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On different versions of the exact subgraph hierarchy for the stable set problem[☆]

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ABSTRACT

Let G be a graph with n vertices and m edges. One of several hierarchies towards the stability number of G is the exact subgraph hierarchy (ESH). On the first level it computes the Lovász theta function $\vartheta(G)$ as semidefinite program (SDP) with a matrix variable of order $n+1$ and $n+m+1$ constraints. On the kth level it adds all exact subgraph constraints (ESC) for subgraphs of order k to the SDP. An ESC ensures that the submatrix of the matrix variable corresponding to the subgraph is in the correct polytope. By including only some ESCs into the SDP the ESH can be exploited computationally.

In this paper we introduce a variant of the ESH that computes $\vartheta(G)$ through an SDP with a matrix variable of order n and $m+1$ constraints. We show that it makes sense to include the ESCs into this SDP and introduce the compressed ESH (CESH) analogously to the ESH. Computationally the CESH seems favorable as the SDP is smaller. However, we prove that the bounds based on the ESH are always at least as good as those of the CESH. In computational experiments sometimes they are significantly better.

We also introduce scaled ESCs (SESCs), which are a more natural way to include exactness constraints into the smaller SDP and we prove that including an SESC is equivalent to including an ESC for every subgraph.

1. Introduction

One of the most fundamental problems in combinatorial optimization is the stable set problem. Given a graph $G = (V, E)$, a subset of vertices $S \subseteq V$ is called stable set if no two vertices of S are adjacent. A stable set is called maximum stable set if there is no stable set with larger cardinality. The cardinality of a maximum stable set is called stability number of G and denoted by $\alpha(G)$. The stable set problem asks for a stable set of size $\alpha(G)$. It is an NP-hard and well-studied problem, see for example the survey of Bomze, Budinich, Pardalos and Pelillo [3].

Typically NP-complete combinatorial optimization problems are solved using branch-and-bound or branch-and-cut algorithms. One type of relaxations used in order to obtain bounds are those based on semidefinite programming (SDP), see Helmberg [21] for an introduction. SDPs can be solved to arbitrary precision in polynomial time and numerous SDP solvers are available.

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Lovász [24] laid the foundations for SDP relaxations in 1979 by introducing the Lovász theta function $\vartheta(G)$ of a graph G, which fulfills

$$\alpha(G) \leqslant \vartheta(G) \leqslant \chi(\overline{G})$$

for every graph G, where $\chi(\overline{G})$ is the chromatic number of the complement graph $\overline{G}$ of G. Among his formulations of $\vartheta(G)$ was an SDP with a matrix variable of order n and $m+1$ equality constraints. We will give the rigorous definition of this SDP in Section 3.1 and refer to it as (T_n). As a result, $\vartheta(G)$ can be calculated in polynomial time, even though it is sandwiched between $\alpha(G)$ and $\chi(\overline{G})$, which are both NP-complete to compute. Later Grötschel, Lovász and Schrijver [18] provided an alternative formulation of $\vartheta(G)$ as SDP with a matrix variable of order $n+1$ and $n+m+1$ equality constraints. In Section 2.1 we will give the rigorous definition of this SDP and refer to it as (T_{n+1}).

In 1995 Goemans and Williamson [17] presented an SDP relaxation for the Max-Cut problem which is a provenly good approximation. Since then SDP relaxations have been used for various combinatorial optimization problems and several ways of further tightening them have been developed. Also hierarchies, that consist of several levels, were established, for example by Lovász and Schrijver [25] and by Lasserre [22]. At the first level a simple relaxation is considered, and the higher the level gets, the tighter the bounds become. Usually the computational power it takes to evaluate the level of the hierarchy increases on each level and often the computation of higher levels is beyond reach. They major drawback of most of the SDP based hierarchies is that the order of the matrix variable increases enormously with each level.

In 2015 Adams, Anjos, Rendl and Wiegele [1] introduced the exact subgraph hierarchy (ESH) for combinatorial optimization problems that have an SDP relaxation. They discussed the ESH for the Max-Cut problem and briefly described it for the stable set problem. Here the first level of the hierarchy boils down to (T_{n+1}). They introduced exact subgraph constraints (ESC), which ensure that the submatrix of the matrix variable in (T_{n+1}) corresponding to a subgraph is in the so-called squared stable set polytope. If the problem is solved exactly the submatrix has to be in this polytope, hence the ESC forces the subgraph to be exact. On the kth level of the ESH the ESC for all subgraphs of order k are included into (T_{n+1}). This implies that the order of the matrix variable remains $n+1$ on each level of the ESH. Gaar and Rendl [13–15] computationally exploit the ESH and relaxations of it for the stable set, the Max-Cut and the coloring problem.

To summarize, the ESH from [1] starts from $\vartheta(G)$ formulated as (T_{n+1}) and adds ESCs on higher levels. As $\vartheta(G)$ has two SDP formulations (T_{n+1}) and (T_n), it is a natural question whether it makes sense to build a hierarchy by starting from $\vartheta(G)$ formulated as (T_n) and adding ESCs. It is the aim of this paper to investigate this natural question, which is even more interesting in the light of a recent work by Galli and Letchford [16], who compared the behavior of (T_{n+1}) and (T_n) when they are strengthened or weakened and who showed that the obtained bounds do not always coincide.

In this paper we show that it makes sense to consider this new hierarchy, which we newly introduce as compressed (because the SDP is smaller) ESH (CESH). We prove that both the ESH and the CESH are equal to $\vartheta(G)$ on the first level and equal to $\alpha(G)$ on the nth level. Furthermore, the SDP has a smaller matrix variable and fewer constraints, so intuitively the CESH is computationally favorable. However, we prove that the bounds obtained by including an ESC into (T_{n+1}) are always at least as good as those obtained from including the same ESC into (T_n), demonstrating that the bounds obtained from the ESH are at least as good as those from the CESH. Furthermore, it turns out in our computational comparison that the bounds are sometimes significantly worse for the CESH, but the running times do not significantly decrease. Hence, we confirm that the ESH has the better trade-off between the quality of the bound and the running time.

The intuition behind the SDP (T_n) is different than the one of (T_{n+1}), in particular for the solutions representing stable sets. We show in this paper that there is an alternative intuitive definition of exact subgraphs for (T_n). This leads to our new definition of scaled ESCs (SESC) and our introduction of another new hierarchy, the scaled ESH (SESH). We prove that SESCs coincide with the original ESCs for (T_n), which implies that the ESH and the SESH coincide.

To summarize, in this paper we confirm that even though our new hierarchies based on exactness seem more intuitive and computational favorable, with off the shelve SDP solvers it is the best option to consider the ESH in the way it has been done so far. Our findings are in accordance with the results of [16], where it is observed that (T_{n+1}) typically gives stronger bounds when strengthened.

The rest of the paper is organized as follows. In Section 2 we give rigorous definitions of ESCs and the ESH and explain how they can be exploited computationally. In Section 3 we introduce the CESH and compare it to the ESH, also in the light of the results of [16]. Then we introduce SESCs in Section 4 and investigate how they are related to the ESCs. In Section 5 we present computational results and we conclude our paper in Section 6.

We use the following notation. We denote by $\mathbb{N}_0$ the natural numbers starting with 0. By $\mathbb{1}_d$ and $\mathbb{0}_d$ we denote the vector or matrix of all ones and all zeros of size d, respectively. Furthermore, by $\mathcal{S}_n$ we denote the set of symmetric matrices in $\mathbb{R}^{n\times n}$. We denote the convex hull of a set S by $\operatorname{conv}(S)$ and the trace of a matrix X by $\operatorname{trace}(X)$. Moreover, $\operatorname{diag}(X)$ extracts the main diagonal of the matrix X into a vector. By x^T and X^T we denote the transposed of the vector x and the matrix X, respectively. Moreover, we denote the ith entry of the vector x by x_i and the entry of X in the ith row and the jth column by $X_{i,j}$. Furthermore, we denote the inner product of two vectors x and y by $\langle x, y\rangle = x^T y$. The inner product of two matrices $X = (X_{i,j})_{1\leqslant i,j\leqslant n}$ and $Y = (Y_{i,j})_{1\leqslant i,j\leqslant n}$ is defined as $\langle X, Y\rangle = \sum_{i=1}^{n}\sum_{j=1}^{n} X_{i,j}Y_{i,j}$. Furthermore, the t-dimensional simplex is given as $\Delta_t = \left\{\lambda \in \mathbb{R}^t : \sum_{i=1}^{t}\lambda_i = 1,\ \lambda_i \geqslant 0 \quad \forall 1 \leqslant i \leqslant t\right\}$.

2. The exact subgraph hierarchy

In this section we recall exact subgraph constraints and the exact subgraph hierarchy for combinatorial optimization problems that have an SDP relaxation introduced by Adams, Anjos, Rendl and Wiegele in 2015 [1]. We detail everything for the stable set problem, because in [1] they focused on Max-Cut. Besides motivation and definitions, we provide new examples, discuss the representation of exact subgraph constraints and compare the exact subgraph hierarchy to other hierarchies from the literature.

2.1. Lovász theta function

We start by presenting the Lovász theta function. To do so, it is handy to consider the incidence vectors of stable sets and the polytope they span.

Definition 1. Let $G = (V, E)$ be a graph with $|V| = n$ and $V = \{1, \dots, n\}$. Then the set of all stable set vectors $\mathcal{S}(G)$ and the stable set polytope $\mathrm{STAB}(G)$ are defined as

$$\begin{aligned} \mathcal{S}(G) &= \left\{ s \in \{0, 1\}^n : s_i s_j = 0 \quad \forall \{i, j\} \in E \right\} \text{ and} \\ \mathrm{STAB}(G) &= \mathrm{conv}\,\{s : s \in \mathcal{S}(G)\}\,. \end{aligned}$$

It is easy to see that the stability number $\alpha(G)$ is obtained by solving

$$\alpha(G) = \max_{s \in \mathcal{S}(G)} \mathbb{1}_n^T s = \max_{s \in \mathrm{STAB}(G)} \mathbb{1}_n^T s,$$

but unfortunately $\mathrm{STAB}(G)$ is very hard to describe in general. Several linear relaxations of $\mathrm{STAB}(G)$ have been considered, like the so-called fractional stable set polytope and the clique constraint stable set polytope. We refer to [18] for further details.

We focus on another relaxation, namely the Lovász theta function $\vartheta(G)$, which is an upper bound on $\alpha(G)$. Grötschel, Lovász and Schrijver [18] proved

$$\begin{aligned} \vartheta(G) = \max \quad & \mathbb{1}_n^T x \\ \text{s. t.} \quad & \mathrm{diag}(X) = x \\ & X_{i,j} = 0 \qquad \forall \{i, j\} \in E \\ & \begin{pmatrix} 1 & x^T \\ x & X \end{pmatrix} \succcurlyeq 0 \\ & X \in \mathcal{S}_n, \; x \in \mathbb{R}^n \end{aligned} \tag{T_{n+1}}$$

and hence provided an SDP formulation of $\vartheta(G)$. This SDP has a matrix variable of order $n+1$. Furthermore, there are m constraints of the form $X_{i,j} = 0$, n constraints to make sure that $\mathrm{diag}(X) = x$ and one constraint ensures that in the matrix of order $n+1$ the entry in the first row and first column is equal to 1. Hence, there are $n+m+1$ linear equality constraints in (T_{n+1}).

To formulate (T_{n+1}) in a more compact way we observe the well-known fact that $X - xx^T \succcurlyeq 0$ if and only if $\begin{pmatrix} 1 & x^T \\ x & X \end{pmatrix} \succcurlyeq 0$, see Boyd and Vandenberghe [4, Appendix A.5.5] on Schur complements. Thus, the feasible region of (T_{n+1}) is

$$\mathrm{TH}^2(G) = \left\{ (x, X) \in \mathbb{R}^n \times \mathcal{S}_n \colon \mathrm{diag}(X) = x, \quad X_{i,j} = 0 \quad \forall \{i, j\} \in E, \quad X - xx^T \succcurlyeq 0 \right\}.$$

Clearly for each element (x, X) of $\mathrm{TH}^2(G)$ the projection of X onto its main diagonal is x. The set of all projections

$$\mathrm{TH}(G) = \left\{ x \in \mathbb{R}^n \colon \exists X \in \mathcal{S}_n : (x, X) \in \mathrm{TH}^2(G) \right\}$$

is called theta body. More information on $\mathrm{TH}(G)$ can be found for example in Conforti, Cornuejols and Zambelli [8]. It is easy to see that $\mathrm{STAB}(G) \subseteq \mathrm{TH}(G)$ holds for every graph G, see [18]. Thus, $\vartheta(G)$ is a relaxation of $\alpha(G)$.

2.2. Introduction of the exact subgraph hierarchy

In order to present the exact subgraph hierarchy we need a modification of the stable set polytope $\mathrm{STAB}(G)$, namely the squared stable set polytope.

Definition 2. Let $G = (V, E)$ be a graph. The squared stable set polytope $\mathrm{STAB}^2(G)$ of G is defined as

$$\mathrm{STAB}^2(G) = \mathrm{conv}\left\{ ss^T : s \in \mathcal{S}(G) \right\}.$$

The matrices of the form ss^T for $s \in \mathcal{S}(G)$ are called stable set matrices.

Note that the elements of $\mathrm{STAB}(G)$ are vectors in $\mathbb{R}^n$, whereas the elements of $\mathrm{STAB}^2(G)$ are matrices in $\mathbb{R}^{n\times n}$. In comparison to $\mathrm{STAB}(G)$ the structure of $\mathrm{STAB}^2(G)$ is more sophisticated and less studied. Only if G has no edges a projection of $\mathrm{STAB}^2(G)$ coincides with a well-studied object, the boolean quadric polytope, see Padberg [27]. In particular, by putting the upper triangle with the main diagonal into a vector for all elements of $\mathrm{STAB}^2(G)$ we obtain the elements of the boolean quadric polytope.

Let us now turn back to $\vartheta(G)$. The following lemma turns out to be the key ingredient for defining the exact subgraph hierarchy.

Lemma 1. *If we add the constraint $X \in \mathrm{STAB}^2(G)$ into (T_{n+1}) for a graph G, then the optimal objective function value is $\alpha(G)$, so*

$$\alpha(G) = \max\left\{\mathbb{1}_n^T x : (x, X) \in \mathrm{TH}^2(G),\ X \in \mathrm{STAB}^2(G)\right\}. \tag{1}$$

Proof. Let $(P^{\mathcal{E}})$ be the SDP on the right-hand side of (1), let $z^{\mathcal{E}}$ be its optimal objective function value and let $\mathcal{S}(G) = \{s_1, \ldots, s_t\}$.

Let without loss of generality s_t be the incidence vector of a maximum stable set of G. Then clearly $x = s_t$ and $X = s_t s_t^T$ is feasible for $(P^{\mathcal{E}})$ and has objective function value $\alpha(G)$, so $\alpha(G) \leqslant z^{\mathcal{E}}$ holds.

Furthermore, any feasible solution (x, X) of $(P^{\mathcal{E}})$ can be written as

$$X = \sum_{i=1}^{t} \lambda_i s_i s_i^T$$

for some $\lambda \in \Delta_t$ because $X \in \mathrm{STAB}^2(G)$ holds. Thus, x can be written as

$$x = \mathrm{diag}(X) = \mathrm{diag}\left(\sum_{i=1}^{t} \lambda_i s_i s_i^T\right) = \sum_{i=1}^{t} \lambda_i s_i.$$

In consequence, the objective function value of (x, X) for $(P^{\mathcal{E}})$ is equal to

$$\mathbb{1}_n^T x = \mathbb{1}_n^T \sum_{i=1}^{t} \lambda_i s_i = \sum_{i=1}^{t} \lambda_i \mathbb{1}_n^T s_i \leqslant \sum_{i=1}^{t} \lambda_i \alpha(G) = \alpha(G)$$

and hence $z^{\mathcal{E}} \leqslant \alpha(G)$ holds, which finishes the proof. □

Lemma 1 implies that if we add the constraint $X \in \mathrm{STAB}^2(G)$ to (T_{n+1}), then we get the best possible bound on $\alpha(G)$, namely $\alpha(G)$. Unfortunately, depending on the representation of the constraint, we either include an exponential number of new variables (if we use a formulation as convex hull) or inequality constraints (if we include inequalities representing facets of $\mathrm{STAB}^2(G)$, see Section 2.3) into the SDP. In order to only partially include $X \in \mathrm{STAB}^2(G)$ we exploit a property of stable sets, namely that a stable set of G induces also a stable set in each subgraph of G. To formalize this in an observation, we first need the following definition.

Definition 3. Let $I \subseteq V$ be a subset of the vertices of the graph $G = (V, E)$ with $|V| = n$ and let $k_I = |I|$. We denote by G_I the subgraph of G that is induced by I. Furthermore, we denote by $X_I = (X_{i,j})_{i,j\in I}$ the submatrix of $X \in \mathbb{R}^{n\times n}$ which is indexed by I.

Observation 1. *Let $G = (V, E)$ be a graph. Then*

$$X \in \mathrm{STAB}^2(G) \quad \Leftrightarrow \quad X_I \in \mathrm{STAB}^2(G_I) \quad \forall I \subseteq V.$$

Proof. As $X_I \in \mathrm{STAB}^2(G_I)$ for all $I \subseteq V$ implies $X \in \mathrm{STAB}^2(G)$ for $I = V$, one direction of the equivalence is trivial. For the other direction note that $X \in \mathrm{STAB}^2(G)$ implies that X is a convex combination of ss^T for stable set vectors $s \in \mathcal{S}(G)$. From this one can easily extract a convex combination of ss^T for $s \in \mathcal{S}(G_I)$ for X_I, thus $X_I \in \mathrm{STAB}^2(G_I)$ for all $I \subseteq V$. □

Observation 1 implies that adding the constraint $X \in \mathrm{STAB}^2(G)$ to (T_{n+1}) as in Lemma 1 makes sure that the constraint $X_I \in \mathrm{STAB}^2(G_I)$ is fulfilled for all subgraphs G_I of G. This gives rise to the following definition.

Definition 4. Let $G = (V, E)$ be a graph and let $I \subseteq V$. Then the exact subgraph constraint (ESC) for G_I is defined as $X_I \in \mathrm{STAB}^2(G_I)$.

Finally we consider the hierarchy by Adams, Anjos, Rendl and Wiegele [1].

Definition 5. Let $G = (V, E)$ be a graph with $|V| = n$ and let J be a set of subsets of V. Then $z_J^{\mathcal{E}}(G)$ is the optimal objective function value of (T_{n+1}) with the ESC for every subgraph induced by a set in J, so

$$z_J^{\mathcal{E}}(G) = \max\left\{\mathbb{1}_n^T x : (x, X) \in \mathrm{TH}^2(G),\ X_I \in \mathrm{STAB}^2(G_I) \quad \forall I \in J\right\}. \tag{2}$$

Table 1
The value of $z_k^{\mathcal{E}}(G)$ for three graphs. Values in gray cells are only upper bounds on $z_k^{\mathcal{E}}(G)$.

G	n	$\alpha(G)$	$\vartheta(G)$	$z_2^{\mathcal{E}}(G)$	$z_3^{\mathcal{E}}(G)$	$z_4^{\mathcal{E}}(G)$	$z_5^{\mathcal{E}}(G)$	$z_6^{\mathcal{E}}(G)$	$z_7^{\mathcal{E}}(G)$	$z_8^{\mathcal{E}}(G)$
hamming6_4	64	4	5.333	4.000	4.000	4.000	4.000	4.000	4.000	4.000
$G_{60,0.25}$	60	13	14.282	14.201	14.156	13.945	13.741	13.386	13.209	13.112
Paley61	61	5	7.810	7.810	7.810	7.810	7.810	7.078	6.989	6.990

Furthermore, for $k \in \mathbb{N}_0$ with $k \leqslant n$ let $J_k = \{I \subseteq V : |I| = k\}$. Then the kth level of the exact subgraph hierarchy (ESH) is defined as $z_k^{\mathcal{E}}(G) = z_{J_k}^{\mathcal{E}}(G)$.

In other words the kth level of the ESH is the SDP for calculating the Lovász theta function (T_{n+1}) with additional ESCs for every subgraph of order k. Due to Observation 1 every level of the ESH is a relaxation of (1).

Note that Adams, Anjos, Rendl and Wiegele did not give the hierarchy a name. However, they called the ESCs for all subgraphs of order k and therefore the constraint to add at the kth level of the ESH the k-projection constraint.

Let us briefly look at some properties of $z_k^{\mathcal{E}}(G)$. For example, the next lemma shows that the bound obtained from the ESH is better the higher the level of the ESH is.

Lemma 2. *Let $G = (V, E)$ be a graph with $|V| = n$. Then*

$$\vartheta(G) = z_0^{\mathcal{E}}(G) = z_1^{\mathcal{E}}(G) \geqslant z_{k-1}^{\mathcal{E}}(G) \geqslant z_k^{\mathcal{E}}(G) \geqslant z_n^{\mathcal{E}}(G) = \alpha(G)$$

holds for all $k \in \{1, \dots, n\}$.

Proof. Lemma 1 states that $z_n^{\mathcal{E}}(G) = \alpha(G)$. For $k = 0$ we do not add any additional constraint into (T_{n+1}). For $k = 1$ the ESC for $I = \{i\}$ boils down to $X_{i,i} \in [0, 1]$, which is enforced by $X \succcurlyeq 0$. Therefore, $\vartheta(G) = z_0^{\mathcal{E}}(G) = z_1^{\mathcal{E}}(G)$ holds. Additionally, due to Observation 1 whenever all subgraphs of order k are exact, also all subgraphs of order $k-1$ are exact, which yields the desired result. $\square$

Next, we consider an example in order to get a feeling for the ESH and how good the bounds on $\alpha(G)$ obtained with it are.

Example 1. We consider $z_k^{\mathcal{E}}(G)$ for $k \leqslant 8$ for a Paley graph, a Hamming graph [10] and a random graph $G_{60,0.25}$ from the Erdős–Rényi model in Table 1. It is possible to compute $z_2^{\mathcal{E}}(G)$. For $k \geqslant 3$ we use relaxations (*i.e.* we compute $z_J^{\mathcal{E}}(G)$ by including the ESCs only for a subset J of the set of all subgraphs of order k and determine the sets J as it is described in more detail in Section 5) to get an upper bound on $z_k^{\mathcal{E}}(G)$ or deduce the value.

For hamming6_4 already for $k = 2$ the upper bound $z_k^{\mathcal{E}}(G)$ matches $\alpha(G)$. Thus, $z_k^{\mathcal{E}}(G) = 4$ holds for all $k \geqslant 2$, so $z_k^{\mathcal{E}}(G)$ is an excellent bound on $\alpha(G)$ for this graph. For $G_{60,0.25}$ as k increases $z_k^{\mathcal{E}}(G)$ improves little by little. For $k = 4$ the floor value of $z_k^{\mathcal{E}}(G)$ decreases, which is very important in a branch-and-bound framework, where this potentially reduces the size of the branch-and-bound tree drastically. For the Paley graph on 61 vertices only for $k \geqslant 6$ the value of $z_k^{\mathcal{E}}(G)$ improves towards $\alpha(G)$. This example represents one of the worst cases, where including ESCs for subgraphs of small order does not give an improvement of the upper bound.

Example 1 shows that there are graphs where including ESCs for subgraphs of small order improves the bound very much, little by little and not at all. It is not surprising that the ESH does not give outstanding bounds for all instances, as the stable set problem is NP-hard.

2.3. Representation of exact subgraph constraints

Next, we briefly discuss the implementation of ESCs. In Definition 2 we introduced $\mathrm{STAB}^2(G)$ as convex hull, so the most natural way to formulate the ESC is as a convex combination as in the proof of Lemma 1. We start with the following definition.

Definition 6. Let G be a graph and let G_I be the subgraph induced by $I \subseteq V$. Furthermore, let $|\mathcal{S}(G_I)| = t_I$ and let $\mathcal{S}(G_I) = \left\{s_1^I, \dots, s_{t_I}^I\right\}$. Then the ith stable set matrix S_i^I of G_I is defined as $S_i^I = s_i^I (s_i^I)^T$.

Now the ESC $X_I \in \mathrm{STAB}^2(G_I)$ can be rewritten as

$$X_I \in \mathrm{conv}\left\{S_i^I : 1 \leqslant i \leqslant t_I\right\}$$

and it is natural to implement the ESC for subgraph G_I as

$$X_I = \sum_{i=1}^{t_I} \lambda_i^I S_i^I, \quad \lambda^I \in \Delta_{t_I}.$$

Table 2
The number of facets of $\mathrm{STAB}^2(G_k^0)$ for $k \in \{2, 3, 4, 5, 6\}$.

k	2	3	4	5	6
# facets of $\mathrm{STAB}^2(G_k^0)$	4	16	56	368	116 764

This implies that for the implementation of the ESC for G_I we include t_I additional non-negative variables, one additional equality constraint for λ^I and a matrix equality constraint of size $k_I \times k_I$ that couples X_I and λ^I into (T_{n+1}).

There is also a different possibility to represent ESCs that uses the following fact. The polytope $\mathrm{STAB}^2(G_I)$ is given by its extreme points, which are the stable set matrices of G_I. Due to the Minkowski–Weyl's theorem it can also be represented by its facets, *i.e.* by (finitely many) inequalities. A priory different subgraphs induce different stable set matrices and hence also different squared stable set polytopes. The next result allows us to consider the squared stable set polytope of only one graph for a given order.

Lemma 3. *Let $G = (V, E)$ be a graph with $|V| = n$. Let $G_n^0 = (V_n^0, E^0)$ with $V_n^0 = \{1, \ldots, n\}$ and $E^0 = \emptyset$. Let $X \in \mathcal{S}_n$. If $X_{i,j} = 0$ for all $\{i, j\} \in E$, then*

$$X \in \mathrm{STAB}^2(G) \quad \Leftrightarrow \quad X \in \mathrm{STAB}^2(G_n^0).$$

Proof. If $X \in \mathrm{STAB}^2(G)$, then by definition X is a convex combination of stable set matrices of G. Then it is also a convex combination of stable set matrices of G_n^0, which are all possible stable set matrices of order n. Hence, $X \in \mathrm{STAB}^2(G_n^0)$.

If $X \in \mathrm{STAB}^2(G_n^0)$, then X is a convex combination of all possible stable set matrices of order n. Consider an edge $\{i, j\} \in E$, then by assumption $X_{i,j} = 0$. Since all entries of stable set matrices are 0 or 1, this implies that whenever the entry (i, j) of a stable set matrix in the convex combination is not equal to zero, its coefficient is zero. Therefore, in the convex combination only stable set matrices which are also stable set matrices of G have non-zero coefficients and thus $X \in \mathrm{STAB}^2(G)$. □

As a consequence of Lemma 3 we can replace the ESC $X_I \in \mathrm{STAB}^2(G_I)$ by the constraint $X_I \in \mathrm{STAB}^2(G_{k_I}^0)$ whenever we add the ESC to (T_{n+1}). Thus, it is enough to have a facet representation of $\mathrm{STAB}^2(G_{k_I}^0)$ in order to include the ESC for G_I represented by inequalities into (T_{n+1}).

In order to obtain all facets of $\mathrm{STAB}^2(G_k^0)$ for a given k we can use the fact that a projection of $\mathrm{STAB}^2(G_k^0)$ is the boolean quadric polytope of size k as already explained in Section 2.2. Deza and Laurent [9] called the boolean quadric polytope of size k the correlation polytope of size k. They showed that the correlation polytope of size k is in one-to-one correspondence with the cut polytope of size $k+1$ via the so-called covariance map. Moreover, they presented a complete list of the facets of the cut polytopes up to a size of $k+1 = 7$, gave several references of other lists of facets and furthermore linked to a web page. The recent version of this web page is maintained by Christof [6] and a conjectured complete facet description of the cut polytope of size $k+1 = 8$ and a possibly complete description of the cut polytope of size $k+1 = 9$ can be found there. Therefore, we could take this list and go back via the covariance map to transfer it into a complete list of facets of $\mathrm{STAB}^2(G_k^0)$.

However, we take a more direct path and use the software PORTA [7] in order to obtain all inequalities that represent facets of $\mathrm{STAB}^2(G_k^0)$ from its extreme points for a given k. The number of facets for all $k \leqslant 6$ is presented in Table 2.

Now we briefly present the inequalities that represent facets of $\mathrm{STAB}^2(G_k^0)$ for $k \in \{2, 3\}$. The ESC for a subgraph G_I of order $k_I = 2$ with $I = \{i, j\}$ is equivalent to

$$0 \leqslant X_{i,j} \tag{3a}$$
$$X_{i,j} \leqslant X_{i,i} \tag{3b}$$
$$X_{i,j} \leqslant X_{j,j} \tag{3c}$$
$$X_{i,i} + X_{j,j} \leqslant 1 + X_{i,j}. \tag{3d}$$

For a subgraph G_I of order $k_I = 3$ with $I = \{i, j, k\}$ the ESCs is equivalent to (3) for all three sets $\{i, j\}$, $\{i, \ell\}$ and $\{j, \ell\}$ and the following inequalities

$$X_{i,j} + X_{i,\ell} \leqslant X_{i,i} + X_{j,\ell} \tag{4a}$$
$$X_{i,j} + X_{j,\ell} \leqslant X_{j,j} + X_{i,\ell} \tag{4b}$$
$$X_{i,\ell} + X_{j,\ell} \leqslant X_{\ell,\ell} + X_{i,j} \tag{4c}$$
$$X_{i,i} + X_{j,j} + X_{\ell,\ell} \leqslant 1 + X_{i,j} + X_{i,\ell} + X_{j,\ell}, \tag{4d}$$

so $3 \cdot 4 + 4 = 16$ inequalities, which matches Table 2. We come back to these inequalities in Sections 2.4 and 3.4.

To summarize, we have discussed two different options to represent ESCs, one as convex combination and one as inequalities that represent facets.

2.4. Comparison to other hierarchies

In this section we compare the ESH for the stable set problem to other hierarchies, as it has never been done before.

The most prominent hierarchies of relaxations for general 0–1 programming problems are the hierarchies by Sherali and Adams [29], by Lovász and Schrijver [25] and by Lasserre [22]. We refer to Laurent [23] for rigorous definitions, comparisons and for details of applying them to the stable set problem.

In fact the Lasserre hierarchy is a refinement of the Sherali–Adams hierarchy which is a refinement of the SDP based Lovász–Schrijver hierarchy. All three hierarchies are exact at level $\alpha(G)$, so after at most $\alpha(G)$ steps STAB(G) is obtained.

Silvestri [30] observed that $z_2^{\mathcal{E}}(G)$ is at least as good as the upper bound obtained at the first level of the SDP hierarchy of Lovász–Schrijver. This is easy to see, because this SDP is (T_{n+1}) with non-negativity constraints for X, and every $X_I \in$ STAB(G_I) is entry-wise non-negative due to (3a). Furthermore, Silvestri proved that the bound on the kth level of the Lasserre hierarchy is at least as good as $z_k^{\mathcal{E}}(G)$, so the Lasserre hierarchy yields stronger relaxations than the ESH.

A drawback of all the above hierarchies is that the size of the SDPs to solve grows at each level. In particular, the SDP at the kth level of the Lasserre hierarchy has a matrix variable with one row for each subset of i vertices of the n vertices for every $1 \leqslant i \leqslant k$. Therefore, the matrix variable is of order $\sum_{i=0}^{k} \binom{n}{i}$. For the ESH this order remains $n+1$ on each level and only the number of constraints increases.

Another big advantage of the ESH over the Lasserre hierarchy is that it is possible to include partial information of the kth level of the hierarchy, which was exploited by Gaar and Rendl [13–15]. In the case of the Lasserre hierarchy one needs the whole huge matrix in order to incorporate the information. Due to that Gvozdenović, Laurent and Vallentin [20] introduced a new hierarchy where they only consider suitable principal submatrices of the huge matrix.

Eventually we want to compare the ESH with other relaxations of $\vartheta(G)$ towards $\alpha(G)$. Lovász and Schrijver [25] proposed to add inequalities that boil down to (3a), and inequalities of the form (4c) and (4d) whenever $\{i,j\} \in E$. Hence, $z_k^{\mathcal{E}}(G)$ is as least as good as this bound for all $k \geqslant 3$. Furthermore, Gruber and Rendl [19] proposed to add inequalities of the form (4c) and (4d) also if $\{i,j\} \notin E$, hence the kth level of the ESH is as least as strong as this relaxation for every $k \geqslant 3$.

Note that Fischer, Gruber, Rendl and Sotirov [12] add triangle inequalities into an SDP relaxation of Max-Cut. Therefore, applying the ESH to the Max-Cut relaxation as it is done by in [15] can be viewed as generalization of the approach in [12].

For a discussion of other approaches for improving a relaxation by including information of smaller polytopes into the relaxation see [1].

3. The compressed exact subgraph hierarchy

In this section we newly introduce a variant of the ESH, namely the compressed ESH, which at first sight is computational favorable to the ESH, as it starts from a smaller SDP formulation of the Lovász theta function. Additionally, we compare this new hierarchy to the ESH and to other hierarchies from the literature.

3.1. Two SDP formulations of the Lovász theta function

The starting point of the new compressed ESH is an SDP formulation of the Lovász theta function $\vartheta(G)$ by Lovász [24], namely

$$\begin{aligned} \vartheta(G) = \max \quad & \langle \mathbb{1}_{n\times n}, X \rangle \\ \text{s.t.} \quad & \operatorname{trace}(X) = 1 \\ & X_{i,j} = 0 \quad \forall \{i,j\} \in E \\ & X \succcurlyeq 0 \\ & X \in \mathcal{S}_n. \end{aligned} \tag{T_n}$$

As the feasible region of (T_n) will be used later, we define

$$\mathrm{CTH}^2(G) = \left\{ X \in \mathcal{S}_n : \operatorname{trace}(X) = 1,\ X_{i,j} = 0 \quad \forall \{i,j\} \in E,\ X \succcurlyeq 0 \right\}.$$

Before we continue, we compare the two SDP formulations (T_{n+1}) and (T_n) of $\vartheta(G)$. As already mentioned (T_{n+1}) is an SDP with a matrix variable of order $n+1$ and $n+m+1$ equality constraints. The formulation (T_n) has a matrix variable of order n and $m+1$ constraints, so both the number of variables and constraints is smaller. Hence, in computations (T_n) seems favorable.

So far, there has been a lot of work on comparing (T_{n+1}) and (T_n). Gruber and Rendl [19] showed the following. If (x^*, X^*) is a feasible solution of (T_{n+1}), then $X' = \frac{1}{\operatorname{trace}(X^*)} X^*$ is a feasible solution of (T_n) which has at least the same objective function value. Hence, an optimal solution of (T_{n+1}) can be transformed into an optimal solution of (T_n). They also proved that whenever X' is optimal for (T_n), then $X^* = \langle \mathbb{1}_{n\times n}, X' \rangle X'$ is optimal for (T_{n+1}). Furthermore, Yildirim and Fan-Orzechowski [31] gave a transformation from a feasible solution X' of (T_n) to obtain x^* of a feasible solution (x^*, X^*) of (T_{n+1}) with at least the same objective function value. Galli and Letchford [16] showed how to construct a corresponding X^*. For an optimal X' the obtained optimal (x^*, X^*) coincides with the one of Gruber and Rendl. Further details can be found in [16], where also the influence of adding certain cutting planes into (T_{n+1}) and (T_n) is discussed. We come back to that later in Section 3.4.

3.2. Introduction of the compressed exact subgraph hierarchy

Next, we newly introduce the compressed exact subgraph hierarchy, a hierarchy similar to the ESH, but it starts from (T_n) instead of starting from (T_{n+1}). First, we verify that it makes sense to build such a hierarchy.

Lemma 4. *If we add the constraint $X \in \mathrm{STAB}^2(G)$ into (T_n) for a graph G, then the optimal objective function value is $\alpha(G)$, so*

$$\alpha(G) = \max\left\{\langle \mathbb{1}_{n\times n}, X\rangle : X \in \mathrm{CTH}^2(G),\ X \in \mathrm{STAB}^2(G)\right\}. \tag{5}$$

Proof. Let $(P^{\mathcal{C}})$ be the SDP on the right-hand side of (5), let $z^{\mathcal{C}}$ be its optimal objective function value and let $\mathcal{S}(G) = \{s_1, \dots, s_t\}$.

Let without loss of generality s_t be the incidence vector of a maximum stable set of G, and s_1 be the incidence vector of the empty set, which is of course stable. Then clearly $X = \frac{1}{\alpha(G)} s_t s_t^T + \left(1 - \frac{1}{\alpha(G)}\right) s_1 s_1^T$ is feasible for $(P^{\mathcal{C}}_\alpha)$ and has objective function value $\alpha(G)$, so $\alpha(G) \leqslant z^{\mathcal{C}}$ holds.

Furthermore, any feasible solution X of $(P^{\mathcal{C}})$ can be written as

$$X = \sum_{i=1}^{t} \lambda_i s_i s_i^T$$

for some $\lambda \in \Delta_t$ because $X \in \mathrm{STAB}^2(G)$ holds, and it fulfills

$$1 = \mathrm{trace}(X) = \sum_{i=1}^{t} \lambda_i \,\mathrm{trace}(s_i s_i^T) = \sum_{i=1}^{t} \lambda_i \mathbb{1}_n^T s_i.$$

In consequence, the objective function value of X for $(P^{\mathcal{C}})$ is equal to

$$\langle \mathbb{1}_{n\times n}, X\rangle = \sum_{i=1}^{t} \lambda_i \langle \mathbb{1}_{n\times n}, s_i s_i^T\rangle = \sum_{i=1}^{t} \lambda_i (\mathbb{1}_n^T s_i)^2 \leqslant \alpha(G) \sum_{i=1}^{t} \lambda_i \mathbb{1}_n^T s_i = \alpha(G)$$

and hence $z^{\mathcal{C}} \leqslant \alpha(G)$ holds, which finishes the proof. □

Lemma 4 corresponds to Lemma 1 for the ESH and justifies the introduction of the compressed exact subgraph hierarchy.

Definition 7. Let $G = (V, E)$ be a graph with $|V| = n$ and let J be a set of subsets of V. Then $z_J^{\mathcal{C}}(G)$ is the optimal objective function of (T_n) with the ESC for every subgraph induced by a set in J, so

$$z_J^{\mathcal{C}}(G) = \max\left\{\langle \mathbb{1}_{n\times n}, X\rangle : X \in \mathrm{CTH}^2(G),\ X_I \in \mathrm{STAB}^2(G_I) \quad \forall I \in J\right\}. \tag{6}$$

For $k \in \mathbb{N}_0$ with $k \leqslant n$ the kth level of the compressed exact subgraph hierarchy (CESH) is defined as $z_k^{\mathcal{C}}(G) = z_{J_k}^{\mathcal{C}}(G)$.

As in the case of the ESH we can deduce the following result for the CESH.

Lemma 5. *Let $G = (V, E)$ be a graph with $|V| = n$. Then*

$$\vartheta(G) = z_0^{\mathcal{C}}(G) = z_1^{\mathcal{C}}(G) \geqslant z_{k-1}^{\mathcal{C}}(G) \geqslant z_k^{\mathcal{C}}(G) \geqslant z_n^{\mathcal{C}}(G) = \alpha(G)$$

holds for all $k \in \{1, \dots, n\}$.

Proof. Analogous to the proof of Lemma 2. □

Hence, due to Lemmas 2 and 5 both the ESH and the CESH start at $\vartheta(G)$ at level 1 and reach $\alpha(G)$ on level n.

3.3. Comparison to other hierarchies

Before we continue to consider the differences between the ESH and the CESH, we compare the CESH with other relaxations of $\alpha(G)$ based on (T_n).

Schrijver [28] suggested to add non-negativity constraints into (T_n) to obtain stronger bounds. Galli and Letchford [16] proved that it is equivalent to include non-negativity constraints into (T_{n+1}) and (T_n), so $z_2^{\mathcal{E}}(G)$ is a stronger bound than this one because it induces non-negativity in (T_{n+1}). Lemma 3 implies that also for (T_n) it is equivalent to include $X_I \in \mathrm{STAB}^2(G_I)$ and $X_I \in \mathrm{STAB}^2(G_{k_I}^0)$, so $z_2^{\mathcal{C}}(G)$ induces non-negativity due to (3a). Hence, also $z_2^{\mathcal{C}}(G)$ is as least as good as the bound of Schrijver.

Dukanovic and Rendl [11] proposed to add so-called triangle inequalities to (T_n). Silvestri [30] showed that $z_3^{\mathcal{C}}(G)$ is at least as good as upper bound as the bound of Dukanovic and Rendl. This is intuitive, because the triangle inequalities correspond to (4a), (4b) and (4c) and therefore represent faces of $\mathrm{STAB}^2(G_I)$ for $k_I = 3$. As a result, the CESH can be seen as a generalization of the relaxation of [11].

3.4. Comparison of the CESH and the ESH

Now we continue our comparison of the bounds based on the ESH and our new CESH.

Theorem 1. *Let $G = (V, E)$ be a graph with $|V| = n$ and let J be a set of subsets of V. Then $z_J^{\mathcal{E}}(G) \leqslant z_J^{\mathcal{C}}(G)$.*

Proof. We consider the transformation of an optimal solution of (T_{n+1}) into an optimal solution of (T_n) by Gruber and Rendl [19]. We show that this transformation applied to the optimal solution of (2) yields a feasible solution of (6) with at least the same objective function value, thus $z_J^{\mathcal{E}}(G) \leqslant z_J^{\mathcal{C}}(G)$ holds.

Towards that end, let (x^*, X^*) be an optimal solution of (2) and $\gamma = z_J^{\mathcal{E}}(G) = \mathbb{1}_n^T x^*$ its objective function value. Let $X' = \frac{1}{\gamma} X^*$.

First, we show that X' is feasible for (6). Clearly $X^* - x^*(x^*)^T \succcurlyeq 0$ and $\gamma \geqslant 0$ imply $X' \succcurlyeq 0$. Furthermore, due to $X^*_{i,j} = 0$ for all $\{i, j\} \in E$ we have $X'_{i,j} = 0$ for all $\{i, j\} \in E$. Additional to that

$$\operatorname{trace}(X') = \frac{1}{\gamma}\operatorname{trace}(X^*) = \frac{1}{\gamma}\mathbb{1}_n^T x^* = \frac{1}{\gamma}\gamma = 1,$$

so X' is feasible for (T_n).

What is left to check for feasibility are the ESCs. We can rewrite $X_I^* \in \mathrm{STAB}^2(G_I)$ as $X_I^* = \sum_{i=1}^{t_I} \lambda_i^I S_i^I$ for $\sum_{i=1}^{t_I} \lambda_i^I = 1$ and $\lambda_i^I \geqslant 0$ for all $1 \leqslant i \leqslant t_I$. Let w.l.o.g. S_1^I be the zero matrix of dimension $k_I \times k_I$, *i.e.* the first stable set matrix corresponds to the empty set. Then we define

$$\lambda_i^{I\prime} = \begin{cases} \frac{1}{\gamma}\lambda_i^I & \text{for } 2 \leqslant i \leqslant t_I \\ \frac{1}{\gamma}\lambda_i^I + \frac{\gamma-1}{\gamma} & \text{for } i = 1. \end{cases}$$

It is easy to see that $\lambda_i^{I\prime} \geqslant 0$ for all $1 \leqslant i \leqslant t_I$ and that

$$\sum_{i=1}^{t_I} \lambda_i^{I\prime} = \frac{1}{\gamma}\lambda_1^I + \frac{\gamma-1}{\gamma} + \frac{1}{\gamma}\sum_{i=2}^{t_I}\lambda_i^I = \frac{1}{\gamma} + \frac{\gamma-1}{\gamma} = 1$$

holds. Furthermore, because S_1^I is a zero matrix and so $\frac{\gamma-1}{\gamma}S_1^I = 0$, we have

$$X_I' = \frac{1}{\gamma}X_I^* = \sum_{i=1}^{t_I}\frac{1}{\gamma}\lambda_i^I S_i^I = \left(\frac{1}{\gamma}\lambda_i^I + \frac{\gamma-1}{\gamma}\right)S_1^I + \sum_{i=2}^{t_I}\lambda_i^{I\prime}S_i^I = \sum_{i=1}^{t_I}\lambda_i^{I\prime}S_i^I.$$

As a consequence $X_I' \in \mathrm{STAB}^2(G_I)$ and thus X_I' is feasible for (6).

It remains to determine the objective function value of X_I' for (6). From $X^* - x^*(x^*)^T \succcurlyeq 0$ it follows that $\mathbb{1}_n^T(X^* - x^*(x^*)^T)\mathbb{1}_n \geqslant 0$ and hence $\langle \mathbb{1}_{n\times n}, X^* - x^*(x^*)^T\rangle \geqslant 0$. This implies that

$$\langle \mathbb{1}_{n\times n}, X^*\rangle \geqslant \langle \mathbb{1}_{n\times n}, x^*(x^*)^T\rangle = \mathbb{1}_n^T x^*(x^*)^T\mathbb{1}_n = (\mathbb{1}_n^T x^*)^2 = \gamma^2$$

holds, thus

$$\langle \mathbb{1}_{n\times n}, X'\rangle = \frac{1}{\gamma}\langle \mathbb{1}_{n\times n}, X^*\rangle \geqslant \frac{1}{\gamma}\gamma^2 = \gamma.$$

To summarize, X' is a feasible solution of (6) with objective function value $\gamma = z_J^{\mathcal{E}}(G)$. Therefore, the optimal objective function value of the maximization problem (6) is at least $z_J^{\mathcal{E}}(G)$, so $z_J^{\mathcal{E}}(G) \leqslant z_J^{\mathcal{C}}(G)$. □

Theorem 1 states that the bounds obtained by starting from (T_{n+1}) and including some ESCs is always at least as good as the bound obtained by starting from (T_n) and including the same ESCs. In particular, this implies that the relaxation on the kth level of the ESH is at least as good as the relaxation on the kth level of the CESH, which is formalized in the following corollary.

Corollary 1. *Let $G = (V, E)$ be a graph with $|V| = n$ and let $k \in \mathbb{N}_0$, $k \leqslant n$. Then $z_k^{\mathcal{E}}(G) \leqslant z_k^{\mathcal{C}}(G)$.*

We now further investigate the theoretical difference between the ESH and the CESH, especially in the light of the results of Galli and Letchford [16]. They proved that whenever a collection of homogeneous inequalities is added to (T_{n+1}), the resulting optimal solution yields a feasible solution for (T_n) with the same collection of inequalities, which has at least the same objective function value. This implies that adding homogeneous inequalities to (T_{n+1}) gives stronger bounds on $\alpha(G)$ than adding the same inequalities to (T_n).

If we consider the ESCs in more detail as we did in Section 2.3, then in turns out that for $k = 2$ the inequalities (3a), (3b) and (3c) are homogeneous, while (3d) is inhomogeneous, so inhomogeneous inequalities are needed to represent ESCs.

Next, we give an intuition for the different behavior of inhomogeneous inequalities for the two SDP formulations of the Lovász theta function (T_{n+1}) and (T_n). Let (x^*, X^*) be an optimal solution of (T_{n+1}) with additional constraints (3). From the proof of Theorem 1 we know that $X' = \frac{1}{\gamma}X^*$ is a feasible solution of (T_n) with additional constraints (3). Indeed, the homogeneous inequalities (3a), (3b) and (3c) are preserved under scaling, matching [16]. Scaling (3d) with $\frac{1}{\gamma}$ yields that X' satisfies

$$X'_{i,i} + X'_{j,j} \leqslant \frac{1}{\gamma} + X'_{i,j}$$

and since $\frac{1}{\gamma} \leqslant 1$ it follows that X' satisfies (3d).

If X' is an optimal solution of (T_n) with additional constraints (3) and we use the transformation $X^* = \gamma X'$, then clearly X^* satisfies (3a), (3b) and (3c). Scaling (3d) with γ yields that

$$X^*_{i,i} + X^*_{j,j} \leqslant \gamma + X^*_{i,j}$$

holds for X^*. This does not imply that X^* fulfills (3d) as $\gamma \geqslant 1$.

To summarize, this consideration confirms that the ESCs for $k_I = 2$ yield a stronger restriction in (T_{n+1}) than they do in (T_n). This gap of the bounds gets even larger for larger k_I, so for example for $k_I = 3$ the inequality (4d) is inhomogeneous. This concludes our investigation of the new CESH.

4. The scaled exact subgraph hierarchy

In Section 3 we saw that including an ESC into (T_{n+1}) as in the ESH gives a stronger bound than including the same ESC into (T_n) as in the CESH. In this section we investigate whether this is due to a suboptimal definition of the ESCs for the later case. In particular, we go back to the intuition behind ESCs for (T_{n+1}) and transfer this intuition to (T_n). This will lead to the new definitions of scaled ESCs and the scaled ESH. We will explore this hierarchy and compare the CESH and the scaled ESH in detail.

4.1. Introduction of the scaled exact subgraph hierarchy

To start, observe the following. It can be confirmed easily that both (T_{n+1}) and (T_n) are upper bounds on $\alpha(G)$. Let $s \in \mathcal{S}(G)$ be a stable set vector that corresponds to a maximum stable set. Then $X^* = ss^T$ is feasible for (T_{n+1}) and has objective function value $\alpha(G)$. Therefore, intuitively $\mathrm{STAB}^2(G)$ defines exactly the appropriate polytope for (T_{n+1}).

For (T_n) the matrix $X' = \frac{1}{s^Ts}ss^T$ yields a feasible solution with objective function value $\alpha(G)$, whereas $X^* = ss^T$ is not feasible unless $\alpha(G) = 1$. Hence, intuitively it makes more sense to consider the polytope spanned by matrices of the form $\frac{1}{s^Ts}ss^T$ for $s \in \mathcal{S}(G)$ for (T_n) than to consider $\mathrm{STAB}^2(G)$. This leads to the following definition.

Definition 8. Let $G = (V, E)$ be a graph with $|V| = n$. Then the scaled squared stable set polytope $\mathrm{SSTAB}^2(G)$ of G is defined as

$$\mathrm{SSTAB}^2(G) = \mathrm{conv}\left(\left\{\frac{1}{s^Ts}ss^T : s \in \mathcal{S}(G),\ s \neq \mathbb{0}_n\right\} \cup \{\mathbb{0}_{n\times n}\}\right).$$

The goal of this section is to investigate a new modified version of the CESH based on the scaled squared stable set polytope defined in the following way.

Definition 9. Let $G = (V, E)$ be a graph and let $I \subseteq V$. Then the scaled exact subgraph constraint (SESC) for G_I is defined as $X_I \in \mathrm{SSTAB}^2(G_I)$. Furthermore, let $|V| = n$ and let J be a set of subsets of V. Then $z_J^{\mathcal{S}}(G)$ is the optimal objective function value of (T_n) with the SESC for every subgraph induced by a set in J, so

$$z_J^{\mathcal{S}}(G) = \max\left\{\langle \mathbb{1}_{n\times n}, X\rangle : X \in \mathrm{CTH}^2(G),\ X_I \in \mathrm{SSTAB}^2(G_I) \quad \forall I \in J\right\}. \tag{7}$$

For $k \in \mathbb{N}_0$ with $k \leqslant n$ the kth level of the scaled exact subgraph hierarchy (SESH) is defined as $z_k^{\mathcal{S}}(G) = z_{J_k}^{\mathcal{S}}(G)$.

Note that with the considerations above it does not make sense to include the SESC for the whole graph G into (T_{n+1}), as this SDP does not yield an upper bound on $\alpha(G)$, because all solutions corresponding to $\alpha(G)$ are not feasible. Hence, we introduce a hierarchy based on SESCs only starting from (T_n) and not from (T_{n+1}).

Additionally, note that a priory we do not know whether the SESH has as nice properties as the ESH and the CESH.

4.2. Comparison of the SESH and the CESH

The next lemma is the key ingredient to compare the SESH to the CESH.

Lemma 6. *Let $G = (V, E)$ be a graph. Then $X \in \mathrm{SSTAB}^2(G)$ holds if and only if $X \in \mathrm{STAB}^2(G)$ and $\mathrm{trace}(X) \leqslant 1$.*

Proof. Let $\mathcal{S}(G) = \{s_1, \dots, s_t\}$ and let w.l.o.g. $s_1 = \mathbb{0}_n$, *i.e.* the first stable set is the empty set.

If $X \in \mathrm{SSTAB}^2(G)$, then X can be written as

$$X = \widetilde{\lambda}_1 \mathbb{0}_{n\times n} + \sum_{i=2}^{t} \widetilde{\lambda}_i \frac{1}{s_i^T s_i} s_i s_i^T$$

for some $\widetilde{\lambda} \in \Delta_t$. It is easy to see that

$$\mathrm{trace}(X) = \widetilde{\lambda}_1 \,\mathrm{trace}(\mathbb{0}_{n\times n}) + \sum_{i=2}^{t} \widetilde{\lambda}_i \frac{1}{s_i^T s_i}\, \mathrm{trace}(s_i s_i^T) = \sum_{i=2}^{t} \widetilde{\lambda}_i \leqslant 1$$

holds. We define $\lambda_i = \widetilde{\lambda}_i \frac{1}{s_i^T s_i}$ for $2 \leqslant i \leqslant t$. Then clearly $\widetilde{\lambda}_i \geqslant \widetilde{\lambda}_i \frac{1}{s_i^T s_i} = \lambda_i \geqslant 0$ holds because $s_i^T s_i \geqslant 1$ for all $2 \leqslant i \leqslant t$. Let $\lambda_1 = 1 - \sum_{i=2}^{t} \lambda_i$, then $\lambda_1 \geqslant 1 - \sum_{i=2}^{t} \widetilde{\lambda}_i = \widetilde{\lambda}_1 \geqslant 0$ holds. Hence

$$X = \lambda_1 \mathbb{0}_{n\times n} + \sum_{i=2}^{t} \lambda_i s_i s_i^T$$

for $\lambda \in \Delta_t$ and therefore $X \in \mathrm{STAB}^2(G)$. Hence, $X \in \mathrm{SSTAB}^2(G)$ implies that $X \in \mathrm{STAB}^2(G)$ and $\mathrm{trace}(X) \leqslant 1$ holds.

Now assume $X \in \mathrm{STAB}^2(G)$ and $\mathrm{trace}(X) \leqslant 1$. Then X can be rewritten as

$$X = \lambda_1 \mathbb{0}_{n\times n} + \sum_{i=2}^{t} \lambda_i s_i s_i^T$$

for some $\lambda \in \Delta_t$. Then, because $\mathrm{trace}(s_i s_i^T) = s_i^T s_i$, we have

$$1 \geqslant \mathrm{trace}(X) = \lambda_1 \,\mathrm{trace}(\mathbb{0}_{n\times n}) + \sum_{i=2}^{t} \lambda_i \,\mathrm{trace}(s_i s_i^T) = \sum_{i=2}^{t} \lambda_i s_i^T s_i. \tag{8}$$

We define $\widetilde{\lambda}_i = \lambda_i s_i^T s_i$ for $2 \leqslant i \leqslant t$ and $\widetilde{\lambda}_1 = 1 - \sum_{i=2}^{t} \widetilde{\lambda}_i$. Then clearly $\widetilde{\lambda}_i \geqslant 0$ holds for $2 \leqslant i \leqslant t$. Furthermore, (8) implies that $\widetilde{\lambda}_1 \geqslant 0$ holds, so $\widetilde{\lambda} \in \Delta_t$. This together with

$$X = \widetilde{\lambda}_1 \mathbb{0}_{n\times n} + \sum_{i=2}^{t} \widetilde{\lambda}_i \frac{1}{s_i^T s_i} s_i s_i^T$$

implies that $X \in \mathrm{SSTAB}^2(G)$. □

Lemma 6 allows us to prove the following.

Theorem 2. *Let $G = (V, E)$ be a graph and let J be a set of subsets of V. Then $z_J^{\mathcal{S}}(G) = z_J^{\mathcal{C}}(G)$. In particular, $z_k^{\mathcal{S}}(G) = z_k^{\mathcal{C}}(G)$.*

Proof. Due to Lemma 6 the SESC $X_I \in \mathrm{SSTAB}^2(G_I)$ in $z_J^{\mathcal{S}}(G)$ can be replaced by the ESC $X_I \in \mathrm{STAB}^2(G_I)$ and $\mathrm{trace}(X_I) \leqslant 1$. The latter is redundant, as $\mathrm{trace}(X) = 1$ is fulfilled by all $X \in \mathrm{CTH}^2(G)$ and all elements on the main diagonal of X are non-negative because $X \succcurlyeq 0$. Thus, $z_J^{\mathcal{S}}(G) = z_J^{\mathcal{C}}(G)$ and $z_k^{\mathcal{S}}(G) = z_k^{\mathcal{C}}(G)$ hold. □

Theorem 2 implies that the SESH and the CESH coincide and in particular that the SESH has the same properties as the CESH stated in Lemma 2, which we now formulate explicitly.

Corollary 2. *Let $G = (V, E)$ be a graph with $|V| = n$. Then*

$$\vartheta(G) = z_0^{\mathcal{S}}(G) = z_1^{\mathcal{S}}(G) \geqslant z_{k-1}^{\mathcal{S}}(G) \geqslant z_k^{\mathcal{S}}(G) \geqslant z_n^{\mathcal{S}}(G) = \alpha(G)$$

holds for all $k \in \{1, \dots, n\}$.

Hence, even though intuitively it makes more sense to add SESCs into (T_n) instead of ESCs, both versions give the same bound and the SESH and the CESH coincide.

5. Computational comparison

In the previous sections we have theoretically investigated first the original ESH, which starts from (T_{n+1}) and includes ESCs. Next, we introduced the CESH, which starts from (T_n) and includes ESCs and finally the SESH which starts from (T_n) and includes SESCs. Each of these hierarchies can be exploited computationally by including a wisely chosen subset J of all possible ESCs or SESCs. We denote the resulting bounds based on the ESH, the CESH and the SESH by $z_J^{\mathcal{E}}(G)$, $z_J^{\mathcal{C}}(G)$ and

$z_J^{\mathcal{S}}(G)$, respectively. So far we have proven in Theorems 1 and 2 that $z_J^{\mathcal{S}}(G) = z_J^{\mathcal{C}}(G) \geqslant z_J^{\mathcal{E}}(G)$ holds for all graphs G and for all set of subsets J, hence the bounds based on the CESH and the SESH coincide and the bounds based on the ESH are always as least as good as those bounds.

In this section we compare the ESH and the CESH computationally. We refrain from computations with SESH since both the obtained bounds and the sizes of the SDPs are the same for SESH and CESH. First, we are interested in whether $z_J^{\mathcal{E}}(G)$ is significantly better than $z_J^{\mathcal{C}}(G)$. Second, we are interested in the running times. In theory, the running times for $z_J^{\mathcal{C}}(G)$ should be smaller, because the matrix variable is of order n instead of $n+1$ and the number of equality constraints is n less.

We consider several graphs in various settings. Some graphs are from the Erdős–Rényi model $G(n, p)$ for different values of n and p (the probability that an edge is present in the graph), some are complement graphs of graphs of the second DIMACS implementation challenge [10] and some come from the house of graphs collection [5]. Furthermore, there is a spin glass graph (see [12]), a Paley graph, a circulant and a cubic graph among the instances. In the computations we always compare including all ESCs of the same set J into (T_{n+1}) and (T_n), so we compute $z_J^{\mathcal{E}}(G)$ and $z_J^{\mathcal{C}}(G)$. The source code and all the used graphs are available online at https://arxiv.org/src/2003.13605/anc.

All computations are done on an Intel(R) Core(TM) i7-7700 CPU @ 3.60 GHz with 32 GB RAM with MATLAB. We use the interior point solver MOSEK [26] for solving the SDPs. Note that there is a lot of research on how to solve SDPs of the form (2) much faster using the bundle method, see Gaar [13] and Gaar and Rendl [14,15]. We refrain from using these involved methods, as we are interested in comparing the bounds in a simple way.

In the first experiment, we compare levels of the ESH and the CESH. For including all possible ESCs of order k into a graph of order n we have $\binom{n}{k}$ additional ESCs to the SDPs (T_{n+1}) and (T_n), so these computations are out of reach rather quickly. Table 3 summarizes the values of $z_J^{\mathcal{C}}(G)$ and $z_J^{\mathcal{E}}(G)$ for including all ESCs for $k \in \{0, 2, 3, 4\}$ and presents the running times in seconds to solve the corresponding SDPs.

First, we note that indeed the computation of $\vartheta(G)$ (corresponds to the column $k = 0$) yields the same value for computing it via (T_{n+1}) and (T_n). Furthermore, the computations confirm that $z_J^{\mathcal{E}}(G) \leqslant z_J^{\mathcal{C}}(G)$ holds for all graphs G. On the second level of the ESH and the CESH the two values coincide for almost all graphs. Only the instances HoG_34272, HoG_34274 and HoG_34276 show a significant difference. On the third and fourth level the difference is more substantial. This is not surprising, as there are more inhomogeneous facets defining STAB^2 in these cases. In the running times there is almost no difference for small graphs with not so many ESCs. Only if the number of ESCs becomes larger, typically the computation time for $z_J^{\mathcal{C}}(G)$ is significantly shorter. However, most of the times this comes with a worse bound.

Computing the kth level of the ESH and the CESH by including all ESCs of order k is beyond reach rather soon, so in the next experiments we want to include the ESCs only for some subgraphs of a given order k. In order to determine the set J of subgraphs for which to include the ESCs we follow the approach of Gaar and Rendl [14,15]. In particular, we start with $J = \emptyset$ and iteratively solve an SDP for computing the Lovász theta function (either (T_{n+1}) and (T_n)) with the already determined ESCs induced by J. Then we use the optimal solution of the SDP in order to search for violated ESCs. To find potentially violated subgraphs we perform a heuristic search among all subgraphs that tries to minimize the inner product of the optimal solution corresponding a subgraph and certain matrices (*e.g.*, matrices that induce facets of $\mathrm{STAB}^2(G_k^0)$). We refer to [14,15] for more details. We perform 10 iterations with including at most 200 ESCs of order k in each iteration, so in the end for each graph and for each k we have a set J of at most 2000 ESCs. Of course it makes a difference whether we do the search starting from (T_{n+1}) and (T_n) as different subgraphs might be violated. We denote by $J_{\mathcal{E}}$ and $J_{\mathcal{C}}$ the set of subsets obtained by using (T_{n+1}) and (T_n) in order to search for violated subgraphs. The used sets $J_{\mathcal{E}}$ and $J_{\mathcal{C}}$ are available online at https://arxiv.org/src/2003.13605/anc. Table 4 summarizes the cardinalities of $J_{\mathcal{E}}$ and $J_{\mathcal{C}}$. The values of $z_J^{\mathcal{E}}(G)$ and $z_J^{\mathcal{C}}(G)$ and the running time for the sets $J = J_{\mathcal{E}}$ can be found in Tables 5 and 6. The analogous computational results when considering $J = J_{\mathcal{C}}$ are presented in Tables 7 and 8.

First, observe in Table 4 that the cardinality of $J_{\mathcal{C}}$ is typically larger compared to the cardinality of $J_{\mathcal{E}}$. This is plausible, because due to the additional row and column in (T_{n+1}) and the SDP constraint in this formulation some ECSs might be satisfied, which are violated in the version with (T_n).

When we turn to the values of $z_J^{\mathcal{E}}(G)$ and $z_J^{\mathcal{C}}(G)$ in Tables 5 and 7 we observe for both $J = J_{\mathcal{E}}$ and $J = J_{\mathcal{C}}$ that (a) the larger k becomes, the better the bounds are, (b) for $k = 0$, so for computing $\vartheta(G)$, we have $z_J^{\mathcal{E}}(G) = z_J^{\mathcal{C}}(G)$ as expected, (c) for a fixed set J we have $z_J^{\mathcal{E}}(G) \leqslant z_J^{\mathcal{C}}(G)$ in accordance with the theory derived earlier and (d) typically the difference between $z_J^{\mathcal{E}}(G)$ and $z_J^{\mathcal{C}}(G)$ increases with increasing k. This behavior is observable for both $J = J_{\mathcal{E}}$ and $J = J_{\mathcal{C}}$, hence the choice of the set J has no significant influence on the behavior of the values of $z_J^{\mathcal{E}}(G)$ and $z_J^{\mathcal{C}}(G)$.

However, we observe that usually the values of $z_J^{\mathcal{E}}(G)$ for $J_{\mathcal{E}}$ are the best bounds, then $z_J^{\mathcal{E}}(G)$ for $J_{\mathcal{C}}$ are the second best bounds, $z_J^{\mathcal{C}}(G)$ for $J_{\mathcal{C}}$ are the third best bounds and $z_J^{\mathcal{C}}(G)$ for $J_{\mathcal{E}}$ yields the worst bounds — even if the differences are typically very small. This behavior is not surprising, because we know that for a fixed set J we have $z_J^{\mathcal{E}}(G) \leqslant z_J^{\mathcal{C}}(G)$ and it makes sense that the final bounds obtained are better when using the same formulation of $\vartheta(G)$ to obtain the bounds that was used to obtain J.

Looking at the running times in Tables 6 and 8 we see that our expectations are not met: Even though the order of the matrix variable and the number of constraints of the SDP to compute $z_J^{\mathcal{C}}(G)$ are smaller than those to compute $z_J^{\mathcal{E}}(G)$, the running times are typically larger. So apparently the highly sophisticated interior point solver MOSEK can deal better with $z_J^{\mathcal{E}}(G)$. If we compare the running times for the set $J = J_{\mathcal{E}}$ and $J = J_{\mathcal{C}}$ we see that the running times for $J_{\mathcal{E}}$ typically

Table 3
The values of $z_J^{\mathcal{E}}(G)$ and $z_J^{\mathcal{C}}(G)$ for different graphs G with including all ESCs of order 0 (corresponds to $\vartheta(G)$), 2, 3 and 4 and the running times to compute the values.

Name	n / m		Value of $z_J^{\mathcal{E}}/z_J^{\mathcal{C}}$				Running time			
			$\vartheta(G)$	$J=J_2$	$J=J_3$	$J=J_4$	$\vartheta(G)$	$J=J_2$	$J=J_3$	$J=J_4$
HoG_34272	9	$z_J^{\mathcal{E}}$	3.3380	3.2729	3.0605	3.0000	0.03	0.04	0.35	0.42
	17	$z_J^{\mathcal{C}}$	3.3380	3.2763	3.1765	3.0000	0.03	0.04	0.10	0.19
HoG_15599	20	$z_J^{\mathcal{E}}$	7.8202	7.8202	7.4437	7.0000	0.05	0.12	15.63	2545.20
	44	$z_J^{\mathcal{C}}$	7.8202	7.8202	7.4761	7.4291	0.04	0.11	16.27	3439.99
CubicVT26_5	26	$z_J^{\mathcal{E}}$	11.8171	11.8171	10.9961	–	0.04	0.25	101.19	–
	39	$z_J^{\mathcal{C}}$	11.8171	11.8171	11.0035		0.04	0.22	99.11	
HoG_34274	36	$z_J^{\mathcal{E}}$	13.2317	13.0915	12.1661	–	0.05	1.27	4026.75	–
	72	$z_J^{\mathcal{C}}$	13.2317	13.1052	12.5881		0.05	1.39	3700.50	
HoG_6575	45	$z_J^{\mathcal{E}}$	15.0530	15.0530	–	–	0.07	2.18	–	–
	225	$z_J^{\mathcal{C}}$	15.0530	15.0530			0.05	2.18		
MANN_a9	45	$z_J^{\mathcal{E}}$	17.4750	17.4750	–	–	0.05	2.38	–	–
	72	$z_J^{\mathcal{C}}$	17.4750	17.4750			0.04	2.70		
Circulant47_30	47	$z_J^{\mathcal{E}}$	14.3022	14.3022	–	–	0.07	3.80	–	–
	282	$z_J^{\mathcal{C}}$	14.3022	14.3022			0.06	3.34		
G_50_025	50	$z_J^{\mathcal{E}}$	13.5642	13.4554	–	–	0.09	5.71	–	–
	308	$z_J^{\mathcal{C}}$	13.5642	13.4555			0.07	5.36		
G_60_025	60	$z_J^{\mathcal{E}}$	14.2815	14.2013	–	–	0.13	12.40	–	–
	450	$z_J^{\mathcal{C}}$	14.2815	14.2013			0.11	12.19		
Paley61	61	$z_J^{\mathcal{E}}$	7.8102	7.8102	–	–	0.23	6.52	–	–
	915	$z_J^{\mathcal{C}}$	7.8102	7.8102			0.17	6.22		
hamming6_4	64	$z_J^{\mathcal{E}}$	5.3333	4.0000	–	–	0.36	10.60	–	–
	1312	$z_J^{\mathcal{C}}$	5.3333	4.0000			0.29	8.44		
HoG_34276	72	$z_J^{\mathcal{E}}$	26.4635	26.1831	–	–	0.06	30.70	–	–
	144	$z_J^{\mathcal{C}}$	26.4635	26.2105			0.07	32.67		
G_80_050	80	$z_J^{\mathcal{E}}$	9.4353	9.3812	–	–	0.87	60.25	–	–
	1620	$z_J^{\mathcal{C}}$	9.4353	9.3812			0.85	60.63		
G_100_025	100	$z_J^{\mathcal{E}}$	19.4408	19.2830	–	–	0.61	170.61	–	–
	1243	$z_J^{\mathcal{C}}$	19.4408	19.2830			0.52	178.05		
spin5	125	$z_J^{\mathcal{E}}$	55.9017	55.9017	–	–	0.17	309.35	–	–
	375	$z_J^{\mathcal{C}}$	55.9017	55.9017			0.10	309.61		
G_150_025	150	$z_J^{\mathcal{E}}$	23.7185	23.4720	–	–	3.34	2049.99	–	–
	2835	$z_J^{\mathcal{C}}$	23.7185	23.4720			2.81	1461.60		
keller4	171	$z_J^{\mathcal{E}}$	14.0122	13.4659	–	–	10.05	5386.19	–	–
	5100	$z_J^{\mathcal{C}}$	14.0122	13.4659			8.85	4367.68		

Table 4
The number of included ESCs $|J_{\mathcal{E}}|$ and $|J_{\mathcal{C}}|$ for $J=J_{\mathcal{E}}$ and $J=J_{\mathcal{C}}$ for the computations of Table 5 and Table 7, respectively.

Name	n / m		$\lvert J\rvert$ for subgraphs of order k					
			$k=0$	$k=2$	$k=3$	$k=4$	$k=5$	$k=6$
HoG_34272	9	$\lvert J_{\mathcal{E}}\rvert$	0	9	57	116	126	84
	17	$\lvert J_{\mathcal{C}}\rvert$	0	8	56	110	120	84
HoG_15599	20	$\lvert J_{\mathcal{E}}\rvert$	0	0	141	1428	2000	2000
	44	$\lvert J_{\mathcal{C}}\rvert$	0	0	138	1240	1977	2000
CubicVT26_5	26	$\lvert J_{\mathcal{E}}\rvert$	0	0	515	1189	1824	2000
	39	$\lvert J_{\mathcal{C}}\rvert$	0	0	458	1761	2000	1515
HoG_34274	36	$\lvert J_{\mathcal{E}}\rvert$	0	25	823	1700	2000	2000
	72	$\lvert J_{\mathcal{C}}\rvert$	0	24	704	1593	1930	2000
HoG_6575	45	$\lvert J_{\mathcal{E}}\rvert$	0	0	260	1025	1378	1785
	225	$\lvert J_{\mathcal{C}}\rvert$	0	0	268	1439	1563	1490

(continued on next page)

Table 4 (*continued*).

Name	n / m		$\lvert J \rvert$ for subgraphs of order k					
			$k=0$	$k=2$	$k=3$	$k=4$	$k=5$	$k=6$
MANN_a9	45	$\lvert J_{\mathcal{E}} \rvert$	0	0	718	1102	1449	2000
	72	$\lvert J_{\mathcal{C}} \rvert$	0	0	734	1750	1950	2000
Circulant47_30	47	$\lvert J_{\mathcal{E}} \rvert$	0	0	827	1337	1635	2000
	282	$\lvert J_{\mathcal{C}} \rvert$	0	0	761	1276	1796	2000
G_50_025	50	$\lvert J_{\mathcal{E}} \rvert$	0	82	413	707	1146	2000
	308	$\lvert J_{\mathcal{C}} \rvert$	0	88	521	928	1645	2000
G_60_025	60	$\lvert J_{\mathcal{E}} \rvert$	0	93	492	901	1366	2000
	450	$\lvert J_{\mathcal{C}} \rvert$	0	96	486	1233	1665	2000
Paley61	61	$\lvert J_{\mathcal{E}} \rvert$	0	0	0	0	0	48
	915	$\lvert J_{\mathcal{C}} \rvert$	0	0	0	0	0	37
hamming6_4	64	$\lvert J_{\mathcal{E}} \rvert$	0	247	1665	2000	2000	2000
	1312	$\lvert J_{\mathcal{C}} \rvert$	0	251	1579	1970	1955	2000
HoG_34276	72	$\lvert J_{\mathcal{E}} \rvert$	0	49	1402	1415	1873	2000
	144	$\lvert J_{\mathcal{C}} \rvert$	0	76	602	1398	1916	2000
G_80_050	80	$\lvert J_{\mathcal{E}} \rvert$	0	158	704	1132	1854	2000
	1620	$\lvert J_{\mathcal{C}} \rvert$	0	220	1391	1766	2000	2000
G_100_025	100	$\lvert J_{\mathcal{E}} \rvert$	0	228	590	901	1658	2000
	1243	$\lvert J_{\mathcal{C}} \rvert$	0	235	1197	1630	1961	2000
spin5	125	$\lvert J_{\mathcal{E}} \rvert$	0	0	1204	1975	2000	2000
	375	$\lvert J_{\mathcal{C}} \rvert$	0	0	982	1829	2000	2000
G_150_025	150	$\lvert J_{\mathcal{E}} \rvert$	0	275	496	804	1759	2000
	2835	$\lvert J_{\mathcal{C}} \rvert$	0	338	718	1474	1969	2000
keller4	171	$\lvert J_{\mathcal{E}} \rvert$	0	482	1332	1959	2000	2000
	5100	$\lvert J_{\mathcal{C}} \rvert$	0	457	1630	1931	2000	2000
G_200_025	200	$\lvert J_{\mathcal{E}} \rvert$	0	307	688	884	1498	2000
	4905	$\lvert J_{\mathcal{C}} \rvert$	0	345	812	1398	2000	2000
brock200_1	200	$\lvert J_{\mathcal{E}} \rvert$	0	325	571	849	1406	2000
	5066	$\lvert J_{\mathcal{C}} \rvert$	0	365	673	1395	1958	2000
c_fat200_5	200	$\lvert J_{\mathcal{E}} \rvert$	0	1860	1913	2000	2000	2000
	11 427	$\lvert J_{\mathcal{C}} \rvert$	0	1827	1999	2000	2000	2000
sanr200_0_9	200	$\lvert J_{\mathcal{E}} \rvert$	0	267	530	844	1483	2000
	2037	$\lvert J_{\mathcal{C}} \rvert$	0	337	636	1252	2000	2000

Table 5
The values of $z_J^{\mathcal{E}}(G)$ and $z_J^{\mathcal{C}}(G)$ for different graphs G and sets $J = J_{\mathcal{E}}$ for subgraphs of order k for $k \in \{0, 2, 3, 4, 5, 6\}$.

Name	n / m		$J = J_{\mathcal{E}}$ for subgraphs of order k					
			$k=0$	$k=2$	$k=3$	$k=4$	$k=5$	$k=6$
HoG_34272	9	$z_J^{\mathcal{E}}$	3.3380	3.2729	3.0605	3.0000	3.0000	3.0000
	17	$z_J^{\mathcal{C}}$	3.3380	3.2763	3.1864	3.0000	3.0000	3.0000
HoG_15599	20	$z_J^{\mathcal{E}}$	7.8202	7.8202	7.4437	7.0000	7.0000	7.0000
	44	$z_J^{\mathcal{C}}$	7.8202	7.8202	7.4771	7.4667	7.3458	7.0000
CubicVT26_5	26	$z_J^{\mathcal{E}}$	11.8171	11.8171	10.9961	10.7210	10.4214	10.3357
	39	$z_J^{\mathcal{C}}$	11.8171	11.8171	11.0037	11.0035	10.7778	10.6519
HoG_34274	36	$z_J^{\mathcal{E}}$	13.2317	13.0915	12.3174	12.0525	12.0000	12.0000
	72	$z_J^{\mathcal{C}}$	13.2317	13.1052	12.7491	12.2346	12.0000	12.0000
HoG_6575	45	$z_J^{\mathcal{E}}$	15.0530	15.0530	14.3178	14.0257	13.8179	12.7257
	225	$z_J^{\mathcal{C}}$	15.0530	15.0530	14.3178	14.1817	14.1489	13.4104
MANN_a9	45	$z_J^{\mathcal{E}}$	17.4750	17.4750	17.1203	17.0727	16.9964	16.8635
	72	$z_J^{\mathcal{C}}$	17.4750	17.4750	17.1644	17.1163	17.0654	17.0342
Circulant47_30	47	$z_J^{\mathcal{E}}$	14.3022	14.3022	13.6103	13.1817	13.1806	13.0734
	282	$z_J^{\mathcal{C}}$	14.3022	14.3022	13.6172	13.2008	13.1943	13.0907
G_50_025	50	$z_J^{\mathcal{E}}$	13.5642	13.4554	13.1310	12.9420	12.7749	12.6210
	308	$z_J^{\mathcal{C}}$	13.5642	13.4555	13.2743	13.1118	12.9279	12.7287

(*continued on next page*)

Table 5 (*continued*).

Name	n / m		$J = J_{\mathcal{E}}$ for subgraphs of order k					
			$k=0$	$k=2$	$k=3$	$k=4$	$k=5$	$k=6$
G_60_025	60	$z_J^{\mathcal{E}}$	14.2815	14.2013	14.0450	13.8738	13.6876	13.6702
	450	$z_J^{\mathcal{C}}$	14.2815	14.2013	14.1038	13.9800	13.7834	13.7648
Paley61	61	$z_J^{\mathcal{E}}$	7.8102	7.8102	7.8102	7.8102	7.8102	7.7480
	915	$z_J^{\mathcal{C}}$	7.8102	7.8102	7.8102	7.8102	7.8102	7.7720
hamming6_4	64	$z_J^{\mathcal{E}}$	5.3333	4.0000	4.0000	4.0000	4.0000	4.0000
	1312	$z_J^{\mathcal{C}}$	5.3333	4.0000	4.0000	4.0000	4.0000	4.0000
HoG_34276	72	$z_J^{\mathcal{E}}$	26.4635	26.1831	25.5429	24.8186	24.1331	24.1348
	144	$z_J^{\mathcal{C}}$	26.4635	26.2105	25.9856	25.6362	24.8086	24.7730
G_80_050	80	$z_J^{\mathcal{E}}$	9.4353	9.3812	9.3775	9.3521	9.3152	9.2633
	1620	$z_J^{\mathcal{C}}$	9.4353	9.3812	9.3790	9.3626	9.3364	9.2949
G_100_025	100	$z_J^{\mathcal{E}}$	19.4408	19.2866	19.2606	19.2302	19.1807	19.1196
	1243	$z_J^{\mathcal{C}}$	19.4408	19.2866	19.2692	19.2516	19.2153	19.1630
spin5	125	$z_J^{\mathcal{E}}$	55.9017	55.9017	50.4661	50.1027	50.0000	50.0000
	375	$z_J^{\mathcal{C}}$	55.9017	55.9017	51.8181	50.6352	50.0000	50.0081
G_150_025	150	$z_J^{\mathcal{E}}$	23.7185	23.5355	23.4744	23.4693	23.4637	23.4555
	2835	$z_J^{\mathcal{C}}$	23.7185	23.5355	23.4753	23.4704	23.4663	23.4602
keller4	171	$z_J^{\mathcal{E}}$	14.0122	13.7260	13.5252	13.4909	13.4786	13.4801
	5100	$z_J^{\mathcal{C}}$	14.0122	13.7261	13.5253	13.4909	13.4786	13.4811
G_200_025	200	$z_J^{\mathcal{E}}$	28.2165	28.0436	27.9630	27.9427	27.9326	27.9345
	4905	$z_J^{\mathcal{C}}$	28.2165	28.0436	27.9630	27.9427	27.9333	27.9354
brock200_1	200	$z_J^{\mathcal{E}}$	27.4566	27.2969	27.2250	27.2036	27.1949	27.1925
	5066	$z_J^{\mathcal{C}}$	27.4566	27.2969	27.2250	27.2040	27.1955	27.1937
c_fat200_5	200	$z_J^{\mathcal{E}}$	60.3453	60.3453	58.0000	58.0000	58.0000	58.0000
	11 427	$z_J^{\mathcal{C}}$	60.3453	60.3453	58.0142	58.0000	58.0000	58.0000
sanr200_0_9	200	$z_J^{\mathcal{E}}$	49.2735	49.0388	48.9195	48.8546	48.7465	48.7206
	2037	$z_J^{\mathcal{C}}$	49.2735	49.0388	48.9312	48.8811	48.8137	48.8035

Table 6
The running times for the results of Table 5.

Name	n / m		$J = J_{\mathcal{E}}$ for subgraphs of order k					
			$k=0$	$k=2$	$k=3$	$k=4$	$k=5$	$k=6$
HoG_34272	9	$z_J^{\mathcal{E}}$	0.26	0.07	0.08	0.18	0.36	0.38
	17	$z_J^{\mathcal{C}}$	0.04	0.04	0.08	0.15	0.29	0.36
HoG_15599	20	$z_J^{\mathcal{E}}$	0.04	0.04	0.21	95.64	869.93	1624.17
	44	$z_J^{\mathcal{C}}$	0.04	0.03	0.20	123.77	1005.30	2413.69
CubicVT26_5	26	$z_J^{\mathcal{E}}$	0.04	0.03	2.18	73.75	727.67	2307.93
	39	$z_J^{\mathcal{C}}$	0.04	0.03	1.88	61.06	822.95	2980.21
HoG_34274	36	$z_J^{\mathcal{E}}$	0.04	0.06	12.79	349.74	1035.69	2205.90
	72	$z_J^{\mathcal{C}}$	0.04	0.06	11.20	284.22	977.60	2773.10
HoG_6575	45	$z_J^{\mathcal{E}}$	0.05	0.05	0.78	43.73	243.83	1163.78
	225	$z_J^{\mathcal{C}}$	0.05	0.04	0.77	45.97	275.98	1139.69
MANN_a9	45	$z_J^{\mathcal{E}}$	0.04	0.05	7.09	76.40	465.01	2891.53
	72	$z_J^{\mathcal{C}}$	0.05	0.04	6.39	76.05	494.98	3391.76
Circulant47_30	47	$z_J^{\mathcal{E}}$	0.07	0.06	10.56	116.63	490.99	2181.69
	282	$z_J^{\mathcal{C}}$	0.07	0.06	11.18	109.49	430.87	2321.85
G_50_025	50	$z_J^{\mathcal{E}}$	0.08	0.18	2.43	23.40	200.74	2377.75
	308	$z_J^{\mathcal{C}}$	0.08	0.18	2.49	22.07	209.83	2606.79
G_60_025	60	$z_J^{\mathcal{E}}$	0.13	0.29	4.36	43.88	326.96	2495.65
	450	$z_J^{\mathcal{C}}$	0.12	0.27	4.19	52.47	380.22	2323.79
Paley61	61	$z_J^{\mathcal{E}}$	0.23	0.22	0.22	0.23	0.22	0.67
	915	$z_J^{\mathcal{C}}$	0.17	0.16	0.17	0.18	0.16	0.56

(*continued on next page*)

Table 6 (*continued*).

Name	n		$J = J_{\mathcal{E}}$ for subgraphs of order k					
	m		$k=0$	$k=2$	$k=3$	$k=4$	$k=5$	$k=6$
hamming6_4	64	$z_J^{\mathcal{E}}$	0.36	1.36	45.30	133.11	318.78	802.02
	1312	$z_J^{\mathcal{C}}$	0.29	1.05	29.49	113.16	366.63	804.42
HoG_34276	72	$z_J^{\mathcal{E}}$	0.07	0.12	63.26	218.38	1845.60	5152.23
	144	$z_J^{\mathcal{C}}$	0.07	0.12	60.17	227.44	1978.86	6327.47
G_80_050	80	$z_J^{\mathcal{E}}$	0.89	1.90	12.99	87.98	713.59	1391.32
	1620	$z_J^{\mathcal{C}}$	0.92	1.94	14.02	96.16	624.19	1497.57
G_100_025	100	$z_J^{\mathcal{E}}$	0.64	1.77	10.03	69.21	691.72	2768.81
	1243	$z_J^{\mathcal{C}}$	0.56	1.69	10.67	68.02	690.08	2709.48
spin5	125	$z_J^{\mathcal{E}}$	0.16	0.17	37.22	342.58	947.04	1972.30
	375	$z_J^{\mathcal{C}}$	0.10	0.10	31.63	296.17	1110.95	3237.65
G_150_025	150	$z_J^{\mathcal{E}}$	3.27	6.70	19.19	91.37	957.42	2867.07
	2835	$z_J^{\mathcal{C}}$	3.05	6.50	16.98	77.65	1041.79	3101.88
keller4	171	$z_J^{\mathcal{E}}$	11.36	24.40	178.18	749.89	1644.06	4040.91
	5100	$z_J^{\mathcal{C}}$	9.51	24.76	150.29	737.29	2023.90	4937.69
G_200_025	200	$z_J^{\mathcal{E}}$	10.04	18.35	54.11	141.27	853.42	3252.01
	4905	$z_J^{\mathcal{C}}$	10.05	18.56	57.54	143.34	972.45	4075.58
brock200_1	200	$z_J^{\mathcal{E}}$	11.81	20.90	44.77	151.79	782.03	3350.39
	5066	$z_J^{\mathcal{C}}$	10.78	20.04	43.04	144.64	855.91	3929.63
c_fat200_5	200	$z_J^{\mathcal{E}}$	49.31	177.02	563.46	755.78	3140.87	3714.74
	11427	$z_J^{\mathcal{C}}$	37.30	156.36	653.76	767.95	3101.51	3333.48
sanr200_0_9	200	$z_J^{\mathcal{E}}$	2.17	4.19	17.45	86.09	867.56	4353.92
	2037	$z_J^{\mathcal{C}}$	1.76	4.43	16.98	81.76	881.66	4631.88

Table 7
The values of $z_J^{\mathcal{E}}(G)$ and $z_J^{\mathcal{C}}(G)$ for different graphs G and sets $J = J_{\mathcal{C}}$ for subgraphs of order k for $k \in \{0, 2, 3, 4, 5, 6\}$.

Name	n		$J = J_{\mathcal{C}}$ for subgraphs of order k					
	m		$k=0$	$k=2$	$k=3$	$k=4$	$k=5$	$k=6$
HoG_34272	9	$z_J^{\mathcal{E}}$	3.3380	3.2729	3.0605	3.0000	3.0000	3.0000
	17	$z_J^{\mathcal{C}}$	3.3380	3.2763	3.1765	3.0000	3.0000	3.0000
HoG_15599	20	$z_J^{\mathcal{E}}$	7.8202	7.8202	7.4472	7.3871	7.0000	7.0000
	44	$z_J^{\mathcal{C}}$	7.8202	7.8202	7.4761	7.4291	7.2500	7.0000
CubicVT26_5	26	$z_J^{\mathcal{E}}$	11.8171	11.8171	11.0035	10.9932	10.5956	10.3201
	39	$z_J^{\mathcal{C}}$	11.8171	11.8171	11.0035	11.0035	10.7189	10.5727
HoG_34274	36	$z_J^{\mathcal{E}}$	13.2317	13.0915	12.3066	12.1338	12.0000	12.0000
	72	$z_J^{\mathcal{C}}$	13.2317	13.1052	12.6217	12.3998	12.0000	12.0000
HoG_6575	45	$z_J^{\mathcal{E}}$	15.0530	15.0530	14.3178	14.1594	14.0495	12.9931
	225	$z_J^{\mathcal{C}}$	15.0530	15.0530	14.3178	14.1595	14.0791	13.2063
MANN_a9	45	$z_J^{\mathcal{E}}$	17.4750	17.4750	17.1332	17.0762	17.0009	16.9167
	72	$z_J^{\mathcal{C}}$	17.4750	17.4750	17.1471	17.1092	17.0591	17.0349
Circulant47_30	47	$z_J^{\mathcal{E}}$	14.3022	14.3022	13.6188	13.1845	13.1827	13.0516
	282	$z_J^{\mathcal{C}}$	14.3022	14.3022	13.6233	13.1934	13.1887	13.0598
G_50_025	50	$z_J^{\mathcal{E}}$	13.5642	13.4554	13.1225	12.9735	12.7355	12.6194
	308	$z_J^{\mathcal{C}}$	13.5642	13.4555	13.2253	13.0803	12.8240	12.7127
G_60_025	60	$z_J^{\mathcal{E}}$	14.2815	14.2013	14.0466	13.9115	13.7271	13.6885
	450	$z_J^{\mathcal{C}}$	14.2815	14.2013	14.1014	13.9727	13.7845	13.7478
Paley61	61	$z_J^{\mathcal{E}}$	7.8102	7.8102	7.8102	7.8102	7.8102	7.7803
	915	$z_J^{\mathcal{C}}$	7.8102	7.8102	7.8102	7.8102	7.8102	7.7945
hamming6_4	64	$z_J^{\mathcal{E}}$	5.3333	4.0000	4.0000	4.0000	4.0000	4.0000
	1312	$z_J^{\mathcal{C}}$	5.3333	4.0000	4.0000	4.0000	4.0000	4.0000
HoG_34276	72	$z_J^{\mathcal{E}}$	26.4635	26.1831	25.7450	24.9159	24.1589	24.0977
	144	$z_J^{\mathcal{C}}$	26.4635	26.2105	26.0414	25.5734	24.7075	24.4902

(*continued on next page*)

Table 7 (*continued*).

Name	n		$J = J_C$ for subgraphs of order k					
	m		$k = 0$	$k = 2$	$k = 3$	$k = 4$	$k = 5$	$k = 6$
G_80_050	80	$z_J^{\mathcal{E}}$	9.4353	9.3814	9.3741	9.3566	9.3182	9.2835
	1620	$z_J^{\mathcal{C}}$	9.4353	9.3814	9.3777	9.3658	9.3367	9.3114
G_100_025	100	$z_J^{\mathcal{E}}$	19.4408	19.2892	19.2639	19.2255	19.1638	19.1260
	1243	$z_J^{\mathcal{C}}$	19.4408	19.2892	19.2716	19.2498	19.2015	19.1730
spin5	125	$z_J^{\mathcal{E}}$	55.9017	55.9017	50.6697	50.2870	50.0000	50.0000
	375	$z_J^{\mathcal{C}}$	55.9017	55.9017	51.2339	50.3559	50.0000	50.0000
G_150_025	150	$z_J^{\mathcal{E}}$	23.7185	23.5122	23.4752	23.4676	23.4641	23.4599
	2835	$z_J^{\mathcal{C}}$	23.7185	23.5122	23.4754	23.4691	23.4667	23.4634
keller4	171	$z_J^{\mathcal{E}}$	14.0122	13.6845	13.5526	13.4896	13.4792	13.4823
	5100	$z_J^{\mathcal{C}}$	14.0122	13.6846	13.5526	13.4896	13.4792	13.4826
G_200_025	200	$z_J^{\mathcal{E}}$	28.2165	28.0139	27.9675	27.9447	27.9342	27.9313
	4905	$z_J^{\mathcal{C}}$	28.2165	28.0139	27.9675	27.9449	27.9345	27.9326
brock200_1	200	$z_J^{\mathcal{E}}$	27.4566	27.2911	27.2212	27.2007	27.1950	27.1928
	5066	$z_J^{\mathcal{C}}$	27.4566	27.2911	27.2212	27.2011	27.1960	27.1941
c_fat200_5	200	$z_J^{\mathcal{E}}$	60.3453	60.3453	58.0000	58.0000	58.0000	58.0000
	11 427	$z_J^{\mathcal{C}}$	60.3453	60.3453	58.0000	58.0000	58.0000	58.0000
sanr200_0_9	200	$z_J^{\mathcal{E}}$	49.2735	49.0222	48.9106	48.8432	48.7635	48.7174
	2037	$z_J^{\mathcal{C}}$	49.2735	49.0222	48.9251	48.8736	48.8124	48.7893

Table 8
The running times for the results of Table 7.

Name	n		$J = J_C$ for subgraphs of order k					
	m		$k = 0$	$k = 2$	$k = 3$	$k = 4$	$k = 5$	$k = 6$
HoG_34272	9	$z_J^{\mathcal{E}}$	0.27	0.04	0.06	0.19	0.28	0.24
	17	$z_J^{\mathcal{C}}$	0.04	0.03	0.07	0.15	0.30	0.28
HoG_15599	20	$z_J^{\mathcal{E}}$	0.05	0.05	0.22	76.07	919.15	1507.33
	44	$z_J^{\mathcal{C}}$	0.04	0.03	0.21	84.53	916.81	2409.14
CubicVT26_5	26	$z_J^{\mathcal{E}}$	0.05	0.04	1.45	175.55	868.47	1183.23
	39	$z_J^{\mathcal{C}}$	0.05	0.03	1.57	174.67	1132.52	1132.77
HoG_34274	36	$z_J^{\mathcal{E}}$	0.05	0.06	8.18	234.84	816.22	2301.95
	72	$z_J^{\mathcal{C}}$	0.04	0.06	9.09	262.06	802.13	1949.73
HoG_6575	45	$z_J^{\mathcal{E}}$	0.05	0.05	0.67	126.05	376.49	653.98
	225	$z_J^{\mathcal{C}}$	0.05	0.05	0.66	126.67	439.78	711.86
MANN_a9	45	$z_J^{\mathcal{E}}$	0.04	0.04	8.14	246.63	997.40	2840.47
	72	$z_J^{\mathcal{C}}$	0.06	0.04	7.46	252.58	1091.76	3095.15
Circulant47_30	47	$z_J^{\mathcal{E}}$	0.08	0.07	9.01	88.89	654.73	2551.06
	282	$z_J^{\mathcal{C}}$	0.07	0.06	8.39	90.83	654.91	2443.97
G_50_025	50	$z_J^{\mathcal{E}}$	0.08	0.19	3.58	50.21	574.86	2578.57
	308	$z_J^{\mathcal{C}}$	0.08	0.17	3.87	44.95	541.70	2449.45
G_60_025	60	$z_J^{\mathcal{E}}$	0.14	0.30	4.05	94.83	591.48	2722.16
	450	$z_J^{\mathcal{C}}$	0.11	0.27	3.97	106.23	566.97	2564.81
Paley61	61	$z_J^{\mathcal{E}}$	0.24	0.22	0.22	0.21	0.22	0.59
	915	$z_J^{\mathcal{C}}$	0.17	0.16	0.17	0.19	0.17	0.55
hamming6_4	64	$z_J^{\mathcal{E}}$	0.36	1.19	36.38	131.06	354.15	783.43
	1312	$z_J^{\mathcal{C}}$	0.30	1.06	41.24	120.08	342.97	783.59
HoG_34276	72	$z_J^{\mathcal{E}}$	0.07	0.15	7.25	204.30	1671.17	4388.30
	144	$z_J^{\mathcal{C}}$	0.06	0.15	8.07	245.84	1819.67	5242.20
G_80_050	80	$z_J^{\mathcal{E}}$	0.91	3.06	60.68	232.45	656.17	1531.83
	1620	$z_J^{\mathcal{C}}$	0.88	2.67	57.14	219.95	689.89	1572.06
G_100_025	100	$z_J^{\mathcal{E}}$	0.66	1.81	40.46	249.57	1151.43	2534.13
	1243	$z_J^{\mathcal{C}}$	0.56	1.83	40.63	269.32	1125.60	2634.70

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Table 8 (*continued*).

Name	n		$J = J_{\mathcal{C}}$ for subgraphs of order k					
	m		$k=0$	$k=2$	$k=3$	$k=4$	$k=5$	$k=6$
spin5	125	$z_J^{\mathcal{E}}$	0.17	0.17	19.30	261.38	1320.40	2529.39
	375	$z_J^{\mathcal{C}}$	0.10	0.10	19.53	251.51	1578.82	3110.74
G_150_025	150	$z_J^{\mathcal{E}}$	3.42	8.32	29.13	224.75	1208.97	2954.46
	2835	$z_J^{\mathcal{C}}$	3.07	6.90	27.63	257.91	1463.41	3219.20
keller4	171	$z_J^{\mathcal{E}}$	11.65	22.97	200.58	677.57	1484.11	5050.42
	5100	$z_J^{\mathcal{C}}$	9.47	24.13	227.81	711.48	1815.60	5073.47
G_200_025	200	$z_J^{\mathcal{E}}$	10.02	18.98	68.21	375.73	1844.91	3730.11
	4905	$z_J^{\mathcal{C}}$	10.07	19.69	74.55	359.11	2011.74	3947.52
brock200_1	200	$z_J^{\mathcal{E}}$	11.79	20.48	53.32	343.51	1596.36	3673.71
	5066	$z_J^{\mathcal{C}}$	9.97	21.54	54.54	364.17	1801.74	3993.45
c_fat200_5	200	$z_J^{\mathcal{E}}$	53.80	164.89	702.13	1060.21	3509.77	3669.49
	11 427	$z_J^{\mathcal{C}}$	37.18	159.80	762.12	1038.43	3252.03	3764.20
sanr200_0_9	200	$z_J^{\mathcal{E}}$	2.18	5.20	20.46	208.74	1615.14	4255.90
	2037	$z_J^{\mathcal{C}}$	1.78	5.57	21.65	211.25	1635.43	4749.57

are shorter, but there are also instances (*e.g.*, G_100_025 for $k = 6$) where the computation of both $z_J^{\mathcal{E}}$ and $z_J^{\mathcal{C}}$ is faster for $J = J_{\mathcal{C}}$ than it is for $J = J_{\mathcal{E}}$.

As a result, we confirm that tightening the Lovász theta function towards the stability number with the help of ESCs typically works better when starting from the Lovász theta function formulation (T_{n+1}) (as it is done in the ESH) as it does when starting with the formulation (T_n) (as it is done in the CESH), even though this is not obvious at first sight as the latter SDPs are smaller. However, in some cases it can be advantageous to use the CESC, but then also the subset J should be determined using (T_n).

6. Conclusions

In this paper we derived two new SDP hierarchies from the Lovász theta function towards the stability number. The classical ESH from the literature starts from the SDP (T_{n+1}) and adds ESCs. We introduced the new CESH starting from (T_n) and including ESCs. We proved that this new hierarchy has some same properties as the ESH. Moreover, we showed that the bounds based on the ESH are at least as good as those from the CESH — not only for including all ESCs of a certain order, but also for including only some of them.

We also newly introduced SESCs, which are a more natural formulation of exactness for (T_n). Including them into (T_n) yields the new SESH. Even though SESCs are more intuitive, the bounds based on the CESH and the SESH coincide.

In our computational results with an off-the-shelve interior point solver we typically obtain the best bounds with the fastest running times when using the ESH. However, for some instances using the CESH is beneficial.

It would be interesting to derive a specialized solver for the CESH as it was done by Gaar and Rendl [14,15] for the ESH. They dualize the ESCs, use the bundle method and instead of solving a huge SDP with all ESCs, they iterate and solve (T_{n+1}) with a modified objective function in each iteration. Since (T_n) has a smaller matrix order and fewer constraints, this approach presumably works even better for the CESH. Such a solver allows to compare the running times for the ESH and the CESH in a more sophisticated way.

Another open question is the more precise relationship of the ESH and the CESH. In this paper we have shown that $z_k^{\mathcal{C}}(G) \geqslant z_k^{\mathcal{E}}(G)$ holds for all $k \in \{1, \ldots, n\}$. It would be interesting to know if there is some constant $\ell \geqslant 1$ such that $z_k^{\mathcal{E}}(G) \geqslant z_{k+\ell}^{\mathcal{C}}(G)$ holds for all graphs G and for all $k \in \{1, \ldots, n\}$, so such that it suffices to add ℓ levels to the CESH to reach the quality of the ESH.

Finally, it would be interesting to investigate which implications it has for the ESH and the CESH to induce the positive semidefiniteness constraint not for the whole matrix X, but only for a submatrix of X like it has been done in the recent work [2].

Data availability

The data and source code is available online.

References

[1] Elspeth Adams, Miguel F. Anjos, Franz Rendl, Angelika Wiegele, A hierarchy of subgraph projection-based semidefinite relaxations for some NP-hard graph optimization problems, INFOR Inf. Syst. Oper. Res. 53 (1) (2015) 40–47.

[2] Grigoriy Blekherman, Santanu S. Dey, Marco Molinaro, Shengding Sun, Sparse PSD approximation of the PSD cone, Math. Program. 191 (2022) 981–1004.

[3] Immanuel M. Bomze, Marco Budinich, Panos M. Pardalos, Marcello Pelillo, The maximum clique problem, in: Handbook of Combinatorial Optimization, Supplement Vol. A, Kluwer Acad. Publ., Dordrecht, 1999, pp. 1–74.
[4] Stephen Boyd, Lieven Vandenberghe, Convex Optimization, Cambridge University Press, Cambridge, 2004, xiv+716.
[5] Gunnar Brinkmann, Kris Coolsaet, Jan Goedgebeur, Hadrien Mélot, House of graphs: A database of interesting graphs, Discrete Appl. Math. 161 (1) (2013) 311–314.
[6] Thomas Christof, SMAPO: Cut Polytope, 2024, http://comopt.ifi.uni-heidelberg.de/software/SMAPO/cut/cut.html. (Accessed 17 April 2024).
[7] Thomas Christof, Andreas Löbel, PORTA: Polyhedron representation transformation algorithm, 1997, http://comopt.ifi.uni-heidelberg.de/software/PORTA/. (Accessed 17 April 2024).
[8] Michele Conforti, Gerard Cornuejols, Giacomo Zambelli, Integer Programming, Springer Publishing Company, Incorporated, 2014.
[9] Michel Marie Deza, Monique Laurent, Geometry of cuts and metrics, in: Algorithms and Combinatorics, vol. 15, Springer-Verlag, Berlin, 1997, p. xii+587.
[10] DIMACS Implementation Challenges, http://dimacs.rutgers.edu/Challenges/. (Accessed 17 April 2024).
[11] Igor Dukanovic, Franz Rendl, Semidefinite programming relaxations for graph coloring and maximal clique problems, Math. Program. 109 (2-3, Ser. B) (2007) 345–365.
[12] Ilse Fischer, Gerald Gruber, Franz Rendl, Renata Sotirov, Computational experience with a bundle approach for semidefinite cutting plane relaxations of Max-Cut and equipartition, Math. Program. 105 (2-3, Ser. B) (2006) 451–469.
[13] Elisabeth Gaar, Efficient Implementation of SDP Relaxations for the Stable Set Problem (Ph.D. thesis), Alpen-Adria-Universität Klagenfurt, 2018.
[14] Elisabeth Gaar, Franz Rendl, A bundle approach for SDPs with exact subgraph constraints, in: Andrea Lodi, Viswanath Nagarajan (Eds.), Integer Programming and Combinatorial Optimization, Springer International Publishing, 2019, pp. 205–218.
[15] Elisabeth Gaar, Franz Rendl, A computational study of exact subgraph based SDP bounds for Max-Cut, stable set and coloring, Math. Program. 183 (2020) 283–308.
[16] Laura Galli, Adam N. Letchford, On the Lovász theta function and some variants, Discrete Optim. 25 (2017) 159–174.
[17] Michel X. Goemans, David P. Williamson, Improved approximation algorithms for maximum cut and satisfiability problems using semidefinite programming, J. Assoc. Comput. Mach. 42 (6) (1995) 1115–1145.
[18] Martin Grötschel, László Lovász, Alexander Schrijver, Geometric algorithms and combinatorial optimization, in: Algorithms and Combinatorics: Study and Research Texts, vol. 2, Springer-Verlag, Berlin, 1988, p. xii+362.
[19] Gerald Gruber, Franz Rendl, Computational experience with stable set relaxations, SIAM J. Optim. 13 (4) (2003) 1014–1028.
[20] Nebojša Gvozdenović, Monique Laurent, Frank Vallentin, Block-diagonal semidefinite programming hierarchies for 0/1 programming, Oper. Res. Lett. 37 (1) (2009) 27–31.
[21] Christoph Helmberg, Semidefinite Programming for Combinatorial Optimization (Habilitation thesis), Konrad-Zuse-Zentrum für Informationstechnik Berlin, 2000.
[22] Jean B. Lasserre, An explicit exact SDP relaxation for nonlinear 0-1 programs, in: Integer Programming and Combinatorial Optimization (Utrecht, 2001), in: Lecture Notes in Comput. Sci., vol. 2081, Springer, Berlin, 2001, pp. 293–303.
[23] Monique Laurent, A comparison of the Sherali-Adams, Lovász-Schrijver, and Lasserre relaxations for 0-1 programming, Math. Oper. Res. 28 (3) (2003) 470–496.
[24] László Lovász, On the Shannon capacity of a graph, IEEE Trans. Inform. Theory 25 (1) (1979) 1–7.
[25] László Lovász, Alexander Schrijver, Cones of matrices and set-functions and 0-1 optimization, SIAM J. Optim. 1 (2) (1991) 166–190.
[26] MOSEK ApS, The MOSEK optimization toolbox for MATLAB manual. Version 8.0, 2017.
[27] Manfred Padberg, The Boolean quadric polytope: Some characteristics, facets and relatives, Math. Program. 45 (1, (Ser. B)) (1989) 139–172.
[28] Alexander Schrijver, A comparison of the Delsarte and Lovász bounds, IEEE Trans. Inform. Theory 25 (4) (1979) 425–429.
[29] Hanif D. Sherali, Warren P. Adams, A hierarchy of relaxations between the continuous and convex hull representations for zero-one programming problems, SIAM J. Discrete Math. 3 (3) (1990) 411–430.
[30] Francesco Silvestri, Spectrahedral Relaxations of the Stable Set Polytope using induced Subgraphs (Master's thesis), Universität Heidelberg, 2013.
[31] E. Alper Yildirim, Xiaofei Fan-Orzechowski, On extracting maximum stable sets in perfect graphs using Lovász's theta function, Comput. Optim. Appl. 33 (2–3) (2006) 229–247.