

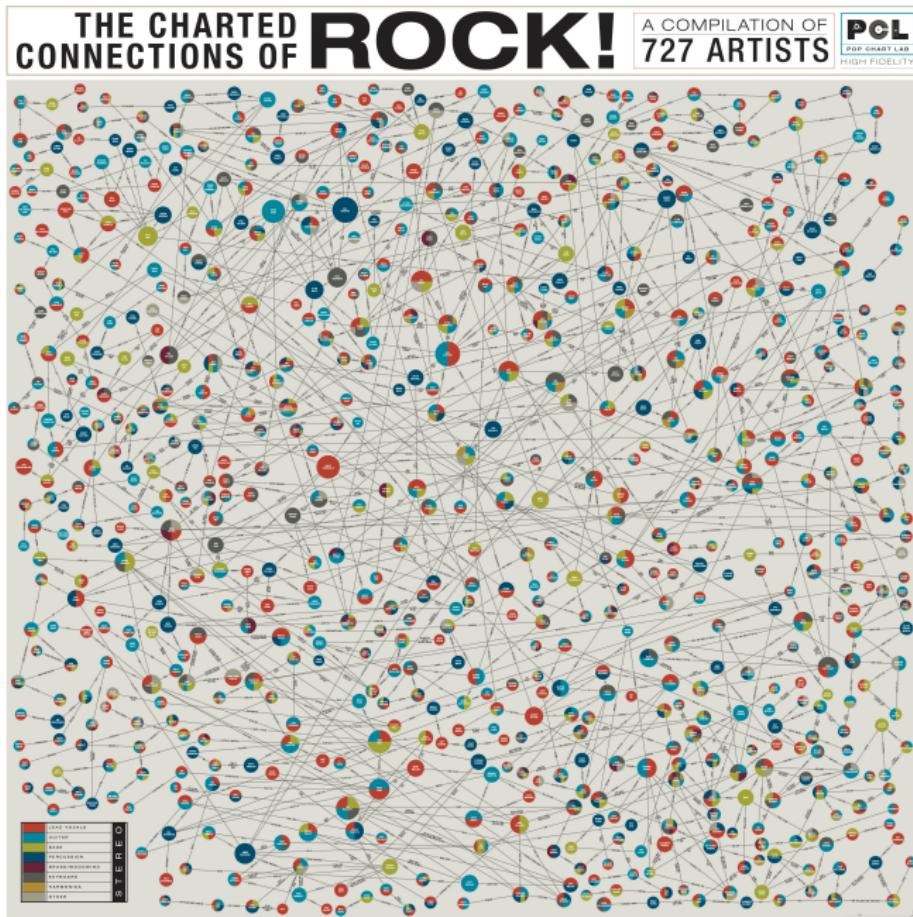
## Parsimonious formulations for low-diameter clusters

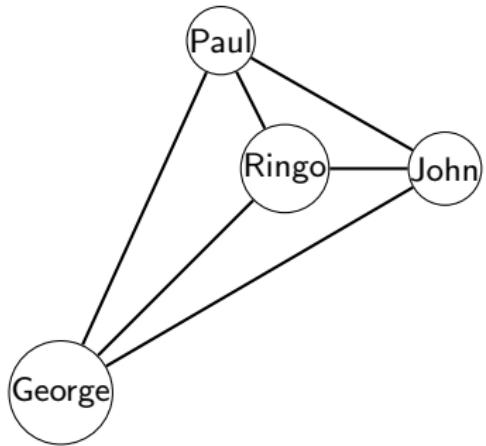
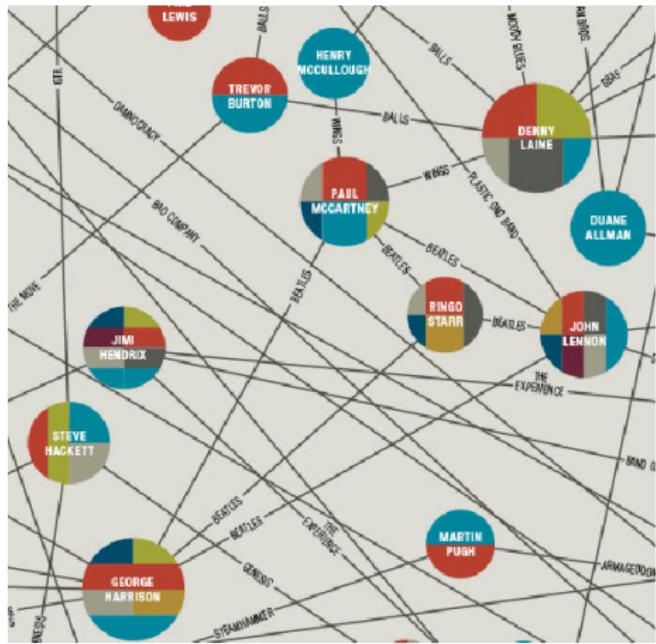
@AustinLBuchanan and @HASalemi

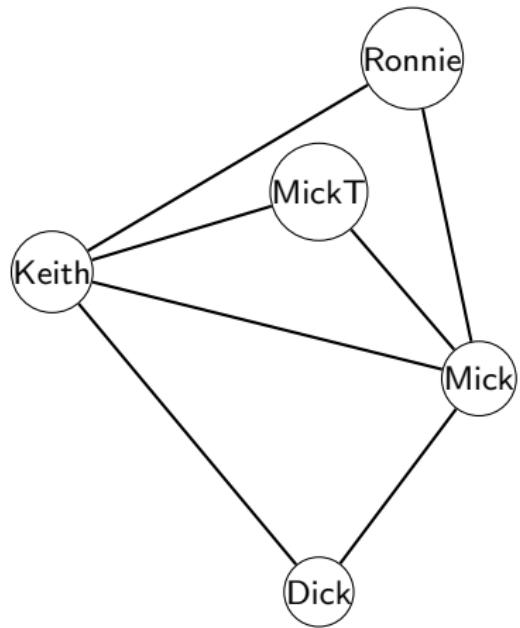
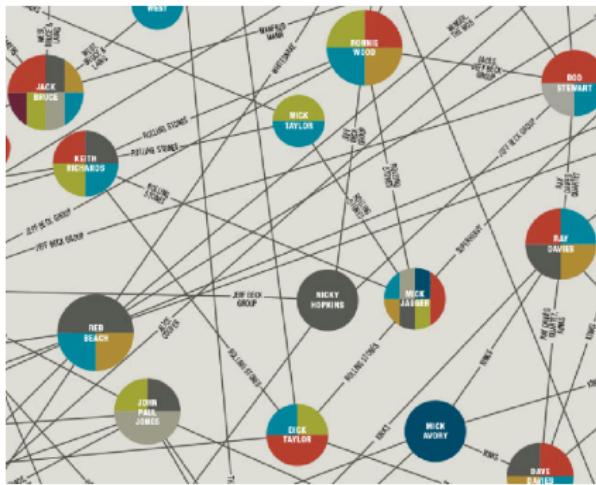
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The rock musician graph  $G = (V, E)$ .







## What is a $k$ -club?

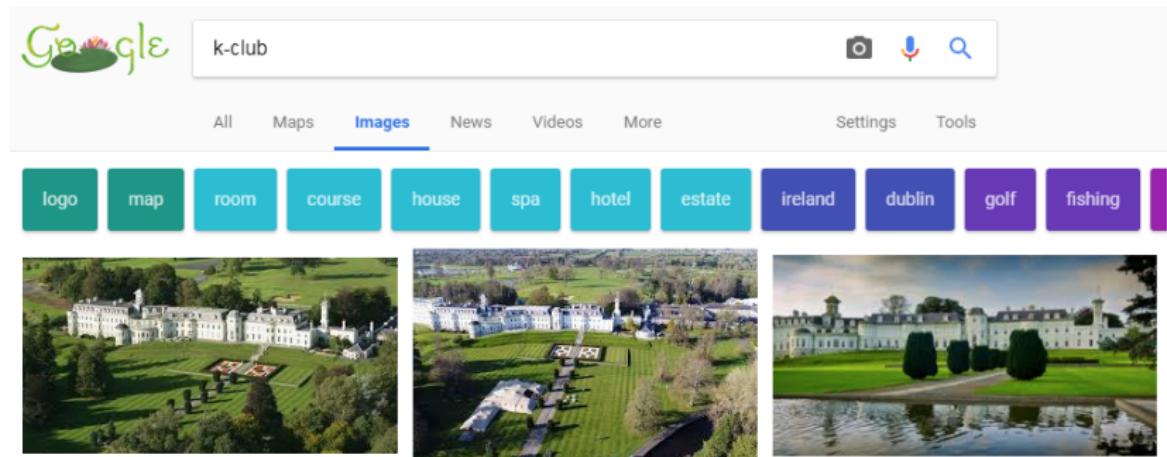
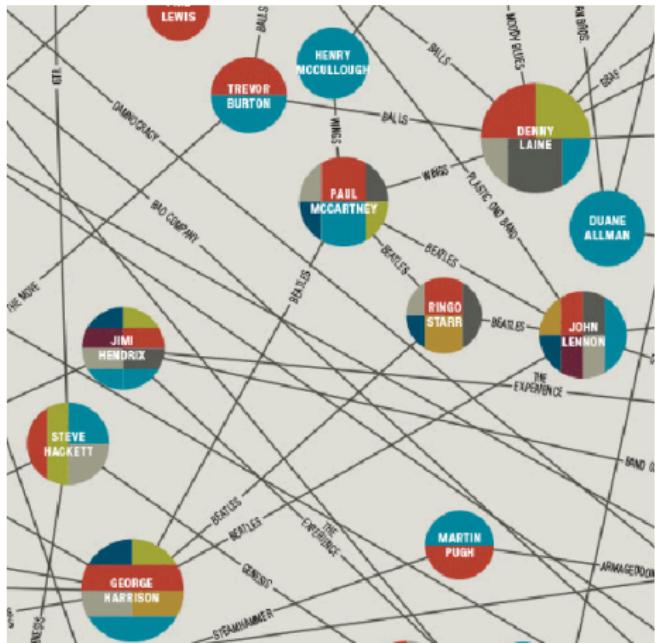


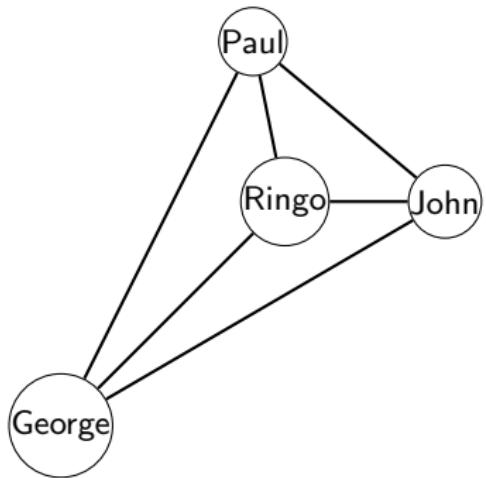
Figure: Did you mean “The K Club Hotel in Straffan, Ireland?”

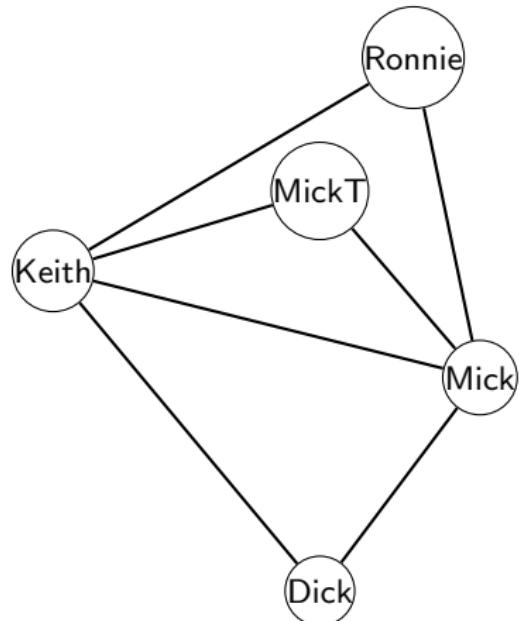
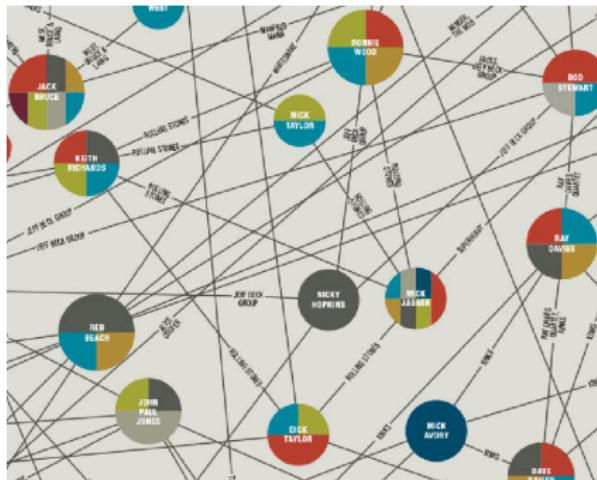
### Definition (Mokken, 1979)

A vertex subset  $S \subseteq V$  is a  $k$ -club in graph  $G = (V, E)$  if  $\text{diam}(G[S]) \leq k$ .



Example 1-club  
THE BEATLES

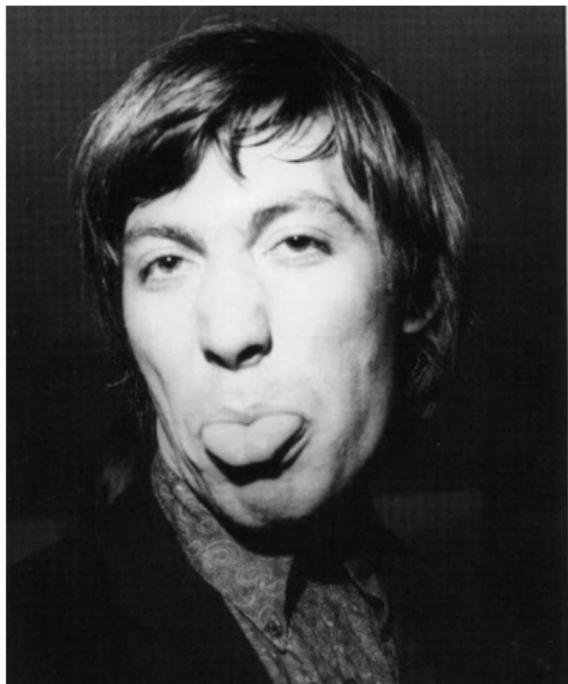




Example 2-club



"You included Ringo, but not me?"



Low-diameter constraints appear in:

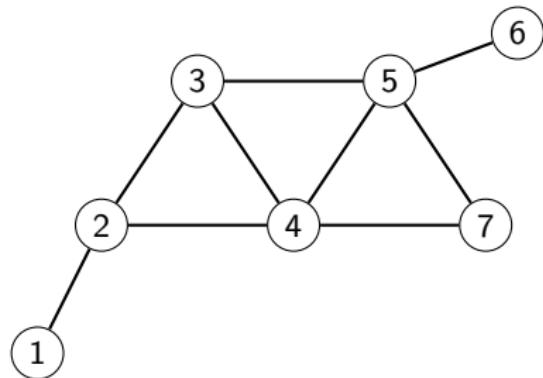
- ▶ sociology/social network analysis
  - ▶ distance  $k$ -clique introduced by Alba (*Journal of Mathematical Sociology*, 1973)
  - ▶  $k$ -club by Mokken (*Quality & Quantity*, 1979)
- ▶ bioinformatics
- ▶ political districting
- ▶ wildlife conservation planning
- ▶ wireless sensor networks

A stylized problem that incorporates these diameter constraints:

**Problem:** Maximum  $k$ -club.

**Input:** A simple graph  $G = (V, E)$  and positive integer  $k$ .

**Output:** A maximum cardinality  $k$ -club  $S \subseteq V$ .

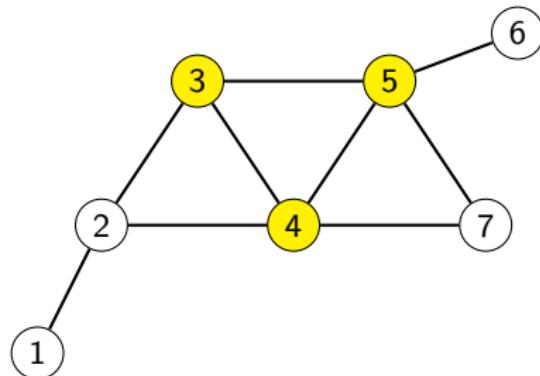


A stylized problem that incorporates these diameter constraints:

**Problem:** Maximum  $k$ -club.

**Input:** A simple graph  $G = (V, E)$  and positive integer  $k$ .

**Output:** A maximum cardinality  $k$ -club  $S \subseteq V$ .



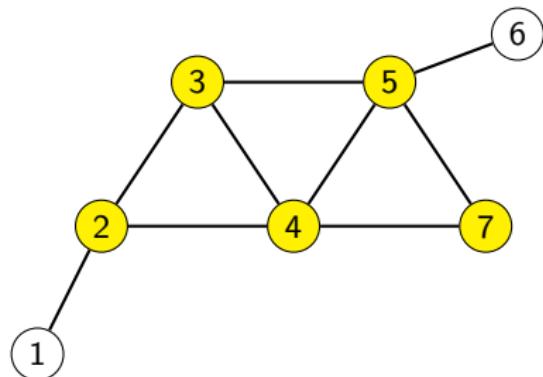
A maximum 1-club

A stylized problem that incorporates these diameter constraints:

**Problem:** Maximum  $k$ -club.

**Input:** A simple graph  $G = (V, E)$  and positive integer  $k$ .

**Output:** A maximum cardinality  $k$ -club  $S \subseteq V$ .



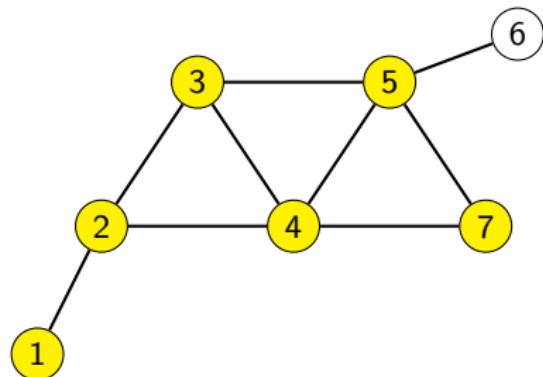
A maximum 2-club

A stylized problem that incorporates these diameter constraints:

**Problem:** Maximum  $k$ -club.

**Input:** A simple graph  $G = (V, E)$  and positive integer  $k$ .

**Output:** A maximum cardinality  $k$ -club  $S \subseteq V$ .



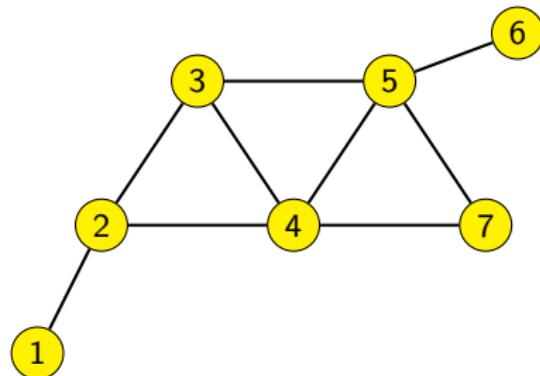
A maximum 3-club

A stylized problem that incorporates these diameter constraints:

**Problem:** Maximum  $k$ -club.

**Input:** A simple graph  $G = (V, E)$  and positive integer  $k$ .

**Output:** A maximum cardinality  $k$ -club  $S \subseteq V$ .



A maximum 4-club

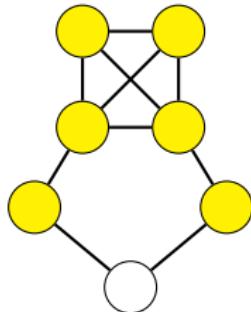
## Definition (Alba, 1973)

$S \subseteq V$  is a (distance)  $k$ -clique if  $\text{dist}_G(i,j) \leq k$  for all  $i,j \in S$ .

maximum 2-clique

$$\max_{S \subseteq V} |S|$$

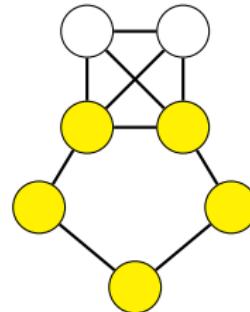
$$\text{dist}_G(i,j) \leq 2 \quad \forall i,j \in S.$$



maximum 2-club

$$\max_{S \subseteq V} |S|$$

$$\text{dist}_{G[S]}(i,j) \leq 2 \quad \forall i,j \in S.$$





Theorem (Håstad (1999), Zuckerman (2006))

When  $k = 1$ , hard to get  $n^{1-\epsilon}$ -approximation for max k-club.

Theorem (Asahiro et al. (2018))

For any fixed  $k \geq 2$ , there are  $n^{1/2}$ -approximation algorithms for k-club and k-clique, and getting an  $n^{1/2-\epsilon}$ -approximation is hard.

Theorem (Mahdavi Pajouh and Balasundaram (2012))

For any fixed  $k \geq 2$ , k-club maximality testing is coNP-complete.

## A history of $k$ -club formulations

The usual variables:

$$x_i = \begin{cases} 1 & \text{vertex } i \text{ is chosen in the } k\text{-club} \\ 0 & \text{otherwise} \end{cases}$$

Some others:

- ▶ Variable  $y_P$  for each path  $P$  of length at most  $k$ 
  - ▶ First described by Bourjolly et al. (EJOR, 2002).
  - ▶ Problem: can be  $\Omega(n^{k+1})$  variables (for hop-based distances).
  - ▶ Improved to  $O(n^{k-1})$  by Wotzlaw (arXiv, 2014).
- ▶ Variable  $y_{ij}^t$  if there exists path of length  $t$  from  $i$  to  $j$ 
  - ▶ First described by Veremyev and Boginski (EJOR, 2012).
  - ▶ Problem: somewhat large at  $O(kn^2)$  variables; weak LP.
  - ▶ Big M's removed by Veremyev et al. (Networks, 2015).



► Formulations for *special k*

- $k = 2$ . Common neighborhood formulation:

$$x_a + x_b \leq 1 + x(N(a) \cap N(b))$$

- $k = 3$ . Node and edge variables, by Almeida & Carvalho (Networks, 2012):

$$x_a + x_b \leq 1 + x(N(a) \cap N(b)) + y(E_{ab})$$

where  $E_{ab} = \{\{u, v\} \in E \mid u \in N(a) \setminus N(b), v \in N(b) \setminus N(a)\}$ .

- $k = 3$ . Use  $n$  variables and exponentially many constraints (ibid):

$$x_a + x_b \leq 1 + x(N(a) \cap N(b)) + x(S)$$

where  $S$  is a vertex cover of the subgraph induced by  $E_{ab}$ .

## Our proposed formulations

### Path-like formulation:

- ▶ Variable  $y_S$  for each *minimal* length- $k$   $a, b$ -connector  $S \subset V$ .
- ▶  $O(m^{(k-1)/2})$  variables when  $k$  is odd;
- ▶  $O(nm^{(k-2)/2})$  variables when  $k$  is even;
- ▶ generalizes  $k = 3$  formulation of Almeida and Carvalho (Networks, 2012)
- ▶ improves upon Bourjolly et al. (EJOR, 2002) and Wotzlaw (arXiv, 2014)
- ▶ for brevity, we skip this one today

### Cut-like formulation:

- ▶ Just the  $x_i$  variables!
- ▶ Constraints have a simple form:

$$x_a + x_b \leq 1 + x(C)$$

- ▶ Generalizes  $k = 2$  common neighbor formulation
- ▶ Generalizes  $k = 3$  formulation of Almeida and Carvalho (Networks, 2012)

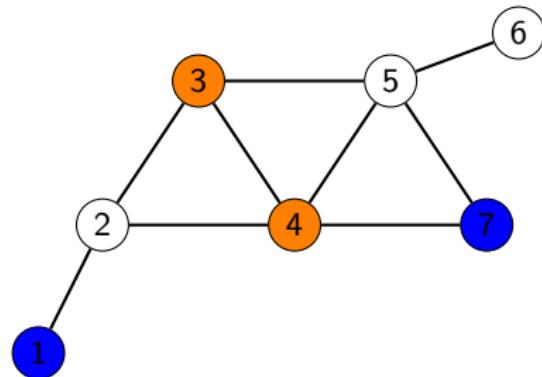
## A digression

Vertex-induced connected subgraph polytope:

$$\text{conv.hull} \left\{ x^S \in \{0, 1\}^n \mid G[S] \text{ is connected} \right\}.$$

Practically useful inequalities for  $a, b$ -separators  $C \subseteq V \setminus \{a, b\}$ :

$$x_a + x_b \leq 1 + x(C).$$

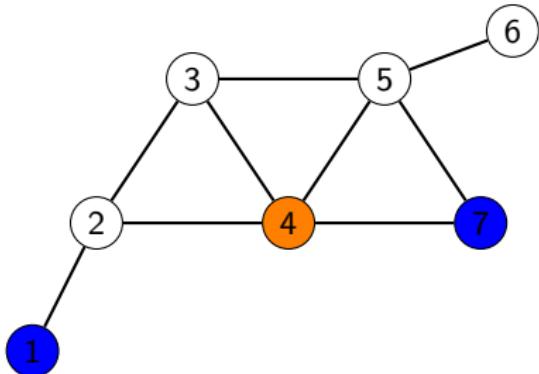


Successfully employed by:

1. Carvajal et al. (OR, 2013) for forest harvest planning
2. Buchanan et al. (IJOC, 2015) for WSNs
3. Fischetti et al. (MPC, 2017) for Steiner problems

See polyhedral study by Wang et al. (MP, 2017).

Is there a **distance-constrained** generalization?



For 3-club we can write:  $x_1 + x_7 \leq 1 + x_4$ .

### Definition

$C \subseteq V \setminus \{a, b\}$  is a length- $k$   $a, b$ -separator if  $\text{dist}_{G-C}(a, b) > k$ .

For any length- $k$   $a, b$ -separator  $C$  we can write:

$$x_a + x_b \leq 1 + x(C).$$

$$\begin{aligned}
 & \max \sum_{i \in V} x_i \\
 & x_a + x_b \leq 1 + x(C) \quad \forall a, b, C \\
 & x_i \in \{0, 1\} \quad \forall i \in V.
 \end{aligned}$$



Here,  $\forall a, b, C$  is shorthand for *minimal* length- $k$   $a, b$ -separators  $C$ .

## Proposition

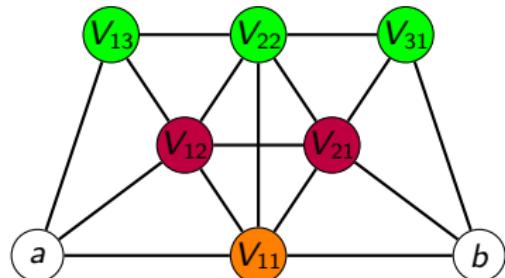
*This formulation is correct.*

Results skipped today:

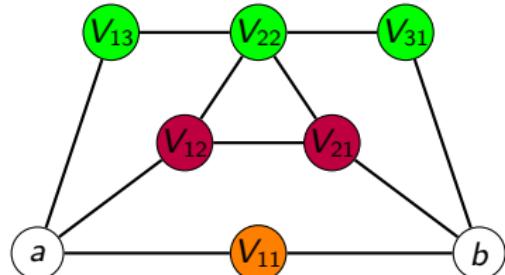
- ▶ Formulation strength:  $\text{CUT} \subsetneq \text{PATH}$
- ▶ Facet characterization
- ▶ Separation is easy for  $k \in \{2, 3, 4\}$  and hard for  $k \geq 5$ .

## Illustration of separation when $k = 4$

$$V_{ij} := \{v \in V \mid \text{dist}(a, v) = i, \text{ dist}(v, b) = j\}$$



If edge is not in minimal length-4  $a, b$ -connector, ignore it:



Direct arcs to right; node split; weight the new arcs; apply min-cut.

## Experiments

PC setup:

- ▶ Windows 10; 64bit; VS 2015; C++; 32 GB RAM;
- ▶ Intel Xeon Processor E52630 v4:
  - ▶ 10 cores (20 threads), 2.2GHz, 3.1GHz Turbo, 25MB cache;
- ▶ Gurobi 7.5.1.

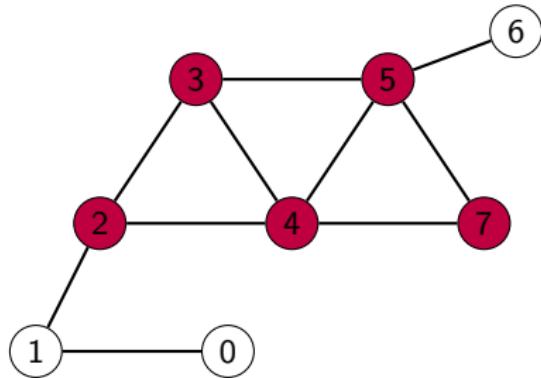
Test instances:

- ▶ some real-life graphs from 10th DIMACS Implementation Challenge;
- ▶ synthetic graphs developed by Veremyev and Boginski (EJOR, 2012)

The union of these was used by Moradi and Balasundaram (OPTL, 2015).

## Heuristic

Might identify this **2-club**.

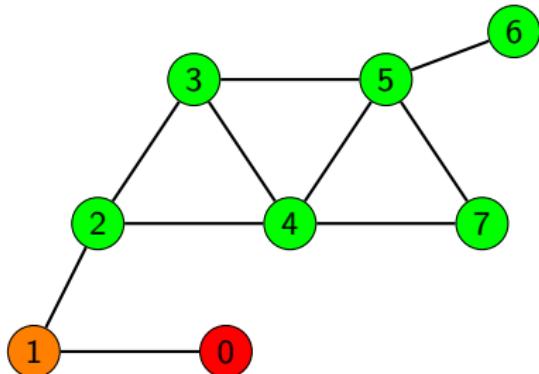


1. initialize  $S \leftarrow V$  and create  $G^k$ ;
2. while  $S$  is not a clique in  $G^k$  do
  - ▶ pick  $v \in S$  of minimum degree in  $G^k[S]$ ;
  - ▶  $S \leftarrow S \setminus \{v\}$ ;
3. while  $S$  is not a  $k$ -club in  $G$  do
  - ▶ pick  $v \in S$  with the fewest nearby nodes  $|N_{G[S]}^k(v) \cap S|$  in  $G[S]$ ;
  - ▶  $S \leftarrow S \setminus \{v\}$ ;
4. return  $S$ .

A poly-time version of ***k*-clique & DROP** by Bourjolly et al. (C&OR, 2000).

## Preprocessing

When  $k = 2$ , red node can be deleted, and then orange node.

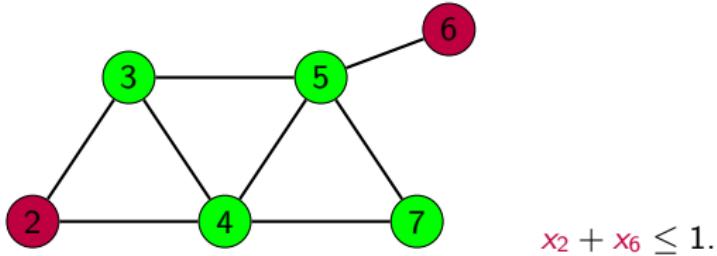


Preprocessing for  $k$ -club when given lower bound  $p$ :

1. create the  $k$ -th power graph  $G^k$ ;
2. find the  $(p - 1)$ -core  $G' = (V', E')$  of  $G^k$ ;
3. return  $G[V']$ .

We initialize the formulation with:

$$\begin{aligned}x_a + x_b &\leq 1 && \text{when } \text{dist}_G(a, b) > k \\x_i &\in \{0, 1\} && i \in V.\end{aligned}$$



Add (violated) length- $k$   $a, b$ -separator inequalities **on-the-fly**.

$$x_a + x_b \leq 1 + x(C).$$

We only separate integral points!

## Our separation routine

Given a possible solution  $x^* \in \{0, 1\}^n$ :

1.  $D := \{i \in V \mid x_i^* = 1\}$ ;
2. If  $D$  is a  $k$ -club, return;
3. For every “far” pair  $\{a, b\} \in \binom{D}{2}$  in  $G[D]$  do
  - ▶  $C := V \setminus D$  is a length- $k$   $a, b$ -separator;
  - ▶ Find  $C' \subseteq C$  **minimal** and add  $x_a + x_b \leq 1 + x(C')$ .

# DIMACS 10 Experiments

Times in seconds using the same heuristic, preprocessing, computer, and solver.

Graph	n	$k = 3$				$k = 4$			
		R	CHC	PATH	CUT	R	CHC	PATH	CUT
karate	34	0.19	0.01	0.02	0.01	0.61	0.01	0.03	0.01
lesmis	77	1.04	0.01	0.04	0.01	2.94	0.01	0.19	0.01
polbooks	105	1.01	0.01	0.07	0.01	13.99	0.03	1.16	0.03
adjnoun	112	6.48	0.03	0.33	0.01	8.90	0.02	1.02	0.02
football	115	[24,63]	[24,67]	9.96	0.27	13.35	0.01	1.35	0.01
celegansm	453	337.12	0.06	5.41	0.07	207.38	0.07	39.14	0.08
email	1133	LPNS	[192,232]	[206,239]	264.41	LPNS	[642,653]	LPNS	1.88
polblogs	1490	LPNS	2.37	960.54	1.56	LPNS	0.78	LPNS	0.72
netscience	1589	1.30	0.03	0.07	0.03	2.38	0.03	0.23	0.03
power	4941	1.21	0.95	1.00	0.99	1.77	0.98	1.41	0.93
hep-th	8361	[114,124]	[114,122]	2622.90	191.30	LPNS	[318,346]	[336,347]	428.68
PGPgiantc	10680	633.09	6.08	25.25	5.54	1556.62	6.38	407.25	5.81

- ▶ R – Recursive, Veremyev et al. (Networks, 2015)
- ▶ CHC – Canonical hypercube cut, Moradi and Balasundaram (OPTL, 2015)

## Synthetic Graph Experiments

Times reported are averages over 10 instances. If not all 10 solved in 1 hour, the number solved is reported in parenthesis.

$n$	$\rho$ (%)	$k = 3$				$k = 4$			
		R	CHC	PATH	CUT	R	CHC	PATH	CUT
100	2	0.56	0.02	0.05	0.02	2.56	0.02	0.15	0.02
	3	6.18	0.14	0.25	0.09	52.42	(7)	1.29	0.13
	4	41.34	(8)	1.33	0.29	550.42	(1)	1.88	0.11
200	1	2.54	0.12	0.27	0.12	6.29	0.14	0.72	0.16
	1.5	16.42	0.70	1.35	0.75	285.07	34.95	6.04	0.70
	2	201.70	2.60	8.00	2.09	(0)	(0)	551.84	21.07
300	0.5	0.13	0.01	0.02	0.01	1.17	0.04	0.10	0.04
	1	33.94	1.88	4.96	1.95	235.45	1.85	10.77	2.03
	1.5	444.22	7.62	23.31	6.60	(0)	(1)	(7)	452.34

PATH, which has many variables, is omitted for larger  $k$ .

$n$	$\rho$ (%)	$k = 5$			$k = 6$			$k = 7$		
		R	CHC	CUT	R	CHC	CUT	R	CHC	CUT
100	2	5.29	(9)	0.02	19.37	0.51	0.02	4.69	0.03	0.01
	3	22.15	(7)	0.03	10.24	0.11	0.01	9.54	0.01	0.01
	4	8.77	0.71	0.01	9.53	0.01	0.01	10.76	0.01	0.01
200	1	86.08	1.19	0.28	(9)	(5)	0.23	(8)	(5)	0.12
	1.5	(2)	(0)	1.02	(4)	(1)	0.12	153.08	(8)	0.04
	2	(4)	(0)	0.17	46.08	0.03	0.02	59.00	0.02	0.02
300	0.5	1.46	0.04	0.04	7.68	0.04	0.05	9.67	0.05	0.05
	1	(0)	(0)	6.72	(0)	(0)	2.23	(6)	(2)	0.14
	1.5	(0)	(0)	1.41	(7)	(9)	0.04	(6)	0.04	0.03

## Conclusion

New formulations for low-diameter clusters ( $k$ -clubs):

- ▶ **path-like** and **cut-like** formulations
- ▶ generalize or strengthen several previous formulations
- ▶ **cut-like** also applies when distances are not hop-based

Top performer is **cut-like** formulation:

- ▶ uses  $n$  variables
- ▶ usually solves in 1 or 2 seconds
- ▶ all 24 real-life instances in < 8 minutes (others fail on 4+)
- ▶ all 450 synthetic instances in < 35 minutes (others fail on 84+)

Manuscript available on Optimization Online:

- ▶ Austin Buchanan and Hosseinali Salemi. Parsimonious formulations for low-diameter clusters. [http://www.optimization-online.org/DB\\_HTML/2017/09/6196.html](http://www.optimization-online.org/DB_HTML/2017/09/6196.html)

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