Approximating the stability number and the chromatic number of a graph via semidefinite programming
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Chapter 3

The Lovász theta number

The Lovász theta function maps a graph $G = (V, E)$ to $\mathbb{R}_+$. It was introduced by Lovász in [64] for bounding the stability number and the Shannon capacity\(^1\) of a graph. Several equivalent formulations using orthonormal representations, eigenvalues, adjacency matrices, semidefinite programming were studied in [54, 61, 64]. Here we define the Lovász theta number via semidefinite programming and we prove ‘the sandwich theorem’. We finalize the chapter with some variations of the Lovász theta number obtained by adding nonnegativity and triangle constraints.

3.1 Equivalent formulations

Given a graph $G = (V, E)$, set $n := |V|$. We define $\vartheta(G)$, the Lovász theta number of $G$, via the SDP

$$\vartheta(G) := \max_{\text{s.t.}} \langle J, X \rangle \quad \text{s.t.} \quad \text{Tr}(X) = 1, \quad X_{ij} = 0 \ (ij \in E(G)), \quad X \succeq 0,$$

where $X$ is a symmetric matrix indexed by $V$ (or $\mathcal{P}_{n1}(V)$).

If $V = \emptyset$ we define $\vartheta(G) := 0$. This is however trivial case.

The dual SDP of (3.1) reads

$$\min \ t \quad \text{s.t.} \quad tI + \sum_{ij \in E} y_{ij} E^{ij} - J = Z,$$

$$Z \succeq 0, \quad t \in \mathbb{R}, \quad y_{ij} \in \mathbb{R} \ (ij \in E(G)),$$

where $E^{ij} \in \mathbb{R}^{V \times V}$, $E^{ij}_{pq} := 1$ if $\{p, q\} = \{i, j\}$ and $E^{ij}_{pq} := 0$ otherwise.

Since $\frac{1}{|V|}I$ is strictly feasible for (3.1) and $(|V| + 1)I - J$ is strictly feasible for (3.2) the minimum in (3.2) is equal to $\vartheta(G)$ (directly from Corollary 2.3.3).

\(^1\)The Shannon capacity of a graph $G$ is defined as $\Theta(G) := \lim_{n \to \infty} (\alpha(G^n))^{\frac{1}{n}}$, where $G^n$ is given by $G^1 := G$ and $G^n := G^{n-1} \cdot G$ for $n \geq 2$. 
Let \((t, Z)\) be feasible for (3.2). Set
\[
Z' := \begin{pmatrix}
t & e^T \\
e & \frac{1}{2}Z + \frac{1}{2}ee^T
\end{pmatrix}.
\tag{3.3}
\]
Consider \(Z'\) to be indexed by \(\mathcal{P}_{\leq 1}(V)\), with the first row corresponding to \(0\) (the empty set). Lemma 2.4.2 yields
\[
\vartheta(G) \leq \min Z' = \min Z'_{00} \quad \text{s.t.} \quad Z'_{0i} + Z'_{i0} = 2 \quad (i \in V) \quad \text{s.t.} \quad Z'_{ii} = Z'_{00} \quad (i \in V)
\]
\[
Z'_{ii} = 1 \quad (i \in V)
\]
\[
Z'_{ij} = 0 \quad (ij \in E(G))
\]
\[
Z' \succeq 0
\]
where variable \(Z'\) is a symmetric matrix indexed by \(\mathcal{P}_{\leq 1}(V)\).

Strict feasibility of (3.2) implies strict feasibility of (3.4) since for \(Z'\) from (3.3) we have \(Z' > 0 \iff Z > 0\). Hence, we can write the dual of (3.4) as
\[
\vartheta(G) = \max \quad -2 \sum_{i \in V} X'_{0i} - \sum_{i \in V} X'_{ii} \quad \text{s.t.} \quad X'_{00} = 1 \quad (i \in V)
\]
\[
X'_{ij} = 0 \quad (ij \in E(G))
\]
\[
X' \succeq 0.
\tag{3.5}
\]

The following lemma leads us to a formulation which is extensively used in the next chapter.

**Lemma 3.1.1.** If \(X'\) is an optimal solution for the program (3.5) then \(X'_{0i} + X'_{ii} = 0\) for all \(i \in V\).

**Proof.** Let \(X'\) be feasible for the program (3.5), and suppose \(a := X'_{0i} + X'_{ii} \neq 0\) for some \(i \in V\). Then \(b := X'_{ii} > 0\) since \(X'_{ii} \succeq (X'_{0i})^2\). Set \(c_{X'} := -2 \sum_{i \in V} X'_{0i} - \sum_{i \in V} X'_{ii}\). The matrix \(X''\) obtained by multiplying the \(i\)th row and the \(i\)th column of \(X'\) by \(1 - \frac{a}{b}\) is feasible for (3.5) with the objective value \(c_{X'} + \frac{a^2}{b}\). \(\square\)

By Lemma 3.1.1 we can restrict the feasible set in (3.5) to the PSD matrices
\[
X' = \begin{pmatrix}
1 & -x^T \\
-x & X
\end{pmatrix},
\tag{3.6}
\]
such that \(\text{diag}(X) = x\), and \(X_{ij} = 0\) for all \(ij \in E(G)\). Moreover, the objective function then reads
\[
\sum_{i \in V} X'_{0i} = \sum_{i \in V} X_{ii} = \sum_{i \in V} x_i.
\]
Multiplying the first row and the first column of \(X'\) by \(-1\) gives
\[
\begin{pmatrix}
1 & -x^T \\
-x & X
\end{pmatrix} \succeq 0 \iff \begin{pmatrix}
1 & x^T \\
x & X
\end{pmatrix} \succeq 0.
\tag{3.7}
\]
The program (3.5) is thus equivalent to:
\[
\vartheta(G) = \max \quad \sum_{i \in V} X'_{ii} \quad \text{s.t.} \quad X'_{00} = 1
\]
\[
X'_{ii} = X'_{0i} \quad (i \in V)
\]
\[
X'_{ij} = 0 \quad (ij \in E)\tag{3.8}
\]
\[
X' \succeq 0.
\]
This program is also strictly feasible. To see this take \( x := \frac{1}{|V| + 1} e \) and 
\( X := \text{Diag}(x) \) and set \( X' := \begin{pmatrix} 1 & x \\ x & X \end{pmatrix} \).

### 3.2 The sandwich theorem

The sandwich theorem \[64\] compares three graph parameters: the stable set
number, the clique cover number and the Lovász theta number.

**Theorem 3.2.1** (The sandwich theorem). For any graph \( G = (V, E) \), one has
\[
\alpha(G) \leq \vartheta(G) \leq \chi(G). \tag{3.9}
\]

**Proof.** Let \( S \subseteq V \) be a stable set in \( G \) such that \( |S| = \alpha(G) \). Set 
\( X' := \begin{pmatrix} 1 & x_S \\ x_S & X \end{pmatrix} \). Here \( x_S \) is the characteristic vector of \( S \) in \( \mathbb{R}^V \), and 
\( \begin{pmatrix} 1 \\ x_S \end{pmatrix} = \chi_{P \leq 1(S)} \) is the characteristic vector of \( P \leq 1(S) \) in \( \mathbb{R}^{P \leq 1(V)} \). Since \( X' \) is feasible 
for the program (3.8) and 
\( \sum_i X'_{ii} = \alpha(G) \), we have 
\( \alpha(G) \leq \vartheta(G) \).

Let \( C_j \subseteq V \) (\( j = 1, 2, \ldots, \chi(G) \)) be disjoint cliques such that \( \bigcup_j C_j = V \). Take 
their characteristic vectors \( \chi_{C_j} \in \mathbb{R}^V \) (\( j = 1, 2, \ldots, \chi(G) \)) and set
\[
Z' := \sum_j \begin{pmatrix} 1 \\ \chi_{C_j} \end{pmatrix} \begin{pmatrix} 1 \\ \chi_{C_j} \end{pmatrix}^T. \tag{3.10}
\]
The matrix \( Z' \) is now feasible for (3.4) and \( Z'_{00} = \overline{\chi}(G) \). This proves 
\( \vartheta(G) \leq \overline{\chi}(G) \). \( \square \)

In fact, we have proved \( \vartheta(G) \leq \overline{\chi}(G) \) by using the following formulation for 
the clique cover number:
\[
\overline{\chi}(G) = \min \sum_{C \text{ clique}} \lambda_C \\
\text{s.t.} \sum_{C \text{ clique}} \lambda_C \chi^C = e \\
\lambda_C \in \{0, 1\} \text{ for each clique } C. \tag{3.11}
\]

Note that \( \lambda \) is indexed by the cliques of \( G \), and observe that the number of 
cliques can be exponential in \( |V| \). Thus the above program is an example of an 
integer linear program with an exponential number of variables. By relaxing 
the discrete variable domain \( \{0, 1\} \) to the interval \( [0, 1] \) we obtain a lower bound 
on \( \overline{\chi}(G) \) called the fractional clique cover number of \( G \):
\[
\overline{\chi}^*(G) := \min \sum_{C \text{ clique}} \lambda_C = \max e^T x \\
\text{s.t.} \sum_{C \text{ clique}} \lambda_C \chi^C = e \\
\lambda_C \geq 0 \text{ for each clique } C. \tag{3.12}
\]

Although the fractional clique cover number is defined to be the optimum of 
the linear program above, it is known to be NP-hard (see [35]). The difficulty
is caused by the fact that the constraints in the ‘primal’ program (3.12) are not polynomial time checkable. For more details about $\chi^*(G)$ consult e.g. [84].

A comparison between $\vartheta(G)$ and $\chi^*(G)$ can be derived by adjusting the proof for $\vartheta(G) \leq \chi(G)$.

**Proposition 3.2.2.** For any graph $G = (V, E)$ one has $\vartheta(G) \leq \chi^*(G)$.

**Proof.** Take an optimal $\lambda$ for the program (3.12), set

$$Z' := \sum_{C \text{ clique}} \lambda_C \left( \frac{1}{\chi_C} \right) \left( \frac{1}{\chi_C} \right)^T,$$

and observe that $Z'$ is feasible for (3.4) with $Z_{00}' = \chi^*(G)$. $\square$

The fractional clique cover number of $\overline{G}$ is called the fractional chromatic number of $G$ and it is denoted by $\chi^*(G)$. Namely,

$$\chi^*(G) := \overline{\chi^*(G)} = \min \sum_{S \text{ stable set}} \lambda_S \quad \text{s.t.} \quad \sum_{S \text{ stable set}} \lambda_S \chi^S = e$$

We can now summarize the results described in this section. For any graph $G$ we have

$$\alpha(G) \leq \vartheta(G) \leq \chi^*(G) \leq \chi(G),$$

and equivalently

$$\omega(G) \leq \vartheta(G) \leq \chi^*(G) \leq \chi(G),$$

after recalling $\omega(G) = \alpha(\overline{G})$ and $\chi(G) = \overline{\chi(G)}$.

**Perfect graphs.** For a perfect graph all the inequalities in (3.15) and (3.16) are equalities. Therefore, the stability number of a perfect graph $G$ can be determined by computing an approximated value for $\vartheta(G)$. It can be done by solving, for instance, the SDP (3.1) with precision $< \frac{1}{2}$, and then rounding the objective value to the nearest integer. Similarly, determining the chromatic number of a perfect graph $G$ can be done by computing $\vartheta(\overline{G})$. Besides these numerical values, one can find a stable set of the maximum size and an optimal colouring of a perfect graph in polynomial time using the Lovász theta number (for details see [35]).

On the other hand, all the inequalities in (3.15) and (3.16) can be strict. The smallest graph for which this happens is $C_5$, since $\alpha(C_5) = 2$, $\vartheta(C_5) = \sqrt{5}$, $\chi^*(C_5) = \frac{5}{2}$, and $\overline{\chi}(C_5) = 3$, and since all graphs smaller than $C_5$ are perfect. Nevertheless, the values $\vartheta(G) - \alpha(G)$, $\chi^*(G) - \vartheta(G)$ and $\chi(G) - \overline{\chi}(G)$ can be arbitrarily large. To see this take, let $G$ be the union of $k$ disjoint copies of $C_5$. We have

- $\alpha(G) = k\alpha(C_5) = 2k$;
- $\vartheta(G) = k\vartheta(C_5) = k\sqrt{5}$;
- $\chi^*(G) = k\chi^*(C_5) = \frac{5}{2}k$;
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\[ \chi(G) = k\chi(C_5) = 3k; \]

since the parameters are additive with respect to the direct sum of graphs. Knuth [54] proves additivity for \( \vartheta \), while for \( \alpha, \chi^* \) and \( \chi \) it follows directly from the definitions.

3.3 Nonnegativity and triangle inequalities

Several variations of the Lovász theta number were proposed in order to get sharper upper bounds for the stability number of a graph and sharper lower bounds for the chromatic number of a graph.

Given a graph \( G = (V,E) \), \( |V| \neq 0 \), set \( n := |V| \). McEliece, Rodemich, and Rumsey [68] and Schrijver [83] give the bound:

\[
\vartheta'(G) := \max \langle J, X \rangle \quad \text{s.t.} \quad \text{Tr}(X) = 1 \\
X_{ij} = 0 \ (ij \in E(G)) \\
X \succeq 0, X \geq 0 \\
X \in \mathcal{D}_n,
\]

(3.17)

where \( X \) is indexed by \( V \).

Schrijver [83] proves the relation of \( \vartheta'(G) \) with the linear programming bound for codes of Delsarte [21].

Among equivalent formulations for \( \vartheta'(G) \) we often use the following:

\[
\vartheta'(G) = \max \sum_i X'_{ii} \quad \text{s.t.} \quad X'_{00} = 1 \\
X'_{ij} = 0 \ (ij \in E(G)) \\
X' \succeq 0, X' \geq 0 \\
X' \in \mathcal{D}_{n+1},
\]

(3.18)

where \( X' \) is indexed by \( P_{\leq 1}(V) \). In order to see the link between (3.17) and (3.18) one should follow the steps given in Section 3.1.

Szegedy [90] presented a sharper bound for the fractional clique cover number:

\[
\vartheta^+(G) := \max \langle J, X \rangle \quad \text{s.t.} \quad \text{Tr}(X) = 1 \\
X_{ij} = 0 \ (ij \in E(G)) \\
X \succeq 0.
\]

(3.19)

The formulation for \( \vartheta^+(G) \) which corresponds to (3.4) is:

\[
\vartheta^+(G) = \min \sum_i Z'_{ii} \quad \text{s.t.} \quad Z'_{i0} = Z'_{0i} \ (i \in V) \\
Z'_{ii} = 1 \ (i \in V) \\
Z'_{ij} = 0 \ (ij \in E(G)) \\
Z' \succeq 0, Z' \geq 0 \\
Z' \in \mathcal{D}_{n+1},
\]

(3.20)

where \( Z' \) is indexed by \( P_{\leq 1}(V) \).
The bounds $\vartheta'(G)$ and $\vartheta^+(G)$ were further strengthened by adding triangle inequalities. Dukanovic and Rendl [25] define:

$$\vartheta^\triangle(G) := \max_{\{J, X\}} \langle J, X \rangle$$

s.t. \[ \begin{align*}
X_{ij} &= 0 \quad (ij \in E(G)) \\
X_{ij} &\leq X_{ii} \quad (i, j \in V) \\
X_{ij} + X_{jk} &\leq X_{ik} + X_{kk} \quad (i, j, k \in V) \\
X &\succeq 0, X \succeq 0.
\end{align*} \] (3.21)

By adding triangle inequalities in (3.20) Meurdesoif [70] defines:

$$\vartheta^+\triangle(G) = \min_{Z'} Z'_{00}$$

s.t. \[ \begin{align*}
Z'_{ii} &= Z'_{0i} \quad (i \in V) \\
Z'_{ii} &= 1 \quad (i \in V) \\
Z'_{ij} &= 0 \quad (ij \in E(\overline{G})) \\
Z'_{ij} + Z'_{jk} - Z'_{ki} &\leq 1 \quad (i, j, k \in V) \\
Z' &\succeq 0, Z' \succeq 0,
\end{align*} \] (3.22)

where $Z'$ is again indexed by $P_{\leq 1}(V)$.

The parameters defined above satisfy

$$\alpha(G) \leq \vartheta^\triangle(G) \leq \vartheta'(G) \leq \vartheta^+(G) \leq \vartheta^+\triangle(G) \leq \overline{\chi}(G).$$

The last inequality follows from the fact that the matrix defined in (3.13) is feasible for the program (3.22) defining $\vartheta^+\triangle(G)$. For proving the first inequality take a maximum size stable set $S$ in $G$ and set $X := \frac{1}{\alpha(G)} \chi^S (\chi^S)^T$. The matrix $X$ is feasible for (3.21) and $\langle J, X \rangle = \alpha(G)$.

The links between the bounds defined for a graph $G$ and for its complement $\overline{G}$ are given in the following theorem.

**Theorem 3.3.1.** For any graph $G$

(a) $\alpha(G)\chi^*(G) \geq |V(G)|$,

(b) $\vartheta(G)\overline{\vartheta}(G) \geq |V(G)|$,

(c) $\vartheta'(G)\vartheta^+(\overline{G}) \geq |V(G)|$,

(d) $\vartheta^\triangle(G)\vartheta^+\triangle(\overline{G}) \geq |V(G)|$.

Moreover, the equality holds in (a),(b),(c) and (d) if $G$ is vertex transitive.

**Proof.** (a) Take an optimal solution $\lambda$ for the program (3.14) defining $\chi^*(G)$. Now $\alpha(G)\chi^*(G) = \alpha(G) \sum_{S \text{ stable}} \lambda_S \geq \sum_{S \text{ stable}} \lambda_S |S| = \sum_{S \text{ stable}} \lambda_S e^T \chi^S = e^T e = |V(G)|$.

Assume that $G$ is vertex transitive and let $S$ be a stable set in $G$ with $|S| = \alpha(G)$. We have $\sum_{\sigma \in \text{Aut}(G)} \chi^\sigma(S) = k_S e$ for some $k_S \in \mathbb{R}_+ \setminus \{0\}$. Note next that $\sigma(S)$ is stable for all $\sigma \in \text{Aut}(G)$, which yields $\chi^*(G) \leq \frac{|\text{Aut}(G)|}{k_S} |V(G)|$. On the other hand we also obtain $k_S |V(G)| = |\text{Aut}(G)|\alpha(G)$, yielding $\frac{|\text{Aut}(G)|}{\alpha(G)} \geq \chi^*(G)$. 


(b) Let $Z'$ be optimal for the program defining $\vartheta(G)$ (see (3.4)). Then $\frac{1}{\vartheta(G)} Z'$ is feasible for (3.8). Now $Z'_i = 1 \ (i \in V(G))$ yields $\vartheta(G) \geq \frac{1}{\vartheta(G)} |V(G)|$.

Assume that $G$ is vertex transitive. As the program (3.8) is invariant under action of $\text{Aut}(G)$, we can restrict $X'$ in (3.8) to be invariant under action of $\text{Aut}(G)$. Let now matrix $X'$ be invariant under action of $\text{Aut}(G)$ and optimal for (3.8). Since $X'_{ii} = \frac{\vartheta(G)}{n}$ as $G$ is vertex transitive, $\frac{1}{\vartheta(G)} X'$ is feasible for (3.4) defining $\vartheta(G)$. Therefore $\vartheta(G) \leq \frac{1}{\vartheta(G)}$.

The proofs for (c) and (d) are analogous to the one of (b). \qed

The relation (b) was proven in [64], (c) in [90], while [25] contains the proof for (d). We will see in Chapter 5 how this theorem can be generalized to more graph parameters which are of interest in this thesis.

**Negative results.** Dukanovic and Rendl [25] compute the bounds defined above for several graph classes. In fact, they test if adding nonnegativity and triangle inequalities often does not give any improvements.

(i) on random graphs (see Section 6.4) adding nonnegativity or triangle inequalities does not improve the Lovász theta number considerably (only in the order of decimals);

(ii) on some vertex transitive graphs the nonnegativity constraints might lead to substantial improvements over the Lovász theta number (see Section 6.2 for some examples), whereas additional inclusion of the triangle constraints often does not give any improvements.

We prove below two negative results about adding additional constraints. We apply the following result in Section 6.1.

**Proposition 3.3.2.** If $G$ is vertex transitive and for any pair of edges $ij$, $i'j'$ there exist $\sigma \in \text{Aut}(G)$ such that $\sigma(\{i, j\}) = \{i', j'\}$ then $\vartheta'(G) = \vartheta(G)$.

**Proof.** Since the program (3.1) defining the parameter $\vartheta(G)$ is invariant under the action of $\text{Aut}(G)$, we can assume that the matrix variable $X$ is invariant under the action of $\text{Aut}(G)$. If $G$ is vertex transitive and $E(G) = \{\{i, j\} \mid \sigma \in \text{Aut}(G)\}$ the program (3.1) reads

$$\vartheta(G) = \max \langle J, X \rangle \text{ s.t. } X = \frac{1}{|V(G)|} I + x A_G \succeq 0, \ X \in \mathbb{R}^{V(G) \times V(G)}, \ x \in \mathbb{R}. $$

Since $X := \frac{1}{\vartheta(G)} I$ is feasible, any optimal solution satisfies $x \geq 0$. This proves $\vartheta'(G) = \vartheta(G)$. \qed

We explain now why adding triangle constraints in a program defining the Lovász theta number of a Hamming graph does not give any improvements.

Given an integer $n \geq 1$ and $D \subseteq N := \{1, \ldots, n\}$, the **Hamming graph** $H(n, D)$ is the graph $G$ with node set $V(G) := \mathcal{P}(N)$ and with an edge $(I, J)$ if $|I \Delta J| := |I| \setminus J + |J| \setminus I \in D$ (for $I, J \in \mathcal{P}(N)$).

**Proposition 3.3.3.** Let $G := H(n, D)$, where $n \geq 2$. Then $\vartheta'(G) = \vartheta'(\triangle)(G)$. 

Proof. Observe first that each permutation \( \sigma \in \text{Sym}(n) \) induces an automorphism of \( G \), by letting \( \sigma(I) := \{ \sigma(i) \mid i \in I \} \) for \( I \in \mathcal{P}(N) \). For any \( K \in \mathcal{P}(N) \), the switching mapping \( s_K \) defined by \( s_K(I) := I \triangle K \) (for \( I \in \mathcal{P}(N) \)) is also an automorphism of \( G \). Let \( X \) be optimal for (3.17) and invariant under action of \( \text{Aut}(G) \). It suffices to show that \( X \) is feasible for (3.21).

Since \( X \) is invariant under action of \( \text{Aut}(G) \), an entry \( X_{IJ} \) depends only on \( I \triangle J \), i.e. the matrix \( X \) belongs to the Bose-Mesner algebra \( B_n \). Therefore \( X_{II} = X_{JJ} \) (\( I,J \in \mathcal{P}(N) \)). We also have \( X_{IJ} \leq X_{II} \) (\( I,J \in \mathcal{P}(N) \)), since

\[
\begin{pmatrix}
  X_{II} & X_{IJ} \\
  X_{IJ} & X_{JJ}
\end{pmatrix} = \begin{pmatrix}
  X_{II} & X_{IJ} \\
  X_{IJ} & X_{II}
\end{pmatrix} \geq 0 \quad (I,J \in \mathcal{P}(N)).
\]

It remains to prove \( X_{IK} + X_{JK} \leq X_{IJ} + X_{KK} \) (\( I,J,K \in \mathcal{P}(N) \)). Let \( I,J,K \in \mathcal{P}(N) \). Set \( L := (I \triangle J) \triangle K \) and consider the submatrix of \( X \) indexed by \( I,J,K,L \). It is PSD, and since \( L \triangle I = J \triangle K \), \( L \triangle J = I \triangle K \), \( L \triangle K = I \triangle J \), we have \( X_{IL} = X_{JK}, X_{IJ} = X_{IK}, X_{KL} = X_{IJ} \). Finally,

\[
\frac{1}{4} \begin{pmatrix}
  1 & 1 & 1 & 1 \\
  1 & 1 & 1 & 1 \\
  -1 & -1 & -1 & -1 \\
  -1 & -1 & -1 & -1
\end{pmatrix}^T \begin{pmatrix}
  X_{KK} & X_{IJ} & X_{IK} & X_{JK} \\
  X_{IJ} & X_{KK} & X_{JK} & X_{IK} \\
  X_{IK} & X_{JK} & X_{KK} & X_{IJ} \\
  X_{IK} & X_{JK} & X_{IJ} & X_{KK}
\end{pmatrix} \begin{pmatrix}
  1 \\
  1 \\
  -1 \\
  -1
\end{pmatrix}
\]

\[
= X_{IJ} + X_{KK} - X_{IK} - X_{JK} \geq 0.
\]

Note that we did not use nonnegativity in the last proof. Namely, the triangle constraints are implied by the positive-semidefiniteness and the membership in the Bose-Mesner algebra.