POSITIVSTELLENSÄTZE FOR QUANTUM MULTIGRAPHS

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Abstract. Studying inequalities between subgraph- or homomorphism-densities is an important topic in graph theory. Sums of squares techniques have proven useful in dealing with such questions. Using an approach from real algebraic geometry, we strengthen a Positivstellensatz for simple quantum graphs by Lovász and Szegedy, and we prove several new Positivstellensätze for nonnegativity of quantum multigraphs. We provide new examples and counterexamples.

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1. Introduction

Let $F, G$ be finite undirected graphs without multiple edges or loops (all graphs in the first part of this paper are of this type). A homomorphism is a mapping $\varphi : V_F \to V_G$ defined on vertices, which preserves the adjacency relation, i.e. whenever $ij \in E_F$ is an edge in $F$, then $\varphi(i)\varphi(j) \in E_G$ is an edge in $G$. The homomorphism density $t(F, G)$ of $F$ in $G$ is the probability that a randomly chosen map $\varphi : V_F \to V_G$ is a homomorphism. So if $\hom(F, G)$ denotes the number of homomorphisms, then

$$t(F, G) = \frac{\hom(F, G)}{|V_G|^{|V_F|}}.$$

The subgraph density $t_{\text{inj}}(F, G)$ is closely related; it is the probability that a random injective map is a homomorphism, i.e.

$$t_{\text{inj}}(F, G) = \frac{\text{inj}(F, G)}{|V_G| \cdot (|V_G| - 1) \cdots (|V_G| - |V_F| + 1)},$$
where \( \text{inj}(F, G) \) is the number of injective homomorphisms. With \( F \) fixed and the number of vertices of \( G \) growing, \( t(F, G) \) and \( t_{\text{inj}}(F, G) \) coincide asymptotically, as for example shown in [12]. Since these densities are often studied in the context of very large graphs \( G \), information about any of the two densities also contains some information about the other. We will mostly be concerned with the homomorphism density \( t(\cdot, \cdot) \) in this paper.

One is interested in the possible values that can occur as homomorphism densities, and the relations between them. In other words, given graphs \( F_1, \ldots, F_n \), one wants to understand the set
\[
\{(t(F_1, G), \ldots, t(F_n, G)) \mid G \text{ graph} \} \subseteq \mathbb{R}^n
\]
(see [2] Section 7.3 for a nice picture in the case \( n = 2, F_1 = K_2, F_2 = K_3 \)). A way of doing this is looking at polynomial inequalities between homomorphism densities. Given a polynomial \( p \in \mathbb{R}[x_1, \ldots, x_n] \), one is interested in the question whether

\[
p(t(F_1, G), \ldots, t(F_n, G)) \geq 0
\]
holds for all graphs \( G \), i.e. whether \( p \) is nonnegative on the above set. Note that the homomorphism density is multiplicative in the first component, meaning that

\[
t(F_1 \sqcup F_2, G) = t(F_1, G) \cdot t(F_2, G),
\]
where \( F_1 \sqcup F_2 \) denotes the disjoint union of graphs \( F_1 \) and \( F_2 \). So (after changing the \( F_i \)) we can restrict to linear inequalities: given graphs \( F_1, \ldots, F_n \) and \( c_1, \ldots, c_n \in \mathbb{R} \), does

\[
\sum_{i=1}^{n} c_i \cdot t(F_i, G) \geq 0
\]
hold for all \( G \)?

**Definition 1.1.** (1) A quantum graph is a formal linear combination of graphs, with real coefficients: \( a = \sum_{i=1}^{n} c_i F_i \).

(2) A quantum graph \( a = \sum_i c_i F_i \) is called nonnegative if \( t(a, G) := \sum_i c_i \cdot t(F_i, G) \geq 0 \) holds for all graphs \( G \).

**Example 1.2.** (1) The following quantum graph is nonnegative:

\[
a = \begin{array}{c}
\bullet & \bullet & \quad - & \bullet & \bullet \\
\end{array}
\]

This is shown in [10], using an easy sums of squares approach; see Example 2.2 below for more details.
(2) The following quantum graph is also nonnegative; we will prove this in Example 3.5 below:

\[ b = \begin{array}{c}
\text{vertex} \\
-2
\end{array} + \begin{array}{c}
\text{vertex}
\end{array} + \begin{array}{c}
\text{vertex}
\end{array} \]

(3) The computation \( c := b + 2a \) results in the following quantum graph, whose nonnegativity is known as Goodman’s Theorem:

\[ c = \begin{array}{c}
\text{vertex} \\
-2
\end{array} \begin{array}{c}
\text{vertex}
\end{array} + \begin{array}{c}
\text{vertex}
\end{array} + \begin{array}{c}
\text{vertex}
\end{array} \]

This is precisely the statement that the polynomial \( y - 2x^2 + x \) is nonnegative on the set

\[ \{(t(K_2, G), t(K_3, G)) \mid G \text{ graph} \} \subseteq \mathbb{R}^2. \]

Nonnegativity of quantum graphs is examined in numerous recent papers. It is in general an undecidable problem [7], but sums of squares techniques have proven useful in attacking it [14]. An extensive account of this topic (and many related others) can be found in the very nice book [10].

Our contribution is the following. By putting the existing sums of squares techniques into a bit more conceptual setting of real algebraic geometry, we simplify and slightly strengthen the Positivstellensatz from [14]. This is done in Section 2. Our main results are Theorem 3.2, Theorem 3.6 and Theorem 3.9 in Section 3, all Positivstellensätze for quantum multigraphs. We obtain new examples, using results from real algebraic geometry.

2. Simple graphs

In this section, every graph is finite, undirected and without multiple edges or loops. We start by explaining the setup of graph algebras and graph parameters. Let us emphasize that hardly any of the results in this section is new; the concepts have been introduced and used by several authors before (see for example [6, 7, 12–14] and also [10] for a thorough overview). Our approach will however simplify some of the proofs, and will most notably allow us to extend the results to the multigraph setup in the next section.

A \( k \)-labeled graph is a graph where \( k \) different vertices are labeled from 1 to \( k \) (a 0-labeled graph is an unlabeled graph). Let \( \mathcal{G}_k \) denote the set of isomorphism classes of \( k \)-labeled graphs, where isomorphisms are supposed to respect the labeling. If \( F, G \) are \( k \)-labeled graphs, then the product

\[ F \ast_k G \]

is defined as first taking the disjoint union of \( F \) and \( G \), then identifying vertices with the same label, and finally reducing possible edge multiplicities to one. So for 0-labeled graphs
it is just the disjoint union. This multiplication turns $G_k$ into an abelian monoid, having the graph $E_k$ with vertices $1, \ldots, k$ and no edges as its identity element.

The $k$-th graph algebra $A_k$ is the monoid algebra of $G_k$ over $\mathbb{R}$, i.e. it has, as a vector space, the elements of $G_k$ as a basis:

$$A_k = \left\{ \sum_{G \in G_k} \alpha_G \cdot G \mid \alpha_G \in \mathbb{R}, \text{ almost all } \alpha_G = 0 \right\}.$$  

The multiplication of $G_k$ extends by distributivity, making $A_k$ a commutative algebra. Note that elements of $A_0$ are precisely quantum graphs as in Definition 1.1.

We can equip $A_k$ with a grading, by defining

$$\deg(G) := \left| V_G \right| - k$$

(i.e. counting the unlabeled vertices) for $G \in G_k$ and setting

$$A_k^d := \left\{ \sum_{\deg(G)=d} \alpha_G \cdot G \right\}.$$  

We obtain

$$A_k = \bigoplus_{d \geq 0} A_k^d$$

and the multiplication is compatible with this direct-sum-decomposition, in the usual way. We will often work with the degree zero part $A_k^0$ only. It is a finite dimensional and real reduced algebra (i.e. 0 is a sum of squares only in the trivial way), in fact the quotient of the polynomial algebra $\mathbb{R}[z_{ij} \mid 1 \leq i < j \leq k]$ by the ideal generated by $z_{ij}^2 - z_{ij}$. Here we identify a monomial

$$z^e = z_{12}^{e_{12}} \cdots z_{23}^{e_{23}} \cdots$$

(where $e_{ij} \in \{0, 1\}$) with the graph having an edge between the vertices labeled $i$ and $j$ if and only if $e_{ij} = 1$. The variety corresponding to $A_k^0$ is finite and consists only of real points:

$$\mathcal{V}(A_k^0) = \{0, 1\}^{k \choose 2}.$$  

From this it is clear that the set of sums of squares $\Sigma^2 A_k^0$ in $A_k^0$ coincides with the set of elements which are nonnegative as polynomial functions on $\mathcal{V}(A_k^0)$.

To a graph in $G_k$ we can add a new isolated vertex labeled $k + 1$, and obtain a graph in $G_{k+1}$. This injective monoid-homomorphism $\boxplus : G_k \to G_{k+1}$ extends to an embedding of graded algebras $\boxplus : A_k \to A_{k+1}$. 

A **graph parameter** is a mapping $t: G_0 \to \mathbb{R}$, i.e. a rule that assigns a real number to each (unlabeled) graph. By ignoring the labels one can extend $t: G_k \to \mathbb{R}$ for all $k$, and thus obtain linear functionals $t: A_k \to \mathbb{R}$.

**Definition 2.1.** A graph parameter $t$ is called
- **isolate indifferent** if the value at a graph does not change when adding an isolated vertex; equivalently, if $t$ is compatible with the mappings $⊞$.
- **reflection positive** if $t(a^2) \geq 0$ holds for all $a \in A_k$ and all $k$.
- **flatly reflection positive** if $t(a^2) \geq 0$ holds for all $a \in A_0^k$ and all $k$.

We list some important observations and results:
- For any graph $G$, the homomorphism density $t(\cdot, G)$ defines an isolate indifferent and reflection positive graph parameter. The first property is obvious, the second follows for example from Remark 2.8 below.
- Every isolate indifferent and reflection positive graph parameter is a conic combination of limits of homomorphism densities $t(\cdot, G)$. This is shown in [14]. So nonnegativity of quantum graphs as in Definition 1.1 could also be defined as nonnegativity at each isolate indifferent and reflection positive graph parameter!
- An isolate indifferent and flatly reflection positive graph parameter is automatically reflection positive. This is also shown in [14]. So nonnegativity of quantum graphs as in Definition 1.1 could also be defined as nonnegativity at each isolate indifferent and flatly reflection positive graph parameter!

Now there is an obvious way to prove nonnegativity of a quantum graph $a$: if it coincides with a sum of squares from some $A_k$ (after removing the labels and possibly adding or removing isolated vertices), then $a$ is nonnegative.

**Example 2.2.** This example is taken from [10]. The quantum graph

$$a = \begin{array}{ccc}
\bullet & \bullet & \bullet \\
\bullet & \circ & \bullet \\
\end{array}$$

is nonnegative, since it coincides up to labels and isolated vertices with the following square in $A_1$:

$$\left( \begin{array}{cc}
\bullet & \bullet \\
\circ & \circ \\
\end{array} \right)^2$$

The Positivstellensatz from [14] states that any nonnegative quantum graph arises in this way, *up to an arbitrarily small error $\epsilon$ in the $\ell_1$-norm of coefficients*. Note that [11] provides
a Positivstellensatz without errors, using infinite sums of squares instead. We give a new proof for the following strong approximation result:

**Theorem 2.3.** A quantum graph $a$ is nonnegative if and only if for all $\epsilon > 0$ there is some $k$ and a sum of squares $\sigma \in \Sigma^2 A^0_k$, such that $a + \epsilon$ and $\sigma$ coincide up to labels and isolated vertices.

The proof of the theorem becomes quite easy, if we equip our graph algebras with some more structure. So first note that permutation of the labels yields an operation $S_k \acts G_k$ of the symmetric group $S_k$ by automorphisms on $G_k$. This operation extends to an operation by graded algebra automorphisms on $A_k$. We denote by $B_k$ the set of invariant elements of this action. $B_k$ is a graded subalgebra of $A_k$, and the inclusion $B_k \subseteq A_k$ admits a left-inverse $B_k$-module homomorphism

$$r : A_k \to B_k$$

$$a \mapsto \frac{1}{|S_k|} \sum_{\sigma \in S_k} a^\sigma$$

which respects the grading, the *Reynolds operator*. As a vector space, $B_k$ is spanned by the elements $r(G)$ with $G \in G_k$. $B^0_k \subseteq A^0_k$ is a subalgebra, which is clearly also finite dimensional and real reduced. The variety of $B^0_k$ consists of finitely many points which are all real, and to the inclusion $B^0_k \subseteq A^0_k$ there corresponds a surjective polynomial mapping $V(A^0_k) \to V(B^0_k)$.

We also obtain injective linear maps

$$\boxplus_r := r \circ \boxplus : B_k \to B_{k+1}$$

making the following diagram commutative:

$$\cdots \to A_k \xrightarrow{r} A_{k+1} \xrightarrow{\boxplus_r} \cdots$$

$$\cdots \to B_k \xrightarrow{r} B_{k+1} \xrightarrow{\boxplus_r} \cdots$$

Note that the mappings $\boxplus_r$ are just linear, not multiplicative; they are however compatible with the grading on $B_k$, and we often consider the degree zero part of the above diagram only. We denote by $B^0$ the direct limit of the chain

$$\cdots \to B^0_k \to B^0_{k+1} \to \cdots$$

in the category of $\mathbb{R}$-vector spaces. We next consider

$$C_k := r(\Sigma^2 A^0_k) = \Sigma^2 A^0_k \cap B^0_k.$$
From the fact that the mapping $\mathcal{V}(\mathcal{A}_k^0) \to \mathcal{V}(\mathcal{B}_k^0)$ is surjective we see that $C_k$ is the set of nonnegative functions on $\mathcal{V}(\mathcal{B}_k^0)$, and thus also coincides with $\Sigma^2\mathcal{B}_k^0$ (a fact which is not true for Reynolds operators of group actions in general!). Clearly, 1 is an interior point of the convex cone $C_k$ in $\mathcal{B}_k^0$, meaning that $1 + \epsilon b$ belongs to $C_k$, for each $b \in \mathcal{B}_k^0$ and $\epsilon > 0$ small enough. We have $\varpi_r(C_k) \subseteq C_{k+1}$. In the direct limit $\mathcal{B}^0$ we obtain the convex cone $C := \bigcup_k C_k$, of which 1 is also an interior point. Since a graph parameter $t$ ignores labels, it factors through $\mathcal{B}_k$ via $r$:

$$A_k \xrightarrow{r} B_k \xrightarrow{t} \mathbb{R}.$$ 

**Lemma 2.4.** A family of linear functionals $\varphi: \mathcal{B}_k^0 \to \mathbb{R}$ (for all $k \geq 0$) comes from a flatly reflexion positive and isolate indifferent graph parameter if and only if it is compatible with the embeddings $\varpi_r$ and satisfy $\varphi(C_k) \geq 0$ for all $k$ (equivalently, if it comes from a linear functional on $\mathcal{B}^0$ which is nonnegative on $C$).

**Proof.** Easy exercise. □

**Proof of Theorem 2.3.** One direction is clear. For the other, let $a$ be a nonnegative quantum graph. Choose some $\tilde{a} \in \mathcal{A}_d^0$ which coincides with $a$ up to isolated vertices when all labels are removed. Then $b := r(\tilde{a}) \in \mathcal{B}_d^0$ also coincides with $a$ up to isolated vertices and labels, and is thus nonnegative at each isolate indifferent, flatly reflection positive graph parameter. In view of Lemma 2.4, it belongs to the double dual of $C$ in $\mathcal{B}^0$, and the isolation theorem for convex sets with nonempty interior (see for example [5], Proposition 1.3 for this standard fact) implies $b + \epsilon \in C$ for all $\epsilon > 0$. Since $\mathcal{B}^0$ is the direct limit of the $\mathcal{B}_k^0$ and $C = \bigcup_k C_k$, this proves the claim. □

**Remark 2.5.** The proof even shows that if $a$ is strictly positive at each nontrivial, isolate indifferent and reflection positive graph parameter, then $a$ coincides with a sum of squares from some $\mathcal{A}_k^0$ without error (see again [5], Proposition 1.3).

One can ask whether the $\epsilon$ in Theorem 2.3 is really necessary. It is in fact, as was shown in [7]; there exist nonnegative quantum graphs which do not coincide up to labels and isolated vertices with a sum of squares from some $\mathcal{A}_k^0$ or even $\mathcal{A}_k$. We sketch the idea from [7].

For two graphs $F, G$ we consider a parametrized version of $t(F, G)$. We assign a variable $x_w$ to each of the vertices $w$ of $G$, set $g := \sum_{w \in V_G} x_w$ and define

$$\bar{t}(F, G) := \frac{\sum_{\varphi: V_F \to V_G} \Pi_{v \in V_F} x_{\varphi(v)}}{g|V_F|}.$$
Note that \( \widetilde{t}(F, G)(1, \ldots, 1) = t(F, G) \) is just the usual homomorphism density. Also note that \( \widetilde{t}(\cdot, G) \) is isolate indifferent. We thus obtain linear maps

\[
\widetilde{t}(\cdot, G) : A_k \to \mathbb{R}\left[ \frac{x_w}{g} \mid w \in V_G \right]
\]

which are compatible with \( \boxplus \). Given \( F \in G_k \) and a mapping \( \psi : [k] \to V_G \) there is a relative version

\[
\widetilde{t}_\psi(F, G) := \sum_{\varphi \supseteq \psi} \prod_{v \in V_F \setminus [k]} x_{\varphi(v)}
\]

The relative version is multiplicative on \( G_k \), i.e.

\[
\widetilde{t}_\psi(F \ast_k F', G) = \widetilde{t}_\psi(F, G) \cdot \widetilde{t}_\psi(F', G)
\]

holds; so \( \widetilde{t}_\psi(\cdot, G) : A_k \to \mathbb{R}[x_w/g] \) maps sums of squares to sums of squares. On \( A_k \) we have

\[
\widetilde{t}(\cdot, G) = \sum_{\psi : [k] \to V_G} \widetilde{t}_\psi(\cdot, G) \cdot \frac{\prod_{i \in [k]} x_{\psi(i)}}{g^k}.
\]

**Definition 2.6.** (1) A subset \( P \subseteq R \) of a commutative ring \( R \) is called a preorder if \( P + P \subseteq P \), \( P \cdot P \subseteq P \) and \( P \) contains all squares from \( R \).

(2) For \( r_1, \ldots, r_m \in R \), the set

\[
\text{PO}(r_1, \ldots, r_m) := \left\{ \sum_{e \in \{0,1\}^m} \sigma_e \cdot r_1^{e_1} \cdots r_m^{e_m} \mid \sigma_e \in \Sigma R^2 \right\}
\]

is the smallest preorder containing \( r_1, \ldots, r_m \). It is called the preorder generated by \( r_1, \ldots, r_m \).

So after clearing denominators in \( \widetilde{t}(\cdot, G) \) we get:

**Theorem 2.7.** Let \( a \) be a quantum graph, which coincides (after unlabeling and up to isolated vertices) with a sum of squares from some \( A_k \). Then there is some \( N \) large enough, such that for all graphs \( G \)

\[
\left( \sum_{w \in V_G} x_w \right)^N \cdot \widetilde{t}(a, G) \in \text{PO}(x_w \mid \omega \in V_G) \subseteq \mathbb{R}[x_w \mid \omega \in V_G].
\]

If \( a \) coincides with a sum of squares from \( A_k^0 \), then \( (\sum_{w \in V_G} x_w)^k \cdot \widetilde{t}(a, G) \) has nonnegative coefficients, for all graphs \( G \).

**Remark 2.8.** The theorem shows that homomorphism densities \( t(\cdot, G) \) are reflection positive. We have \( t(\cdot, G) = \widetilde{t}(\cdot, G)(1, \ldots, 1) \), and polynomials from the preorder generated by the \( x_w \) are nonnegative at this point.
Example 2.9. We have seen in Example 2.2 that the following quantum graph comes from a sum of squares in \( A_1 \):

\[
a = \begin{array}{c}
\bullet \\
\bullet
\end{array} - \begin{array}{c}
\bullet \\
\bullet
\end{array}
\]

It is also shown in [10] that \( a \) does not come from a sum of squares in some \( A_k^0 \). Here is another proof: for \( G = K_2 \) we compute \((x_1 + x_2)^4 \cdot \tilde t(a, G) = (x_1 - x_2)^2 x_1 x_2 \), and this homogeneous polynomial has a zero in the interior of the positive orthant. It can thus clearly not have the Pólya property, i.e. multiplication with powers of \( x_1 + x_2 \) will never lead to only nonnegative coefficients (see [3] for more details on the Pólya property).

The paper [7] uses the described method to show that there even exist nonnegative quantum graphs that are not sums of squares from any \( A_k \).

Now that we have explained the setup for simple graphs in some detail, we pass to multigraphs, and prove some new results.

3. Multigraphs

In this section, a graph is still finite, undirected and loopless, but may now have multiple edges. Note that the case of loops and even directed edges is quite similar, and the results have straightforward extensions.

We define \( k \)-labeled graphs and their multiplication as before, except that we don’t erase multiple edges after multiplication. All structures as the graph algebras \( A_k, A_k^0, B_k, B_k^0 \) and the Reynolds operator \( r \) can be defined just as before. This time \( A_k^0 \) is not finite dimensional, but \( A_k^0 = \mathbb{R}[z_{ij} \mid 1 \leq i < j \leq k] \) is the full polynomial algebra, and thus \( \mathcal{V}(A_k^0) = \mathbb{R}^{(k)} \).

The algebra \( B_k^0 \) of \( S_k \)-invariants is finitely generated (by a standard result of Hilbert, see for example [19] for a nice exposition), and to the embedding into \( A_k^0 \) there corresponds a polynomial mapping \( \mathcal{V}(A_k^0) \rightarrow \mathcal{V}(B_k^0) \). We denote by \( B^0 \) the direct limit of the chain

\[
\cdots \rightarrow B_k^0 \rightarrow B_{k+1}^0 \rightarrow \cdots
\]

again in the category of vector spaces.

We again consider \( C_k := r(\Sigma^2 A_k^0) = (\Sigma^2 A_k^0) \cap B_k^0 \) and this is a preorder of \( B_k^0 \), which is now larger than \( \Sigma^2 B_k^0 \) in general. We still have \( \oplus_r(C_k) \subseteq C_{k+1} \) and we obtain a convex cone \( C = \bigcup_k C_k \) in \( B^0 \). More general, let \( P_k \subseteq A_k^0 \) be an \( S_k \)-invariant preorder. Then \( r(P_k) = P_k \cap B_k^0 \) is a preorder and a \( C_k \)-module. If \( \oplus_r(P_k) \subseteq P_{k+1} \) holds, then also \( \oplus_r(r(P_k)) \subseteq r(P_{k+1}) \). So \( B^0 \) contains the convex cone \( \mathcal{P} = \bigcup_k r(P_k) \). If \( 1 \) is an interior point of each \( P_k \) in \( A_k^0 \) (recall this means \( 1 + \epsilon a \in P_k \) for all \( a \) and \( \epsilon \) small; this is sometimes also referred to as \( P_k \) being archimedean), then the same is true for \( r(P_k) \) in \( B_k^0 \) and \( P \) in \( B^0 \). We will mostly consider
the preorders
\[ P_k(d) := \text{PO}(d \pm z_{ij} \mid 1 \leq i < j \leq k) \subseteq A_k^0, \]
of which 1 is an interior point (see [15] or [16]). The induced cone in \( B^0 \) is denoted by \( P(d) \) in this case.

Graph parameters and their properties are defined as before. Furthermore, a graph parameter is called \( d \)-bounded, if \( |t(K^k_2)| \leq d^k \) holds for all \( k \), where \( K^k_2 \) is the graph with two vertices and \( k \) edges between them. With a suitable notion of homomorphism for multigraphs, the homomorphism density \( t(\cdot, G) \) into a multigraph \( G \) with edge-multiplicity at most \( d \) is an example of such a \( d \)-bounded parameter. The following Lemma is the straightforward extension of Lemma 2.4 to the multigraph setting.

Lemma 3.1. (1) A family of linear functionals \( \varphi : B^0_k \rightarrow \mathbb{R} \) comes from a flatly reflection positive and isolate indifferent graph parameter if and only if it is compatible with the embeddings \( \boxplus_r \) and satisfy \( \varphi(C_k) \geq 0 \) for all \( k \). Equivalently, if it comes from a linear functional on \( B^0 \) which is nonnegative on \( \mathcal{C} \).

(2) The family comes from a \( d \)-bounded such parameter, if and only if it comes from a linear functional on \( B^0 \) which is nonnegative on \( P(d) \).

Proof. Again an exercise. For (2) use the fact the boundedness just means \( |\varphi(z_{ij}^k)| \leq d^k \) for all \( k, i, j \). This is equivalent to having representing measures on \([-d, d]^k \) for all \( k \) (by Theorem 2.2 in [13] for example), and this is equivalent to being nonnegative on each \( P_k(d) \), \( r(\mathcal{P}(d)) \) and \( \mathcal{P}(d) \), respectively (by [18]). \( \square \)

The following is our first main theorem. Also compare to Theorem 3.9 below, which provides a more complicated approximation, but avoids the preorder.

Theorem 3.2. A quantum multigraph \( a \) is nonnegative at each isolate indifferent, flatly reflection positive and \( d \)-bounded graph parameter if and only if for each \( \epsilon > 0 \) there is some \( k \) and some \( \sigma \in \mathcal{P}_k(d), \)

such that \( a + \epsilon \) and \( \sigma \) coincide up to labels and isolated vertices.

Proof. One direction is clear. For the other, let \( a \) be nonnegative. Choose some \( \tilde{a} \in A_k^0 \) which coincides with \( a \) up to isolated vertices, when all labels are removed. Then \( b := r(\tilde{a}) \in B^0_d \)
also coincides with \( a \) up to isolated vertices and labels, and is thus nonnegative at each isolate indifferent, flatly reflection positive and \( d \)-bounded graph parameter. In view of Lemma 3.1, it belongs to the double dual of \( \mathcal{P}(d) \) in \( B^0 \), and the isolation theorem for convex sets with nonempty interior again implies \( b + \epsilon \in \mathcal{P}(d) \) for all \( \epsilon > 0 \). Since \( B^0 \) is the direct limit of the \( B^0_k \) and \( \mathcal{P}(d) = \bigcup_k r(\mathcal{P}_k(d)) \), this proves the claim. \( \square \)
Remark 3.3. Again the proof shows that if $a$ is strictly positive at each nontrivial, isolate indifferent, flatly reflexion positive and $d$-bounded parameter, then $a$ comes from an element in some $\mathcal{P}_k(d)$ without error.

It is maybe not very surprising that the error $\epsilon$ cannot be removed here as well. To see this, let $F$ be a multigraph. For any $n \in \mathbb{N}$ we set $g = \sum_{i=1}^{n} x_i$ and define

$$\tilde{t}(F, n) := \frac{\sum_{\varphi : V_F \to [n]} \prod_{i \in V_F} x_{\varphi(i)} \prod_{uv \in E_F} y_{\varphi(v)\varphi(w)}}{g |V_F|} \in \mathbb{R} \left[ \frac{x_i}{g}, y_{ij} \mid 1 \leq i \leq j \leq n \right].$$

This counts the number of vertex-edge-homomorphisms into the complete graph with vertex weights $x_i$ and edge weights $y_{ij}$. Again $\tilde{t}(\cdot, n)$ is isolate indifferent and defines linear maps on all $\mathcal{A}_k$, compatible with $\boxplus$. For $F \in \mathcal{G}_k$ and $\psi : [k] \to [n]$ there is again a relative version

$$\tilde{t}_\psi(F, n) = \frac{\sum_{\varphi \supseteq \psi} \prod_{i \in V_F \setminus [k]} x_{\varphi(i)} \prod_{uv \in E_F} y_{\varphi(v)\varphi(w)}}{g |V_F| - k}$$

which is multiplicative on $\mathcal{A}_k$ and fulfills

$$\tilde{t}(\cdot, n) = \sum_{\psi : [k] \to [n]} \tilde{t}_\psi(\cdot, n) \cdot \frac{\prod_{i=1}^{k} x_{\psi(i)}}{g^k}.$$

Note that $\tilde{t}_\psi(z_{ij}, n) = y_{\psi(i)\psi(j)}$. After clearing denominators we obtain:

**Theorem 3.4.** Let $a$ be a quantum multigraph which coincides up to labels and isolated vertices with an element $\sigma \in \text{PO}(d \pm z_{ij} \mid 1 \leq i < j \leq k) \subseteq \mathcal{A}_k$. Then there is some $N \in \mathbb{N}$ such that for any $n \in \mathbb{N}$ we have

$$\left( \sum_{i=1}^{n} x_i \right)^N \tilde{t}(a, n) \in \text{PO}(x_i, d \pm y_{ij} \mid 1 \leq i \leq j \leq n) \subseteq \mathbb{R}[x_i, y_{ij}].$$

If $a$ comes from an element of some $\mathcal{P}_k(d) \subseteq \mathcal{A}_k^0$, then in $g^k \cdot \tilde{t}(a, n)$ the coefficient of each monomial in $x$ is from $\text{PO}(d \pm y_{ij}) \subseteq \mathbb{R}[y_{ij}]$.

It is often enough to substitute $x_i = 1/n$ and $y_{ii} = 0$ and obtain an element of the preorder $\text{PO}(d \pm y_{ij} \mid 1 \leq i < j \leq n)$.

**Example 3.5.** (1) We consider the Robinson quantum multigraph

$$a = \begin{array}{c}
\bullet \\
\bullet + \end{array} \quad -2 \begin{array}{c}
\bullet \\
\bullet - \end{array}$$

which coincides (up to labels, isolated nodes and dividing by 3) with the fully labeled graph coming from the Robinson polynomial

$$R = z_{12}^6 + z_{13}^6 + z_{23}^6 - (z_{12}^4 z_{13}^2 + z_{12}^4 z_{23}^2 + z_{12}^2 z_{13}^4 + z_{12}^2 z_{23}^4 + z_{13}^2 z_{23}^2 + z_{13}^2 z_{23}^4 + z_{13}^4 z_{23}^4 + z_{13}^4 z_{23}^2 + 3 z_{12}^2 z_{13}^2 z_{23}^2) \in \mathcal{A}_3^0.
For details on the Robinson polynomial see [17]. Since the Robinson polynomial is nonnegative on \( \mathbb{R}^3 \), we have \( R + \epsilon \in \mathcal{P}_3(d) \subseteq \mathcal{A}_0^3 \) for all values of \( d \). This follows for example from the archimedean Positivstellensatz in [18]. Thus \( a \) is nonnegative at each \( d \)-bounded, flatly reflexion positive and isolate indifferent graph parameter.

On the other hand, if we compute \( \hat{\tau}(a, 3) \) and set \( x_i = 1/3 \) as well as \( y_{ii} = 0 \) for all \( i \), then we obtain \( R \) again (up to a positive multiple and in the variables \( y_{ij} \) instead of \( z_{ij} \)). Since \( R \) is homogeneous and not a sum of squares, it does also not belong to the preorder generated by \( d \pm y_{ij} \) (compare the lowest degree parts in a possible representation). So \( a \) does not coincide up to labels and isolated nodes with an element from some \( \text{PO}(d \pm z_{ij}) \) in \( \mathcal{A}_k \) (and thus also not from some \( \mathcal{P}_k(d) \subseteq \mathcal{A}_k^0 \)).

Reducing all edge multiplicities in the Robinson example to one yields the simple quantum graph from Example 1.2 (2), and thus proves its nonnegativity. In particular, it implies Goodman’s Theorem.

(2) Several generalizations of the Robinson polynomial appear under the name \( H_\mu \) in [4], Remark 2.5 and Proposition 2.7. They can be used to produce generalizations of the above example. For any odd integer \( \mu \) we obtain the following nonnegative quantum graph, where the little numbers indicate the multiplicities of the simply drawn edge:

\[
a = \begin{array}{cccc}
2\mu + 4 & 2\mu & -2 & 2\mu + 2 \\
\end{array}
\]

(3) Another related polynomial appears under the name \( h_4 \) in [4], Section 2. It gives rise to the following nonnegative quantum graph:

\[
a = \begin{array}{cc}
\circ & \circ \\
\end{array}
\]

We proceed and want to prove another Positivstellensatz. Let us call a graph parameter \( t \) slowly growing, if

\[
\sum_{i=0}^{\infty} \frac{1}{i!} t \left(K_2^{2i}\right) < \infty
\]

where again \( K_2^j \) is the graph with two vertices and \( j \) edges between them.

**Theorem 3.6.** A quantum multigraph \( a \) is nonnegative at each isolate indifferent, flatly reflection positive and slowly growing graph parameter, if and only if for all \( \epsilon > 0 \) there exists \( r \in \mathbb{N} \) such that

\[
a + \epsilon \sum_{i=0}^{r} \frac{1}{i!} K_2^{2i}
\]

coincides with a sum of squares from \( \mathcal{A}_r^0 \), up to labels and isolated nodes.
Proof. The "if"-direction is clear. For the "only if"-direction we can assume that $a$ is strictly positive at each normalized such parameter (i.e. $t(K_1) = 1$), by adding some $\epsilon > 0$ to $a$ first.

We consider the finite dimensional subspace $V_k = \mathbb{R}[z_{ij}] \subseteq A_k^0$ of polynomials of degree at most $k$, set $\Sigma^2 V_k = \{ \sum_i c_i^2 \mid c_i \in V_k \}$, and finally

$$\Sigma_k := r(\Sigma^2 V_k) \subseteq B_k^0.$$ 

This is a convex cone in a finite dimensional subspace of $B_k^0$. For any fixed $M \geq 1$ we next consider

$$K_k(M) := \Sigma_k + \mathbb{R}_{\geq 0} \left( \binom{k}{2} \cdot M - \sum_{1 \leq i < j \leq k} \sum_{s=0}^k \frac{1}{s!} z_{ij}^{2s} \right),$$

which is also a finite dimensional cone in $B_k^0$. We have $\mathbb{B}(K_k(M)) \subseteq K_{k+1}(M)$.

As usual, we choose some $b \in B_k^0$ that coincides with $a$ up to labels and isolated nodes. We then claim that $\mathbb{B}(b)$ belongs to $K_k(M)$, for some $k$ large enough. Indeed if it does not, there are $K_k(M)$-positive functionals $\varphi_k : B_k^0 \to \mathbb{R}$ with $\varphi_k(b) \leq 0$ for all $k$ large enough. We can ensure $\varphi_k(1) > 0$ (and thus $\varphi_k(1) = 1$): if $b$ is not in the linear hull of $K_k(M)$ then first choose $\varphi_k \equiv 0$ on $K_k(M)$ and negative on $b$, then add some small multiple of the evaluation at the origin; otherwise choose $\varphi_k$ nontrivial on $K_k(M)$, and use Lemma 4.3 from [9] to see that $\varphi_k(1) \neq 0$ is automatic.

Again using Lemma 4.3 from [9] one checks that $\varphi_s(\mathbb{B}(c))$ remains bounded for each fixed $c$ from some $B_k^0$ and all $s$. Choosing a non-principal ultrafilter $\omega$ on $\mathbb{N}$ and setting

$$\psi_k(c) := \lim_{s \to \omega} \varphi_s(c)$$

for all $k$ and $c \in B_k^0$ defines a new compatible family of linear functionals, nonnegative on all $C_k$. This family thus comes from a normalized, flatly reflection positive and isolate indifferent graph parameter $t$, which is obviously slowly growing, in fact

$$\sum_{i=0}^{\infty} \frac{1}{i!} t(K_2^{2i}) \leq M$$

holds. We also have $t(a) \leq 0$, a contradiction.

What we have shown so far is that for each $M \geq 1$ there exists some $k$ large enough such that $b \in K_k(M)$. This means we find a representation

$$b + c \sum_{1 \leq i < j \leq k} \sum_{s=0}^k \frac{1}{s!} z_{ij}^{2s} = \sigma + c \binom{k}{2} M$$

with some $c \geq 0$ and $\sigma \in \Sigma_k$. If we plug in 0 for each $z_{ij}$ and let $M$ go to infinity, we see $c \binom{k}{2} \to 0$. This proves the claim. □
Remark 3.7. (1) Theorem 3.6 gives an explicit $\ell_1$-norm approximation of $a$ via sums of squares. In this setup, the approximation cannot be strengthened to a simple $"+\epsilon"$ approximation, as we will see.

(2) From the main result of [8] we see that a globally nonnegative polynomial $p \in \mathbb{R}[z_{ij}] = \mathcal{A}_k^0$ gives rise to a quantum graph that is nonnegative in the sense of Theorem 3.6.

(3) Whether the perturbation is really necessary is checked as before; if $\tilde{t}(a,n)$ is not a sum of squares (after setting $x_i = 1/n$ and $y_{ii} = 0$ often), then $a$ does not coincide with a sum of squares from some $\mathcal{A}_k$.

Example 3.8. The Robinson example $a$ from Example 3.5 (1) is nonnegative in the sense of Theorem 3.6, since it comes from a globally nonnegative polynomial in $\mathcal{A}_3^0$. As argued before, neither $a$ nor $a + \epsilon$ is a sum of squares in some $\mathcal{A}_k$, since $\tilde{t}(a,3)$ is the Robinson polynomial again.

In a similar fashion, we can prove the following variant of Theorem 3.2. We get a more complicated approximation, but avoid the preorder:

Theorem 3.9. A quantum multigraph $a$ is nonnegative at each isolate indifferent, flatly reflection positive and $d$-bounded graph parameter if and only if for all $\epsilon > 0$ there is some $r$ such that

$$a + \epsilon \left( 1 + \frac{1}{d^{2r}} K_{2r}^2 \right)$$

coincides with a sum of squares from $\mathcal{A}_r^0$, up to labels and isolated nodes.

Proof. By scaling the edge-weights we can restrict to the case $d = 1$. The "if"-direction is clear. For the other direction we again assume that $a$ is strictly positive at each normalized such parameter (this is why we need 1 in the approximation). We proceed as in the proof of Theorem 3.6, this time setting

$$K_k(M) := \Sigma_k + \mathbb{R}_{\geq 0} \left( \binom{k}{2} \cdot M - \sum_{1 \leq i < j \leq k} z_{ij}^{2k} \right).$$

Using Lemma 4.1 and Lemma 4.3 from [9] we obtain $b \in K_k(M)$ for some $k$. Note that the functionals $\psi_k$ that we define as before fulfill $\psi_k(z_{ij}^{2r}) \leq M$ on $\mathcal{A}_k^0$; by Theorem 2.5 in Chapter 4 of [1] they have representing measures on $[-1,1]^{(k)}$ and thus lead to a 1-bounded parameter. We obtain representations

$$b + c \sum_{1 \leq i < j \leq k} z_{ij}^{2k} = \sigma + c \binom{k}{2} M$$

and again $c^{(k)}$ goes to zero for $M \to \infty$. $\square$
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