Relaxations for some NP-hard problems based on exact subproblems

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The Max-Cut Problem

Unconstrained quadratic 1/-1 optimization:

$$\max\ x^T L x \text{ such that } x \in \{-1, 1\}^n$$

This is Max-Cut as a binary quadratic problem.
Unconstrained quadratic 0/1 minimization:

$$\min\ x^T Q x + c^T x \text{ such that } x \in \{0, 1\}^n$$

This is equivalent to Max-Cut, by simple variable transformation.
Q could either be assumed to be upper triangular, or symmetric, with zero diagonal.

Polyhedral Relaxations

Consider the Cut polytope CUT:=conv$\{xx^T : x \in \{-1, 1\}^n\}$.

Max-Cut now reads

$$z_{mc} = \max\{x^T Lx : \ x \in \{-1, 1\}^n\} = \max\{\langle L, X\rangle : \ X \in CUT\}.$$

A simple observation:

$$x \in \{-1, 1\}^n, \ \ f = (1, 1, 1, 0, \ldots, 0)^T \ \ \Rightarrow |f^T x| \geq 1.$$

Results in $x^T f \ f^T x = \langle (xx^T), (ff^T)\rangle = \langle \mathbf{X}, \mathbf{ff^T} \rangle \geq \mathbf{1}$.
Can be applied to any **triangle** $i < j < k$. Nonzeros of f can also be -1. We collect all the triangle inequalities in the metric polytope M

$$M := \{X : f^T X f \geq 1 \text{ where } f \text{ has 3 nonzeros} \in \{-1, 1\}\}$$

Polyhedral Relaxations (2)

There are $4\binom{n}{3}$ such triangle inequality constraints. The number of variables is $\binom{n}{2}$.

Optimizing over M results in a difficult (highly degenerate) LP.

Barahona, Mahjoub (1986): CUT=M for graphs without K_5-minor.

Barahona, Jünger, Reinelt (1989): computational experiments, LP relaxation very efficient for sparse graphs.

Pardella, Liers (2008): computations with 2d spinglass problems of sizes larger than 1000×1000.

Weak results once density of graph grows.

Polyhedral relaxations (3)

Other classes of cutting planes available.

If $f \in \{-1, 0, 1\}$ with $f^T f = t$, and t odd, we get odd-clique inequalities

$$M_t := \{X : f^T X f \geq 1 \text{ where } f \text{ has t nonzeros} \in \{-1, 1\}\}.$$

Deza, Grishukin, Laurent (1993) consider the hypermetric cone and show that it is in fact polyhedral.

Many other classes of facets of CUT, but they are often difficult to separate, no substantial computational experiments available.

Basic semidefinite relaxation

Consider the Cut polytope CUT:=conv$\{xx^T : x \in \{-1,1\}^n\}$. It is contained in the set

$$C := \{X : diag(X) = e,\ X \succeq 0\}$$

of correlation matrices. Since $x^T Lx = \langle L, xx^T \rangle$ we get

$$\max\{\langle L, X\rangle : X \in CUT\} \leq \max\{\langle L, X\rangle : X \in C\} := z_C$$

Goemans, Williamson (1995): worst-case error analysis (at most 14 % above optimum if weights nonnegative).

This is best possible approximation if the Unique Game Conjecture would hold (Khot, 2007) and $P \neq NP$.

Optimizing over C

We solve $\max\{\langle L, X\rangle : X \in C\}$.
Matrices of order n and $C = \{X : diag(X) = e,\ X \succeq 0\}$

n	seconds
1000	12
2000	102
3000	340
4000	782
5000	1570

h	n	seconds
10	1000	3
15	3375	37
20	8000	273
25	15625	1395

Computing times on my laptop. Implementation in MATLAB, 30 lines of source code, Interior-Point Method based on the Newton Method (left). Larger problems can also be solved with the spectral bundle method, see Helmberg, Overton, R. (2012), 3d-grids of size $h \times h \times h$. Relative accuracy 10^{-6}.

Practical experience with $C \cap M$

graph	n	C	$C \cap M$	time(min)	cut
g1d	100	396.1	352.374	1.10	324
g2d	200	1268.9	1167.978	7.00	1050
g3d	300	2359.6	2215.233	14.01	1953
g1s	100	144.6	130.007	2.60	126
g2s	200	377.3	343.149	8.24	318
g3s	300	678.5	635.039	13.73	555
spin5	125	125.3	109.334	11.40	108

All relaxations solved exactly. The cut value is not known to be optimal.

$C, M, C \cap M$

graph	n	C	M	$C \cap M$	cut
g1d	100	396.1	786.3	352.374	324
g2d	200	1268.9	n.a.	1167.978	1050
g3d	300	2359.6	n.a.	2215.233	1953
g1s	100	144.6	137.5	130.007	126
g2s	200	377.3	410.0	343.149	318
g3s	300	678.5	854.4	635.039	555
spin5	125	125.3	110.3	109.334	108

The LP over M is 'harder' than the SDP over $C \cap M$:
Largest possible violation for $X \in M$: $f^T X f = -3$, but should be ≥ 1.
Violation for $X \in C$: $f^T X f \geq 0$, but should be ≥ 1.

Higher order relaxations

There are several hierarchies of relaxations for 0-1 optimization problems, see Lovasz, Schrijver lifting, the RLT procedure by Sherali, Adams and the hierarchy introduced by Anjos, Wolkowicz (2002) and Lasserre (2002).

They get in n lifting steps to the integer optimum, but in each step, the dimension of the problem grows.

Even the first nontrivial lifting step in the SDP hierarchies leads to SDP problems which are computationally out of reach for very modest sizes ($n \approx 50$).

Now: A hierarchy where the matrix dimension stays n.

A new relaxation hierarchy

Recall CUT:=conv$\{xx^T : x \in \{-1,1\}^n\}$.
Let $I \subseteq \{1,\ldots,n\}$ with $|I| = k$.
Set $X_I := X(I,I)$ (submatrix indexed by I).

Key observation: If $X \in CUT$ and $|I| = k$, then

$$X_I \in CUT_k.$$

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This translates into

$$X_I = \sum_j \lambda_j c_j c_j^T, \ \lambda_j \geq 0, \ \sum_j \lambda_j = 1.$$

Here, $c_j \in \{-1,1\}^k$ and $c_j c_j^T$ runs through all cuts in CUT_k.
There are 2^{k-1} distinct cut matrices $c_j c_j^T$.
The additional variables are the λ_j.

Exact subgraph idea

This idea works nicely for problems which have the property that the restriction to subgraph results in a similar problem of smaller dimension.

Candidate problems:

- Max-Cut
- Stable-Set, Max-Clique, Coloring
- Ordering

Not directly applicable to:

- Assignment Problems
- Traveling Salesman Problems

because restriction to subproblem changes the problem structure.

Related Work

Previous work using this idea in connection with polyhedral relaxations:

Buchheim, Liers, Oswald (2008) use this idea to generate target cuts by projecting the polyhedron onto subsets.

A similar idea also used by Bonato, Jünger, Reinelt, Rinaldi (2012) to tighten relaxations for the cut polytope.

In both cases, an outer description of the small polytope is used to lift local cuts to cuts for the original problem.

We show that an inner description for the small polytope has algorithmic advantages.

The new Relaxation

$$z_{C\cap M,k} := \max\{\langle L, X\rangle : X \in C \cap M,$$

$$X_I \in CUT_k \; \forall I \text{ with } |I| = k\}$$

For k fixed, the resulting relaxation is polynomially solvable (with fixed precision).

As k approaches n, we get the exact solution.

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Theorem: For $k \le 4$ we have $z_M = z_{CUT}$.
This follows from the fact that $M = CUT$ for graphs without K_4-minor. Thus the metric polytope is equal to the cut polytope for $k \le 4$.

Smallest interesting case: $k = 5$, but there are $\binom{n}{5}$ subsets to consider.

Some Observations

- Contrary to Cutting Plane approaches, which add constraints valid for CUT, we include an inner description of CUT_k for small k. This can be seen as a variant of Column Generation (new variables are the λ_j).

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- Contrary to Cutting Plane approaches, which add constraints valid for CUT, we include an inner description of CUT_k for small k. This can be seen as a variant of Column Generation (new variables are the λ_j).

- For each I we add 2^{k-1} nonnegative variables and $\binom{k}{2}$ new equations.

- Adding all possible choices for I at once is computationally inefficient, so the challenge is to identify good choices for I.

Selecting I

Given $X \in C \cap M$ we would like to identify a subset I with $|I| = 5$, such that $X_I \notin CUT_5$.

For I fixed this can be determined by projection (solve convex QP with 16 variables).

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Our heuristic: Given I, check whether there exists a violated 5-clique inequality $f^T X f < 1.$
We determine the minimum of

$$f^T X f$$

over all 2^4 vectors f with support on I and denote it by s_I.

We select those I where s_I is significantly smaller than 1.

General Computational Setup

Start:

- Find optimal solution $X \in C \cap M$

Iteration:

(a) Determine subsets I_r with $|I_r| = 5$ and $s_{I_r} < 1$
(b) Resolve with $X_{I_r} \in CUT_5$ yielding new X
(c) Add triangle inequalities violated by X
(d) purge inactive triangles
(e) Resolve with new triangles added yielding new X

Note that after (e) the condition $X \in C \cap M$ is not garantueed to hold. It could be inforced by repeating (c),(d) and (e) until all triangles inequalities are satisfied again.

Preliminary Computational Results

The relaxation $C \cap M$ is usually quite accurate on smaller instances with n up to $n \approx 50$, so we consider instances with $60 \le n \le 100$.

We use randomized enumeration of all I with $|I| = 5$ and include in one round 50 new subsets I with smallest values s_I.

The resulting SDP is solved using an interior-point code (SDPT3).

Triangles are separated by complete enumeration.

A snapshot

We select $n = 70$ and adjacency matrix with density of 50%, edge weights are integers between -10 and 10.
At start we get:

$$z_C = 996.1 \quad z_{C \cap M} = 872.3, \quad z_{mc} = 856$$

round	bound	min s_I	sets I	triangles
1	868.2	0.41	48	670
2	865.9	0.55	94	602
3	864.1	0.54	138	516
4	862.4	0.56	183	509
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10	858.3	0.76	344	416

Preliminary Results

random graphs, density 50 %, edge weights between -10 and 10

n	C	$C \cap M$	new	cut	gap
70	996.2	872.3	858.3	856	0.14
80	1317.2	1181.6	1162.6	1152	0.36
90	1491.1	1335.6	1307.8	1297	0.28
100	1959.6	1772.2	1745.8	1698	0.64

The last column shows by how much the gap between $C \cap M$ and the cut value (normalized to 1) is reduced by the new bound.

Preliminary Results (2)

random dense graphs, edge weights between 1 and 10

n	C	$C \cap M$	new	cut	gap
70	6807.1	6725.9	6712.9	6693	0.60
80	8741.6	8639.6	8623.2	8604	0.54
90	11217.8	11109.4	11092.6	11070	0.57
100	13718.9	13593.3	13575.1	13530	0.71

The last column shows by how much the gap between $C \cap M$ and the cut value (normalized to 1) is reduced by the new bound.

Preliminary Results (3)

random graphs, density 50 %, edge weights 1

n	C	$C \cap M$	new	cut	gap
70	742.0	727.8	727.0	727	0.00
80	967.7	952.5	949.8	947	0.51
90	1177.5	1158.4	1155.4	1148	0.71
100	1458.3	1436.8	1433.7	1424	0.76

The last column shows by how much the gap between $C \cap M$ and the cut value (normalized to 1) is reduced by the new bound.

C, M, $C \cap M$ and the new bound

graph	n	C	M	$C \cap M$	new	cut
g1s	100	144.6	137.5	130.007	128.46	126
spin5	125	125.3	110.3	109.334	108.90	108

Only preliminary results, after a few rounds of adding subgraph constraints. The number of subgraphs included is less than 300

Last slide

- Fast separation?
- Exploit column generation idea (drop $\lambda_j = 0$)?
- Experiment with subsets of larger sizes?
- How solve resulting SDP more efficiently?
- Application to other problem classes?
- Include in Branch-and-Bound (BiqMac)?