter-gadget edges}} = 2n^3 - 4n^2 + 2n$$

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Half-Chorded Odd Cycle Ineuqalities

Let $5 \leq k \leq n$, let $d = \frac{k-1}{2}$ and $v : \mathbb{Z}_k \to \mathbb{Z}_n$ injective

half-chorded odd cycle inequality [And+22]

$$\sum_{i \in \mathbb{Z}_k} (x_{v_i v_{i+1}} - x_{v_i v_{i+d}}) \leq k - 3$$

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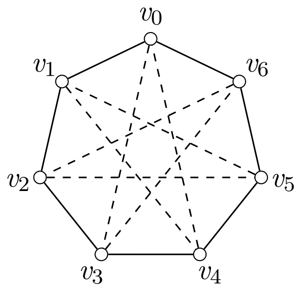
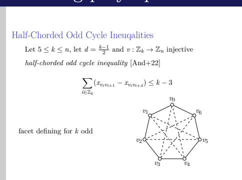
facet defining for k odd

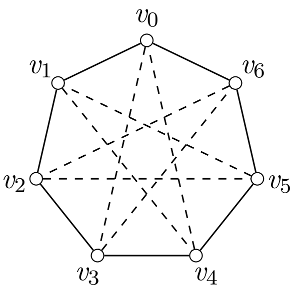


2023-11-21

Evaluation of separation routines for some classes of inequalities of the Clique Partitioning polytope
└─Separating Inequalities
└─Half-Chorded Odd Cycle Ineuqalities



Separating Half-Chorded Odd Cycle Ineuqalities (**half**)



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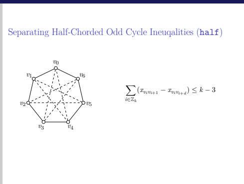

1. half-chords also form a cycle, solid edges are two-chords to that cycle -> relabeling
2. technique with auxiliary graph is exactly the same, except all weights are non-negative
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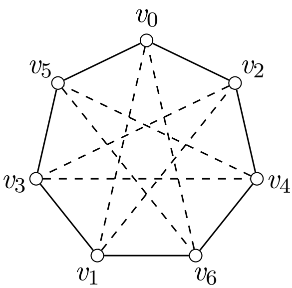

$$\sum_{i \in \mathbb{Z}_k} (x_{v_i v_{i+1}} - x_{v_i v_{i+d}}) \leq k - 3$$

After relabeling

$$\sum_{i \in \mathbb{Z}_k} (x_{v'_i v'_{i+2}} - x_{v'_i v'_{i+1}}) \leq k - 3$$

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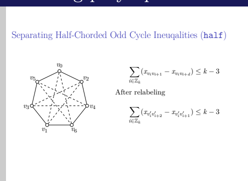
└─Separating Inequalities
└─Separating Half-Chorded Odd Cycle Ineqalities (half)



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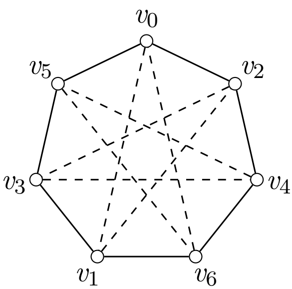

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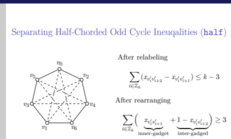
$$\sum_{i\in\mathbb{Z}_k} (x_{v'_i v'_{i+2}} - x_{v'_i v'_{i+1}}) \leq k-3$$

After rearranging

$$\sum_{i\in\mathbb{Z}_k} \Bigg(\underbrace{x_{v'_i v'_{i+1}}}_{\text{inner-gadget}} + \underbrace{1 - x_{v'_i v'_{i+2}}}_{\text{inter-gadged}} \Bigg) \geq 3$$



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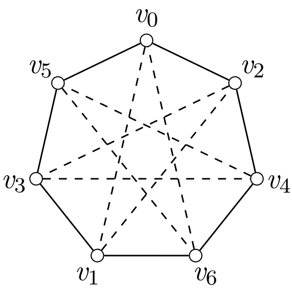

After rearranging

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Dijkstra's Algortihm:
$\mathcal{O}(|E_H| + |V_H| \cdot \log |V_H|) = \mathcal{O}(n^3)$,
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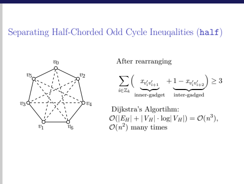

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Run Configurations

	Δ-st-1	Δ-st-2	Δ-st-12	Δ-½	Δ-2	Δ-c	all
1	Δ	Δ	Δ	Δ	Δ	Δ	Δ
2	st[1]	st[2]	st[1]	half	two	half	st[1]
3	—	—	st[2]	—	—	two	st[2]
4	—	—	—	—	—	—	half
5	—	—	—	—	—	—	two

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Evaluation of separation routines for some classes of inequalities of the Clique Partitioning polytope
└Separating Inequalities
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5	—	—	—	—	—	—	two

1. all use Δ first, because they implicitly rely on it
2. ordered them by (expected) run time

Data

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

Data

Natural instances

- `cetacea` (30) [GW89]
- `cats` (36)

Evaluation of separation routines for some classes of inequalities of the Clique Partitioning polytope
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  `size` $\in \{25, 50\}$

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- Normal `r_normal_[size]_[mu]_[sigma]`
  $\texttt{size} \in \{25, 50\}$
  $(\texttt{mu}, \texttt{sigma}) \in \{0, 0.5, 2\} \times \{0.5, 1, 2\}$

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Empirical Results

2023-11-21

Evaluation of separation routines for some classes of inequalities of the Clique Partitioning polytope
└─Empirical Results

Empirical Results

Relative Gap

Relative gap of solution z' to the optimal solution z

$$\mathrm{gap}(z, z') := \frac{|z - z'|}{|z|}$$

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Relative gap of solution z' to the optimal solution z

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1. case $z = 0$ can be ignored
2. only possible to compute when optimal value is known

Example: `adjnoun`

Table 6: Computational results for `adjnoun`

						Δ-st-1			Δ-st-2			Δ-st-12						all		
1		Δ	Δ_∞	$\Delta^{\leq 1}$	$\Delta^{\leq 1}_\infty$	1	2	3	1	2	3	1	2	3	Δ-½	Δ-2	Δ-c	1	2	3
2	# it.	122	**6**	204	45	10,000	10,000	10,000	10,000	10,000	10,000	10,000	10,000	10,000	1,038	1,320	1,200	10,000	10,000	10,000
3	# $\not\Delta$-calls	0	0	0	0	1067	1094	1095	622	613	614	1111	1098	1095	81	97	110	1117	1131	1083
4	cuts																			
5	# total	47,262	12,963	26,027	**8,003**	390,825	392,629	387,427	994,177	994,987	987,904	382,283	391,531	387,849	140,769	171,755	158,097	373,139	372,381	391,373
6	# max	400	8,362	186	500	400	400	400	400	400	400	400	400	400	400	400	400	400	400	400
7	# min	2	16	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
8	# $\not\Delta$-cuts	0	0	0	0	22,493	22,443	23,675	136,047	134,127	134,175	22,847	23,823	22,871	30,158	38,660	39,872	23,366	22,366	23,421
9	# removed	43,535	7,190	23,452	5,379	386,392	388,288	383,042	988,377	988,865	982,200	377,858	387,156	383,454	134,093	165,476	150,739	368,669	367,987	386,963
10	objective																			
11	bound	0.4275	0.4275	0.4275	0.4275	0.391	0.3904	0.3895	0.3865	**0.3863**	0.3866	0.3899	0.389	0.3903	0.398	0.3978	0.3978	0.3891	0.39	0.3893
12	gap	36.1%	36.1%	36.1%	36.1%	24.4%	24.3%	24.0%	23.0%	22.9%	23.0%	24.1%	23.8%	24.2%	26.7%	26.6%	26.6%	23.8%	24.1%	23.9%
13	time																			
14	total 1/s	4.846	**0.794**	5.822	4.210	652.918	657.831	640.986	1234.069	1249.390	1211.961	654.060	668.754	666.687	2322.078	3922.257	4303.249	650.074	623.255	657.059
15	normalized	1.00	**0.16**	1.20	0.87	134.73	135.75	132.27	254.66	257.82	250.10	134.97	138.00	137.57	479.17	809.38	888.00	134.15	128.61	135.59
16	lp time 1/s	4.701	**0.764**	5.566	4.042	618.769	623.890	606.817	1198.666	1213.964	1176.594	619.855	634.372	632.492	67.300	100.684	79.603	615.768	589.009	623.100

Example: adjnoun
Table 6: Computational results for adjnoun

Example: `organoid_160_hard`

Table 11: Computational results for `organoid_160_hard`

						`Δ-st-1`			`Δ-st-2`			`Δ-st-12`						`all`		
1		Δ	Δ_∞	$\Delta^{\leq 1}$	$\Delta^{\leq 1}_\infty$	1	2	3	1	2	3	1	2	3	`Δ-½`	`Δ-2`	`Δ-c`	1	2	3
2	# it.	3,712	**6**	10,000	20	4,060	4,152	3,929	4,000	4,186	4,030	4,037	3,990	3,917	3,712	3,712	3,712	4,081	3,928	3,922
3	# $\not\Delta$-calls	0	0	0	0	1	1	1	2	1	1	2	1	2	1	1	2	4	1	2
4	cuts																			
5	# total	1,482,621	131,841	1,729,012	**15,901**	1,621,281	1,657,361	1,568,785	1,592,542	1,669,574	1,608,612	1,609,391	1,591,066	1,562,088	1,482,621	1,482,621	1,482,621	1,626,670	1,568,107	1,563,353
6	# max	400	65,771	237	1,450	400	400	400	400	400	400	400	400	400	400	400	400	400	400	400
7	# min	16	4	53	21	6	6	6	1	3	6	2	5	3	16	16	16	2	6	5
8	# $\not\Delta$-cuts	0	0	0	0	6	6	6	24	6	6	30	5	9	0	0	0	17	6	15
9	# removed	1,476,839	55,589	1,723,930	10,233	1,615,450	1,652,117	1,563,129	1,586,880	1,663,428	1,602,578	1,602,759	1,584,994	1,556,817	1,476,839	1,476,839	1,476,839	1,619,226	1,561,818	1,558,062
10	objective																			
11	bound	135.5	135.5	136.3	135.5	**135.3**	**135.3**	**135.3**	**135.3**	**135.3**	**135.3**	**135.3**	**135.3**	**135.3**	135.5	135.5	135.5	**135.3**	**135.3**	**135.3**
12	gap	0.1%	0.1%	0.7%	0.1%	0.0%*	0.0%*	0.0%*	0.0%*	0.0%*	0.0%*	0.0%*	0.0%*	0.0%*	0.1%	0.1%	0.1%	0.0%*	0.0%*	0.0%*
13	time																			
14	total 1/s	286.655	140.807	599.619	**14.621**	305.721	309.898	300.815	302.782	311.934	305.005	305.710	302.744	300.734	846.531	1192.236	1752.368	307.655	301.564	300.637
15	normalized	1.00	0.49	2.09	**0.05**	1.07	1.08	1.05	1.06	1.09	1.06	1.07	1.06	1.05	2.95	4.16	6.11	1.07	1.05	1.05
16	lp time 1/s	280.912	140.651	586.847	**14.398**	299.461	303.465	294.748	296.512	305.446	298.737	299.366	296.552	294.604	281.039	281.239	281.777	301.282	295.407	294.493

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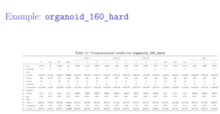
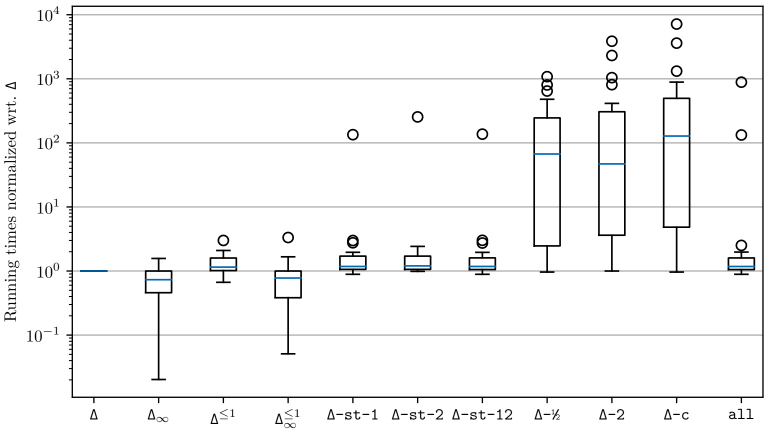
Evaluation of separation routines for some classes of inequalities of the Clique Partitioning polytope
└─Empirical Results
└─Example: `organoid_160_hard`



Run-Times on Natural Instances



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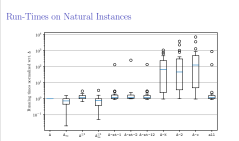
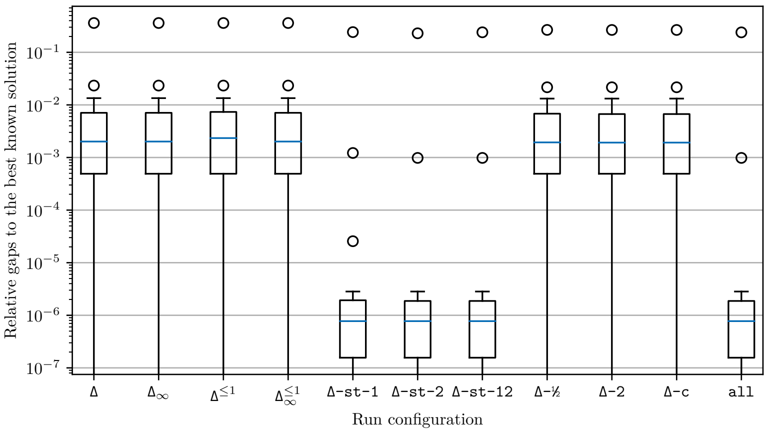
Evaluation of separation routines for some classes of inequalities of the Clique Partitioning polytope
└─Empirical Results
└─Run-Times on Natural Instances



1. Running time of run configurations on non-random instances.
2. For run configurations containing a `st`-separator the results were averaged per instance among the three runs.
3. All results are normalized with respect to the `Δ` run configuration (first column).
4. The ordinate is logarthmically scaled. Box plots are drawn in the standard way, *i.e.*, boxes are from Q_1 to Q_3, the blue mark highlights the median, and whiskers extend by $1.5 * \mathrm{IQR}$.
5. are cycles worth it?

Relative Gaps on Natural Instances



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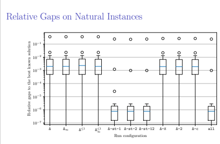
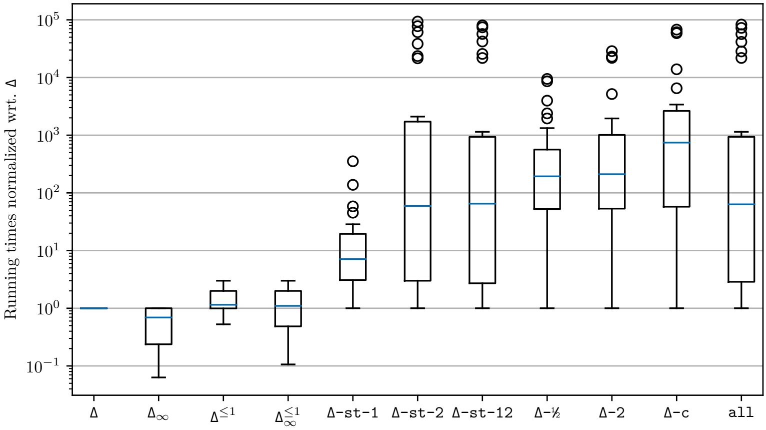
└─Empirical Results
└─Relative Gaps on Natural Instances



1. st-separators artifact of measuring integrality with tolerance parameter

Run-Times on Random Instances



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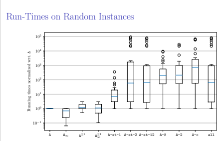
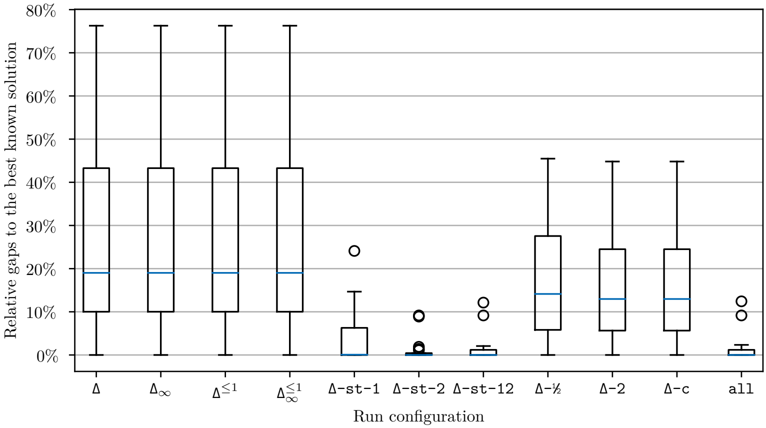
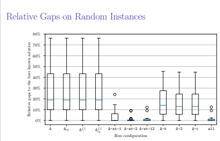
└Empirical Results
└Run-Times on Random Instances



Relative Gaps on Random Instances





1. axis is now linear!
2. explain underlying structure in natural instances to show why they are easier

Conclusion

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

Conclusion

Conclusion

- Δ and `st` often sufficient for integral solutions
- `two` and `half` run longer and do only improve bounds marginally

Conclusion

- Δ and st often sufficient for integral solutions
- two and half run longer and do only improve bounds marginally

1. Everything with a note: on the instances i tested
2. Personal: great fun, learned much
3. would not have started it if i knew how little i knew ((i)lp, optimization, c++), 10/10

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