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ON THE REDUCTION OF A GRAM OPERATOR THAT CORRESPONDS TO A MULTIROOTED GRAPH

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Abstract. Any abstract Gram operator is consistent with some graph. For an arbitrary operator B_Γ that is consistent with a graph Γ, the question arises as to when it is an abstract Gram operator, i.e., whether it is nonnegative. We study this question for certain types of graphs. The simplest case is a star graph. Next, we use the results obtained for star graphs to explore a more general case, where a graph Γ can be treated as a collection of rooted trees, with their roots connected by additional edges into a connected subgraph Γ_0. The work shows that the question about the nonnegativity of an operator B_Γ for such a graph can be reduced to the corresponding question for some operator that is consistent with the subgraph Γ_0.

1. Introduction

Let n be a natural number greater than 1 and $V = \{1, \ldots, n\}$. We consider complex Hilbert spaces H_i, $i \in V$, their external direct sum $H = H_1 \oplus \cdots \oplus H_n$ along with a bounded operator $B : H \to H$. The operator B can be treated as a block matrix $(B_{ij})_{i,j \in V}$ where its block elements are operators $B_{ij} : H_j \to H_i$. If B is nonnegative (and thus self-adjoint) with diagonal block elements being identity operators, we call it an *abstract Gram operator*. The G-construction allows us to build a system of n subspaces for any abstract Gram operator. We denote such a system by $\mathcal{G}(H_1, \ldots, H_n; B)$. Furthermore, for any system of subspaces, the *Gram operator of the system* can be introduced and satisfies all conditions of the abstract Gram operator definition. A system of subspaces built via the G-construction applied to this operator is unitarily equivalent to the original system. Criteria for the irreducibility of a system and the unitary equivalence of two systems can be formulated in terms of their Gram operators. For more details about the G-construction, we refer to [9] and [11].

All this makes the notion of an abstract Gram operator a useful tool for studying classification problems of systems of subspaces (see for example [1, 5, 7–9]). To solve these problems, one builds an operator $B = (B_{ij})_{i,j \in V}$ such that $B_{ii} = I$ and $B_{ij}^* = B_{ji}$. To demonstrate that it is an abstract Gram operator one needs to examine whether B is nonnegative. This problem can be quite challenging but may become easier if some block elements are zero. Note that a block element B_{ij}, $i \neq j$, is zero if and only if related subspaces of the system $\mathcal{G}(H_1, \ldots, H_n; B)$ are orthogonal. Finite simple undirected graphs are useful for encoding the information about which block elements are zero. Namely, for an operator B, where $B_{ii} = I$ and $B_{ij}^* = B_{ji}$, $i, j \in V$, we construct a graph $\Gamma = (V, E)$, where two vertices i and j are considered adjacent (i.e., $\gamma_{ij} \in E$) if and only if the block element B_{ij} is nonzero.

It was initially assumed that the set of indices V consisted of natural numbers from 1 to n, usually with $n > 1$, but all that was actually used was that V is a finite set. This generalization is useful for our further consideration. Therefore, from now on, we assume that V is an arbitrary finite set usually containing two or more elements. We denote by $x = (x_i)_{i \in V}$ a vector in the direct sum of the Hilbert spaces associated with vertices,

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where x_i is the component corresponding to the i-th space. In this paper, we consider only finite simple undirected graphs. For conciseness, we will refer to them as graphs. Additionally, all operators are assumed to be bounded throughout this paper.

Definition 1.1. Let $\Gamma = (V, E)$ be a graph and $B = (B_{ij})_{i,j \in V}$ be an operator in the direct sum H of some Hilbert spaces H_i, $i \in V$. We say that B *is consistent with* Γ if the operators B_{ij} and B_{ji} are nonzero for all edges $\gamma_{ij} \in E$, and the equality

$$\langle Bx, x\rangle = \sum_{i \in V} \|x_i\|^2 + \sum_{\gamma_{ij} \in E} \mathrm{Re}\langle (B_{ij} + B_{ji}^*)x_j, x_i\rangle \tag{1}$$

holds for any $x = (x_i)_{i \in V}$.

Proposition 1.2. *An operator $B = (B_{ij})_{i,j \in V}$ is consistent with a graph $\Gamma = (V, E)$ if and only if its block elements fulfill the following conditions:*

$$B_{ii} = I, \qquad i \in V; \tag{2}$$

$$B_{ij}^* = B_{ji}, \qquad i, j \in V; \tag{3}$$

$$B_{ij} \neq 0 \Leftrightarrow \gamma_{ij} \in E, \qquad i, j \in V,\ i \neq j. \tag{4}$$

Proof. By definition of the inner product in the external direct sum of Hilbert spaces, we have the following equality for any $x = (x_i)_{i \in V}$:

$$\langle Bx, x\rangle = \sum_{i \in V} \langle B_{ii}x_i, x_i\rangle + \sum_{\substack{i,j \in V\\ i<j}} (\langle B_{ij}x_j, x_i\rangle + \langle B_{ji}x_i, x_j\rangle).$$

Condition (2) implies that $\langle B_{ii}x_i, x_i\rangle = \|x_i\|^2$, $i \in V$; condition (3) implies equalities

$$\langle B_{ij}x_j, x_i\rangle + \langle B_{ji}x_i, x_j\rangle = 2\,\mathrm{Re}\langle B_{ij}x_j, x_i\rangle = \mathrm{Re}\langle (B_{ij} + B_{ji}^*)x_j, x_i\rangle, \quad \gamma_{ij} \in E;$$

and condition (4) provides us with a one-to-one correspondence between the set of edges E and the set $\{(i, j) : i, j \in V, i < j, B_{ij} \neq 0\}$. Thus, it follows from these conditions that B is consistent with Γ.

Now, suppose operator B is consistent with Γ.

For a vertex $k \in V$, consider $x = (x_i)_{i \in V}$ such that $x_i = 0$ if $i \neq k$ and x_k is an arbitrary vector in H_k. Then, equality (1) takes the form $\langle B_{kk}x_k, x_k\rangle = \|x_k\|^2$ and we have proved (2).

For vertices $j, k \in V$, $j \neq k$, consider $x = (x_i)_{i \in V}$, such that $x_i = 0$ if $i \notin \{j, k\}$ and x_j, x_k are arbitrary vectors in H_j, H_k correspondingly.

In the case where $\gamma_{jk} \notin E$ equality (1) takes the form $\langle B_{jk}x_k, x_j\rangle + \langle B_{kj}x_j, x_k\rangle = 0$. Thus, by Proposition A.3, we conclude that $B_{jk} = B_{kj}^* = 0$. Taking into account that $\gamma_{ij} \in E$ implies $B_{ij} \neq 0$, we have proved (4).

If $\gamma_{jk} \in E$, equality (1) takes the form

$$\langle B_{jk}x_k, x_j\rangle + \langle B_{kj}x_j, x_k\rangle = \mathrm{Re}\langle (B_{jk} + B_{kj}^*)x_k, x_j\rangle.$$

Then, by Proposition A.4, we obtain $B_{jk} = B_{kj}^*$. Thus, we have proved (3) for adjacent vertices. For the remaining pairs of vertices, this is obvious. □

For brevity, an operator that is consistent with a graph Γ will be denoted by B_Γ. It is clear that such an operator is an abstract Gram operator if and only if it is nonnegative. Note also that condition (3) implies that equality (1) can be shortened to the following form:

$$\langle B_\Gamma x, x\rangle = \sum_{i \in V} \|x_i\|^2 + 2 \sum_{\gamma_{ij} \in E} \mathrm{Re}\langle B_{ij}x_j, x_i\rangle. \tag{5}$$

In [6], the authors consider a unicyclic graph $\Gamma = (C; \Gamma_1, \dots, \Gamma_m)$ and an operator B_Γ such that for each pair of adjacent vertices i and j, there exists a number $\tau_{ij} = \tau_{ji} \in (0, 1)$

such that $\tau_{ij}^{-1}B_{ij}$ is a unitary operator. It was shown that the question of the nonnegativity of B_Γ can be reduced to the same question for some operator B'_C. Later, in [10], this result was generalized to the case where the cycle C is replaced with an arbitrary graph $\Gamma_0 = (V_0, E_0)$, and the blocks B_{ij} are not required to be unitary up to a scalar for adjacent vertices i and j belonging to V_0. In this paper, we further generalize this result by removing restrictions on the block elements B_{ij} for all adjacent vertices i and j.

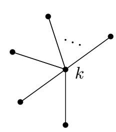
We begin with a star graph $\Gamma_\star$ (Sec. 2). In particular, we prove a criterion for the nonnegativity of $B_{\Gamma_\star}$. Then, we introduce the notion of a root subgraph and describe a class of graphs that can be studied using the proposed approach (Sec. 3). We formulate the main theorem of the paper (Sec. 4) and propose a reduction algorithm (Sec. 5). Choosing a root subgraph in a graph leads to a partial order on vertices and splits them into layers. At each step of the reduction algorithm, one selects a vertex k from the "pre-outer" layer and calculates some operator N_k. To continue, this operator must be nonnegative. If so, vertices adjacent to k from the "outer" layer are removed. For each vertex j not removed and adjacent to k, the block elements B_{kj} are recalculated. This recalculation is simpler and the algorithm more applicable if the operators N_k are invertible. Hence in Sec. 6, we reformulate the main theorem of the paper for two special cases when all operators N_k are guaranteed invertible.

2. Star

Definition 2.1. Let an operator $B_\Gamma = (B_{ij})_{i,j\in V}$ be consistent with a graph $\Gamma = (V, E)$. For any vertex $k \in V$ and any subset of vertices $\mathcal{V} \subset V$ adjacent to vertex k, we define two operators:

$$S_k(B_\Gamma, \mathcal{V}) = \sum_{i\in\mathcal{V}} B_{ki}B_{ik} : H_k \to H_k,$$
$$N_k(B_\Gamma, \mathcal{V}) = I - S_k(B_\Gamma, \mathcal{V}) : H_k \to H_k.$$

Consider the graph $\Gamma_\star = \Gamma_\star(k, \mathcal{V}) = (V_\star, E_\star)$, which is a star with center $k \in V_\star$, i.e., $V_\star = \{k\} \sqcup \mathcal{V}$ and $E_\star = \{\gamma_{ki}\}_{i\in\mathcal{V}}$.



If $V_\star = \{1, \dots, n\}$ then the operator $B_{\Gamma_\star}$ takes the form

$$B_{\Gamma_\star} = \begin{pmatrix} I & \dots & 0 & B_{1k} & 0 & \dots & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & I & B_{k-1k} & 0 & \dots & 0 \\ B_{k1} & \dots & B_{kk-1} & I & B_{kk+1} & \dots & B_{kn} \\ 0 & \dots & 0 & B_{k+1k} & I & \dots & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & 0 & B_{nk} & 0 & \dots & I \end{pmatrix}.$$

For brevity, let the operator $N_k(B_{\Gamma_\star}, \mathcal{V})$ be denoted as $N_\star$.

Proposition 2.2. *For any $x = (x_i)_{i\in V_\star}$*

$$\langle B_{\Gamma_\star}x, x\rangle = \langle N_\star x_k, x_k\rangle + \sum_{i\in\mathcal{V}} \|x_i + B_{ik}x_k\|^2. \tag{6}$$

Proof. By (5) for any x, we have

$$\langle B_{\Gamma_\star}x, x\rangle = \|x_k\|^2 + \sum_{i\in\mathcal{V}} \left(\|x_i\|^2 + 2\,\mathrm{Re}\langle B_{ik}x_k, x_i\rangle\right).$$

Taking into account that

$$\|y\|^2 + 2\,\mathrm{Re}\langle x, y\rangle = \|y + x\|^2 - \|x\|^2$$

we obtain

$$\langle B_{\Gamma_\star} x, x\rangle = \|x_k\|^2 + \sum_{i\in\mathcal{V}} \left(\|x_i + B_{ik}x_k\|^2 - \|B_{ik}x_k\|^2\right).$$

But

$$\|x_k\|^2 - \sum_{i\in\mathcal{V}} \|B_{ik}x_k\|^2 = \langle x_k - S_k(B_{\Gamma_\star}, \mathcal{V})x_k, x_k\rangle,$$

so we get (6). □

Theorem 2.3. *The operator $B_{\Gamma_\star}$ is an abstract Gram operator if and only if the operator $N_\star = N_k(B_{\Gamma_\star}, \mathcal{V})$ is nonnegative.*

Proof. If $\langle N_\star x_k, x_k\rangle \geq 0$ for any $x_k \in H_k$, then for any $x \in H$, by equality (6), we get $\langle B_{\Gamma_\star} x, x\rangle \geq 0$.

Let $B_{\Gamma_\star}$ be nonnegative. For any $x_k \in H_k$, define $x = (x_i)_{i\in V}$ by setting $x_i = -B_{ik}x_k$, $i \in \mathcal{V}$. Then, by equality (6), we obtain $\langle N_\star x_k, x_k\rangle = \langle B_{\Gamma_\star} x, x\rangle \geq 0$. □

Corollary 2.4. *Let $B_{\Gamma_\star}$ be an abstract Gram operator. Then, its kernel consists of all vectors $x = (x_i)_{i\in V_\star}$ such that $x_k \in \ker N_\star$ and $x_i = -B_{ik}x_k$, $i \in \mathcal{V}$.*

Remark. Note that Theorem 2.3 is a corollary of the following statement (to see this, set $H_1 = \oplus_{i\in\mathcal{V}} H_{0,i}$, $H_2 = H_{0,k}$, $A_i = I$ for $i = 1, 2$, and $X = (B_{ik})_{i\in\mathcal{V}}$):

Theorem 2.5. *Let H_1 and H_2 be Hilbert spaces, and let*

$$A = \begin{pmatrix} A_1 & X \\ X^* & A_2 \end{pmatrix} : H_1 \oplus H_2 \to H_1 \oplus H_2,$$

where A_1, A_2, and X are bounded operators. If A_1 is nonnegative and invertible, then $A \geq 0$ if and only if $A_2 \geq X^* A_1^{-1} X$.

This theorem is a well-known result in matrix analysis; see, for example, Theorem 1.3.3 in [2] and the discussion of its history in Section 1.7. In [4], the authors provide three different proofs of this theorem for operators in Hilbert spaces, assuming that H_1 and H_2 coincide (see Theorem 5.1). However, this restriction is not essential for the proofs. Let us note that the proofs of Proposition 2.2 and Theorem 2.3 follow the same ideas as the third proof in [4].

Recall that a subgraph of a graph Γ is called an *induced subgraph* if any two vertices of the subgraph that are adjacent in the graph Γ are adjacent in the subgraph. Let a graph $\bar{\Gamma} = (\bar{V}, \bar{E})$ be an induced subgraph of the graph $\Gamma = (V, E)$, then for any vector $\bar{x} = (\bar{x}_i)_{i\in\bar{V}}$, we can define the vector $x = (x_i)_{i\in V}$ by setting $x_i = \bar{x}_i$ if $i \in \bar{V}$, and $x_i = 0$ otherwise. Thus, the nonnegativity of the operator $B_\Gamma = (B_{ij})_{i,j\in V}$ implies that the operator $B_{\bar{\Gamma}} = (B_{ij})_{i,j\in\bar{V}}$ is nonnegative, since by (5) we have equality $\langle B_{\bar{\Gamma}}\bar{x}, \bar{x}\rangle = \langle B_\Gamma x, x\rangle$. Hence, we get a useful consequence of Theorem 2.3:

Corollary 2.6. *Let B_Γ be an abstract Gram operator. If a star $\Gamma_\star(k, \mathcal{V})$ is an induced subgraph of the graph Γ, then the operator $N_k(B_\Gamma, \mathcal{V})$ is nonnegative.*

Definition 2.7. Let a star $\Gamma_\star = \Gamma_\star(k, \mathcal{V})$ be an induced subgraph of a graph Γ, and let $\check{\mathcal{V}}$ be some nonempty subset of vertices $V \setminus V_\star$. We say that the star $\Gamma_\star$ *can be extended by vertices* $\check{\mathcal{V}}$ if the star $\Gamma_\star(k, \mathcal{V} \sqcup \check{\mathcal{V}})$ is an induced subgraph of the graph Γ. If the set contains only one vertex, we aslo say that the star *can be extended by the vertex.*

Corollary 2.8. *Let an operator B_Γ be a Gram operator, and let a star $\Gamma_\star = \Gamma_\star(k, \mathcal{V})$ be an induced subgraph of the graph Γ. If $\Gamma_\star$ can be extended by some vertices $\check{\mathcal{V}}$ such that the operator $S = S_k(B_\Gamma, \check{\mathcal{V}})$ is invertible, then the operator $N = N_k(B_\Gamma, \mathcal{V})$ is also invertible.*

Proof. Since $\Gamma_\star$ can be extended by vertices $\check{\mathcal{V}}$, it follows from Definition 2.7 that the star $\Gamma_\star(k, \mathcal{V} \sqcup \check{\mathcal{V}})$ is also an induced subgraph of Γ. Hence, by Corollary 2.6, the operator $N_k(B_\Gamma, \mathcal{V} \sqcup \check{\mathcal{V}}) = N - S$ is nonnegative, i.e., $0 \le S \le N$. Thus, if the operator S is invertible, then so is N. □

3. Graph with a root subgraph

Suppose $\Gamma_0 = (V_0, E_0)$ is a connected graph and, for each $r \in V_0$, let $\Gamma_r = (V_r, E_r)$ be a rooted tree. Consider a graph $\Gamma = (V, E)$, formed by identifying each vertex r of the graph Γ_0 with the root of the corresponding tree Γ_r. In other words,

$$V = \bigsqcup_{r \in V_0} V_r \quad \text{and} \quad E \setminus E_0 = \bigsqcup_{r \in V_0} E_r.$$

We call Γ_0 a *root subgraph* of Γ. For a graph with a selected root subgraph, we write $\Gamma = (\Gamma_0; \{\Gamma_r\}_{r \in V_0})$. Usually, depending on the context, we use the symbol Γ to denote both a graph with a selected root subgraph and the graph itself. If we need to distinguish them clearly, we will use the notation $\zeta(\Gamma)$ to refer to the graph itself after disregarding the root subgraph.

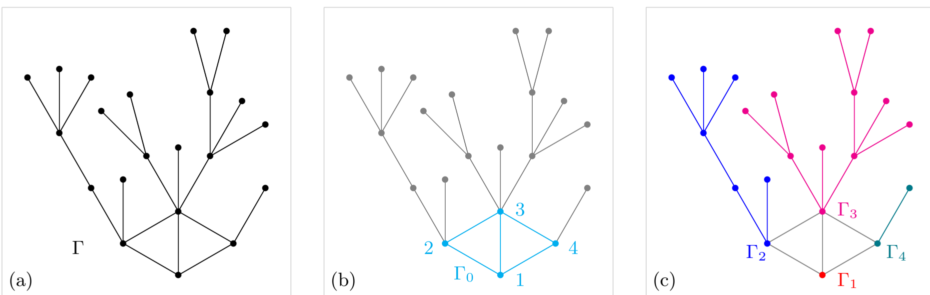


FIGURE 1. A graph (a), a selected root subgraph (b), and the rooted trees (c)

For each vertex $i \in V_r$, there exists a unique path from i to the root of Γ_r. Thus, we can define the distance $d(i) = d(\Gamma, i)$ from that vertex to Γ_0 as the length of this path. The *depth* $d = d(\Gamma)$ of Γ is defined as $\max\{d(i) : i \in V\}$. For each vertex $i \notin V_0$, the *previous vertex* $p(i) = p(\Gamma, i)$ is defined as a vertex in the path from i to the root such that $d(i) = d(p(i)) + 1$. Then, for each vertex $j \in V$, the *set of following vertices* can be defined as

$$\mathcal{V}_j = \mathcal{V}_j(\Gamma) = \{i \in V : p(i) = j\}.$$

The set of all vertices V can be split into layers

$$V = \bigsqcup_{q=0}^{d} \mathcal{L}_q, \qquad \mathcal{L}_q = \mathcal{L}_q(\Gamma) = \{i \in V : d(i) = q\}, \quad q = 0, \dots, d.$$

Note that the following equalities hold:

$$\mathcal{L}_0 = V_0, \qquad \mathcal{L}_q = \bigsqcup_{j \in \mathcal{L}_{q-1}} \mathcal{V}_j, \quad q = 1, \dots, d.$$

Let $V_+ = V_+(\Gamma)$ denote the set of vertices, each of which has a nonempty set of following vertices. Then, for any vertex $j \in V_+$, the star $\Gamma_\star^j = \Gamma_\star(j, \mathcal{V}_j)$ is an induced

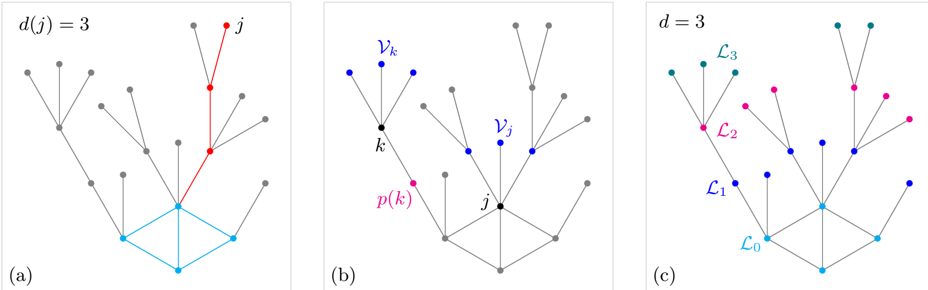


FIGURE 2. Distance from a vertex to the root subgraph (a), following and previous vertices (b), the layers (c)

subgraph of the graph Γ. Moreover, $\Gamma_\star^j$ can be extended by the previous vertex $p(j)$ if $j \notin V_0$, or—taking into account that Γ_0 is assumed to be connected—with at least one vertex from V_0 if $j \in V_0$ and $|V_0| \geq 2$.

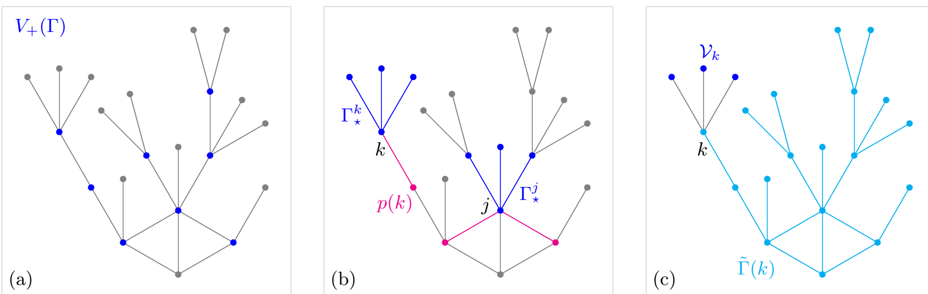


FIGURE 3. The vertices that have a nonempty set of the following vertices (a), examples of extensions of star subgraphs (b), $\tilde{\Gamma}(k)$ as a root subgraph (c)

It is easy to see that a root subgraph is not unique in general. While it is not particularly useful, we can treat any graph as its own root subgraph: $\Gamma' = (\Gamma; \{\Gamma'_r\}_{r\in V})$, where trees Γ'_r are trivial, i.e., $V'_r = \{r\}$ and $E'_r = \varnothing$. In this case, $d = 0$, $V_+(\Gamma') = \varnothing$, and $\zeta(\Gamma') = \zeta(\Gamma)$.

Suppose $d > 0$. By the definition of the depth d, the set $\mathcal{L}_d$ is nonempty. Then, the set $\mathcal{L}_{d-1} \cap V_+$ cannot be empty either. Fix a vertex k from this set and define the induced subgraph $\tilde{\Gamma}(k) = (\tilde{V}, \tilde{E})$ of the graph Γ such that $\tilde{V} = V \setminus \mathcal{V}_k$ and $\tilde{E} = E \setminus \{\gamma_{ki}\}_{i\in\mathcal{V}_k}$. Then, the graph Γ_0 is an induced subgraph of $\tilde{\Gamma}(k)$ and can be selected as a root subgraph of $\tilde{\Gamma}(k)$. Therefore, we set

$$\tilde{\Gamma}(k) = (\Gamma_0; \{\tilde{\Gamma}_r\}_{r\in V_0}) \qquad \tilde{\Gamma}_r = (\tilde{V}_r, \tilde{E}_r) = (V_r \setminus \mathcal{V}_k, E_r \setminus \{\gamma_{ki}\}_{i\in\mathcal{V}_k}). \tag{7}$$

Futhermore, we can select $\tilde{\Gamma}(k)$ to be a root subgraph of graph Γ and define

$$\hat{\Gamma}(k) = (\tilde{\Gamma}(k); \{\hat{\Gamma}_r\}_{r\in\tilde{V}}), \qquad \hat{\Gamma}_r = (\hat{V}_r, \hat{E}_r) = \begin{cases} \Gamma_\star^k, & r = k, \\ (\{r\}, \varnothing), & r \in \tilde{V} \setminus \{k\}. \end{cases} \tag{8}$$

Proposition 3.1. *Let $\tilde{\Gamma} = \tilde{\Gamma}(k)$ and $\hat{\Gamma} = \hat{\Gamma}(k)$ be defined by (7) and (8), respectively. If we denote $\hat{V}_+ = V_+(\hat{\Gamma})$, $\hat{\mathcal{V}}_j = \mathcal{V}_j(\hat{\Gamma})$, $j \in V$, $\tilde{V}_+ = V_+(\tilde{\Gamma})$, and $\tilde{\mathcal{V}}_j = \mathcal{V}_j(\tilde{\Gamma})$, $j \in \tilde{V}$, then*

(i) *$\hat{V}_+ = \{k\}$, $\hat{\mathcal{V}}_j = \varnothing$ if $j \neq k$, and $\hat{\mathcal{V}}_k = \mathcal{V}_k$;*
(ii) *$\tilde{V}_+ = V_+ \setminus \{k\}$, $\tilde{\mathcal{V}}_j = \mathcal{V}_j$ if $j \neq k$, and $\tilde{\mathcal{V}}_k = \varnothing$.*

As a sample (see figures above), we choose a graph containing two cycles and illustrate the introduced notions on it.

4. Reduction theorem

Definition 4.1. Let $\Gamma = (\Gamma_0; \{\Gamma_r\}_{r\in V_0})$. An operator B_Γ, consistent with the graph Γ, *can be reduced on the root subgraph* Γ_0 if there exist

(a) a Hilbert space H_i^0 and an injective operator $T_i : H_i^0 \to H_i$ for each vertex $i \in V$;
(b) an operator $D_{ij} : H_j \to H_i^0$ for each pair of vertices $j \in V_+$ and $i \in \mathcal{V}_j$;
(c) an operator $B^0_{\Gamma_0} = (B^0_{ij})_{i,j\in V_0}$ consistent with Γ_0, where $B^0_{ij} : H_j^0 \to H_i^0$;

and the following conditions hold:

$$B_{ij} = T_i D_{ij}, \qquad j \in V_+,\ i \in \mathcal{V}_j, \tag{9}$$

$$B_{ij} = T_i B^0_{ij} T_j^*, \qquad \gamma_{ij} \in E_0, \tag{10}$$

$$I = B_{jj} = T_j T_j^* + \sum_{i\in\mathcal{V}_j} D_{ij}^* D_{ij}, \qquad j \in V. \tag{11}$$

$B^0_{\Gamma_0}$ is called *a reduction* of B_Γ on Γ_0.

The reduction is not unique. To show this, consider arbitrary unitary operators $U_i : H_i^0 \to \tilde{H}_i^0$, $i \in V$. Then, the operators $\tilde{T}_i = T_i U_i^*$, $i \in V$; $\tilde{D}_{ij} = U_i D_{ij}$, $j \in V_+$, $i \in \mathcal{V}_j$; and $\tilde{B}^0_{ij} = U_i B^0_{ij} U_j^*$, $\gamma_{ij} \in E_0$; fulfill conditions (9), (10), and (11). The following proposition shows that any two reductions are connected in this way and introduces uniquely defined operators N_i, $i \in V$.

Proposition 4.2. *Let* $\Gamma = (\Gamma_0; \{\Gamma_r\}_{r\in V_0})$ *and suppose that* B_Γ *can be reduced on* Γ_0. *Define operators* $N_i = T_i T_i^*$ *and natural embeddings* $J_i : \overline{\operatorname{Im} N_i} \to H_i : x \mapsto x$, $i \in V$. *Then,*

(i) *there exist unitary operators* U_i, $i \in V$, *such that* $T_i = N_i^{1/2} J_i U_i$;
(ii) *the operators* N_i *are uniquely defined;*
(iii) *if* $N_i = 0$ *then* $i \in V_0$ *and it is the only vertex of* V_0.

Proof. (i) Since $\ker T_i = \{0\}$, the partial isometry W_i of the polar decomposition $T_i = N_i^{1/2} W_i$ maps H_i^0 onto $\overline{\operatorname{Im} N_i}$ unitarily. Thus, $T_i = N_i^{1/2} J_i U_i$, where $U_i : H_i^0 \to \overline{\operatorname{Im} N_i} : x \mapsto W_i x$ is a unitary operator.

(ii) Note that for $i \notin V_+$, equality (11) takes the form $N_i = I$. Thus, the operators N_i are uniquely defined for the layer $\mathcal{L}_d$, as this layer does not intersect V_+. Suppose that the operators N_i are uniquely defined for some layer $\mathcal{L}_q$ with $0 < q \le d$. Then the operators $\bar{T}_i = N_i^{1/2} J_i$ are uniquely defined for this layer as well. Since $\ker \bar{T}_i = \{0\}$, the solution $\bar{D}_{ij}$ of the equation $B_{ij} = \bar{T}_i \bar{D}_{ij}$ is unique for any pair of vertices $i \in \mathcal{L}_q$ and $j = p(i) \in \mathcal{L}_{q-1}$. Thus, any T_i and D_{ij} for $i \in \mathcal{L}_q$, $j = p(i) \in \mathcal{L}_{q-1}$, are equal to $\bar{T}_i U_i$ and $U_i^* \bar{D}_{ij}$, respectively, where U_i is a certain unitary operator. Therefore, $D_{ij}^* D_{ij} = \bar{D}_{ij}^* \bar{D}_{ij}$ and equation (11) uniquely determines N_j for $j \in \mathcal{L}_{q-1}$.

(iii) If $N_i = 0$, then $T_i = 0$. Let j be a vertex adjacent to i. It cannot be the previous vertex to i, because otherwise, by (9), we would have $B_{ij} = 0$. This implies $i \in V_0$. Now, the vertex j cannot belong to V_0, because otherwise, by (10), we would again have $B_{ij} = 0$. Since we assume that Γ_0 is connected, we conclude that $V_0 = \{i\}$. □

The main result of the paper is the following theorem.

Theorem 4.3. *Let* $\Gamma = (\Gamma_0; \{\Gamma_r\}_{r\in V_0})$. *The operator* B_Γ *is an abstract Gram operator if and only if it can be reduced on the root subgraph* Γ_0 *with its reduction* $B^0_{\Gamma_0}$ *also being an abstract Gram operator.*

Lemma 4.4. *Let $\Gamma = (\Gamma_0; \{\Gamma_r\}_{r\in V_0})$. The operator B_Γ can be reduced on the root subgraph Γ_0 if and only if there exist objects introduced by items (a), (b), and (c) of Definition 4.1, such that for any vector $x = (x_i)_{i\in V}$, the following equality holds:*

$$\langle B_\Gamma x, x\rangle = \langle B^0_{\Gamma_0} z, z\rangle + \sum_{j\in V_+} \sum_{i\in \mathcal{V}_j} \|T_i^* x_i + D_{ij} x_j\|^2, \quad z = (T_i^* x_i)_{i\in V_0}. \tag{12}$$

The proof of this lemma in one direction relies on equality (5). To prove it in another direction, we use ideas similar to those of Proposition 1.2. For details of the proof, see Appendix B.

Corollary 4.5. *Let $\Gamma = (\Gamma_0; \{\Gamma_r\}_{r\in V_0})$ and let the operator B_Γ can be reduced on the root subgraph Γ_0. Then, B_Γ is an abstract Gram operator if and only if so is its reduction $B^0_{\Gamma_0}$.*

Proof. By the previous lemma, equality (12) holds for any $x = (x_i)_{i\in V}$, since the operator B_Γ can be reduced on Γ_0. Thus, if operator $B^0_{\Gamma_0}$ is nonnegative then the right-hand side of (12) is nonnegative for any x, so operator B_Γ is also nonnegative.

Now suppose that B_Γ is nonnegative while $B^0_{\Gamma_0}$ is not. Since $\ker T_i = \{0\}$, the set $\operatorname{Im} T_i^*$ is dense in H_i^0 for any $i \in V$. Therefore, if for some vector $\bar z = (\bar z_i)_{i\in V_0}$ we have $\langle B^0_{\Gamma_0} \bar z, \bar z\rangle < 0$ then there exists a vector $z = (T_i^* x_i)_{i\in V_0}$ such that $\langle B^0_{\Gamma_0} z, z\rangle < 0$. Fix these vectors x_i, $i \in V_0 = \mathcal{L}_0$, and define positive numbers λ and ε by equalities

$$\lambda = -\langle B^0_{\Gamma_0} z, z\rangle, \qquad \varepsilon = \sqrt{\frac{\lambda}{|V|}}.$$

For each vertex $i \in \mathcal{L}_q$, $q = 1, \dots, d$, there exists a unique previous vertex j. It belongs to the layer $\mathcal{L}_{q-1}$. Since $\operatorname{Im} T_i^*$ is dense in H_i^0 and $-D_{ij} x_j \in H_i^0$, for a given vector $x_j \in H_j$, we can find a vector $x_i \in H_i$ such that $\|T_i^* x_i + D_{ij} x_j\| < \varepsilon$. Fix these vectors. Thus, we have fully defined the vector $x = (x_i)_{i\in V}$ for which by (12) we obtain the estimate

$$\langle B_\Gamma x, x\rangle < -\lambda + \varepsilon^2 |V \setminus V_0| < 0.$$

This contradicts the assumption that B_Γ is nonnegative. □

This corollary implies that proving the following lemma completes the proof of Theorem 4.3.

Lemma 4.6. *Let $\Gamma = (\Gamma_0; \{\Gamma_r\}_{r\in V_0})$. If B_Γ is an abstract Gram operator, then it can be reduced on the root subgraph Γ_0.*

5. Reduction algorithm

Definition 5.1. Let an operator $B_\Gamma = (B_{ij})_{i,j\in V}$ be consistent with a graph $\Gamma = (V, E)$. For a vertex $k \in V$ and a subset of vertices $\mathcal{V} \subset V$ that are adjacent to k, such that the operator $N = N_k(B_\Gamma, \mathcal{V})$ is nonnegative, denote by J the natural embedding of $\overline{\operatorname{Im} N}$ into H_k and define the operator

$$T_k(B_\Gamma, \mathcal{V}) = N^{1/2} J.$$

Proposition 5.2. *Under the conditions of the previous definition, let $T = T_k(B_\Gamma, \mathcal{V})$ and suppose j is a vertex in $V \setminus \mathcal{V}$ that is adjacent to k. If $B_{kj} B_{jk} \le N$, then there exists a unique operator D_j such that $B_{kj} = T D_j$.*

Proof. Note that the operator T is injective and satisfies the equality $N = TT^*$. Then, since $B_{kj} B_{kj}^* \le TT^*$, Douglas' lemma (see [3]) implies that a solution D_j to the equation $B_{kj} = T D_j$ exists. The solution is unique because $\ker T = \{0\}$. □

By $D_{kj}(B_\Gamma, \mathcal{V})$ denote the operator whose existence was established by the previous proposition.

Proposition 5.3. *Suppose the star $\Gamma_\star = \Gamma_\star(k, \mathcal{V})$ is an induced subgraph of Γ and can be extended by a vertex $j \in V \setminus \mathcal{V}$. If B_Γ is an abstract Gram operator, then all conditions required to define the operator $D_j = D_{kj}(B_\Gamma, \mathcal{V})$ are satisfied.*

Proof. It follows from Definition 2.7 that the star $\Gamma_\star(k, \mathcal{V} \sqcup \{j\})$ is an induced subgraph of Γ. Hence, by Corollary 2.6, the operator $N_k(B_\Gamma, \mathcal{V} \sqcup \{j\}) = N - B_{kj}B_{jk}$ is nonnegative, i.e., $0 \le B_{kj}B_{jk} \le N$. □

Corollary 5.4. *Let $\Gamma = (\Gamma_0; \{\Gamma_r\}_{r \in V_0})$ and $V_+ = \{k\}$. If B_Γ is an abstract Gram operator then it can be reduced on the root subgraph Γ_0.*

Proof. Set $N_i = N_i(B_\Gamma, \mathcal{V}_i)$ for $i \in V$. Then all of them are equal to the identity unless $i = k$. In the latter case the operator N_k is nonnegative by Corollary 2.6. Thus, we can define $H_i^0 = \overline{\operatorname{Im} N_i}$ and $T_i = T_i(B_\Gamma, \mathcal{V}_i)$, $i \in V$. Note that $T_i = I$ and $H_i^0 = H_i$ for all $i \ne k$.

To fulfill (9), D_{ik}, $i \in \mathcal{V}_k$, must be equal to B_{ik}. In this case, equalities (11) hold, as $N_k = T_k T_k^*$. Now let i and j be adjacent vertices of Γ_0. To fulfill (10), B_{ij}^0 has to coincide with B_{ij} if neither i nor j equals k, and B_{kj}^0 must be equal to $D_j = D_{kj}(B_\Gamma, \mathcal{V}_k)$. Then $B_{jk}^0 = D_j^*$ and thus B_Γ can be reduced on Γ_0. □

Using this corollary, we prove Lemma 4.6 by induction on the number of elements in the set V_+ (see Appendix C). Therefore, Theorem 4.3 is proved.

Algorithm 1 Reduction algorithm

function IsGramOperator(B_Γ)
  while $d = d(\Gamma) > 0$ **do** ▷ $\Gamma = (\Gamma_0, \{\Gamma_r\}_{r \in V_0})$
    $k \leftarrow$ some element of $\mathcal{L}_{d-1}(\Gamma) \cap V_+(\Gamma)$ $\Gamma_0 = (V_0, E_0)$
    $\mathcal{V} \leftarrow \mathcal{V}_k(\Gamma)$ $\Gamma_r = (V_r, E_r)$, $r \in V_0$
    $\tilde{V} \leftarrow V \setminus \mathcal{V}$ $\zeta(\Gamma) = (V, E)$
    $N \leftarrow N_k(B_\Gamma, \mathcal{V})$ $B_\Gamma = (B_{ij})_{i,j \in V}$
    guard $N \ge 0$ **else**
      return false
    end guard
    for all $j \in \tilde{V}$, $\gamma_{jk} \in E$ **do**
      guard $B_{kj}B_{jk} \le N$ **else**
        return false
      end guard
      $D_j \leftarrow D_{kj}(B_\Gamma, \mathcal{V})$
    end for
    for all $i, j \in \tilde{V}$, $\gamma_{ij} \in E$ **do**
      $$\tilde{B}_{ij} \leftarrow \begin{cases} D_j, & i = k, \\ D_i^*, & j = k, \\ B_{ij}, & \text{otherwise.} \end{cases}$$
    end for
    $\Gamma \leftarrow \big(\Gamma_0; \{(V_r \setminus \mathcal{V},\ E_r \setminus \{\gamma_{ki}\}_{i \in \mathcal{V}})\}_{r \in V_0}\big)$
    $B_\Gamma \leftarrow (\tilde{B}_{ij})_{i,j \in \tilde{V}}$
  end while
  return $(B_\Gamma \ge 0)$ ▷ $\zeta(\Gamma) = \Gamma_0$
end function

Corollary 5.4, together with Corollary 4.5, provides us with Algorithm 1. Let us take a closer look at it. The algorithm is represented as a function that takes an operator B_Γ

consistent with $\Gamma = (\Gamma_0; \{\Gamma_r\}_{r\in V_0})$ and returns *true* or *false*. It assumes (line 22) that we have an effective way to check whether an operator consistent with the root subgraph Γ_0 is a Gram operator.

The core of the function is a while loop (lines 2–21), executed until the graph Γ coincides with Γ_0. At each iteration:

- It chooses an arbitrary vertex k from the pre-outer layer with a nonempty set of following vertices $\mathcal{V}$ (line 3).
- The algorithm checks whether B_Γ can be reduced on the root subgraph $\tilde{\Gamma}(k)$, which is Γ after removing vertices $\mathcal{V}$ together with the corresponding edges, and computes operators D_j for each vertex $j \in V \setminus \mathcal{V}$ adjacent to k (lines 7–15).
- Using operators D_j, it recalculates the block elements related to edges of the induced subgraph $\tilde{\Gamma}(k)$ (lines 16–18).
- It then replaces the graph Γ with $\tilde{\Gamma}(k)$ (line 19) and the operator B_Γ with the one constructed from the updated block elements (line 20).

If B_Γ is a Gram operator at the start of an iteration, then the iteration cannot terminate prematurely, and the updated B_Γ, which is the reduction of B_Γ on $\tilde{\Gamma}(k)$, is also a Gram operator. Conversely, if the iteration proceeds successfully, then the original B_Γ is a Gram operator if and only if the updated operator is. Thus, if some iteration fails, the original operator B_Γ is not a Gram operator. Otherwise, when the loop finishes and Γ coincides with Γ_0, the original and updated operators are either both Gram operators or neither is.

6. Invertibility

Let $\Gamma = (\Gamma_0; \{\Gamma_r\}_{r\in V_0})$ and suppose that B_Γ can be reduced on Γ_0. It follows from Proposition 4.2, that we can assume that $T_i = N_i^{1/2} J_i$ and $H_i^0 = \overline{\operatorname{Im} N_i}$ for $i \in V$. If $\ker N_i = \{0\}$, then $H_i^0 = H_i$ and $T_i = T_i^* = N_i^{1/2}$. Moreover, if for some $i \in V \setminus V_0$ the operator N_i is invertible, then T_i is also invertible, hence $D_{ij} = N_i^{-1/2} B_{ij}$ for $j = p(i)$. If we suppose that the operators N_i are invertible for all $i \in \mathcal{V}_j$, then we have the following relation:

$$N_j = I - \sum_{i\in\mathcal{V}_j} B_{ji} N_i^{-1} B_{ij}, \quad j \in V. \tag{13}$$

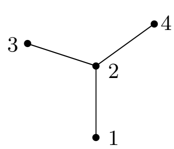
In the case where both N_i and N_j, $i, j \in V_0$, are invertible, we obtain

$$B_{ij}^0 = N_i^{-1/2} B_{ij} N_j^{-1/2}, \quad \gamma_{ij} \in E_0. \tag{14}$$

Proposition 6.1. *Let $\Gamma = (\Gamma_0; \{\Gamma_r\}_{r\in V_0})$. If the operator B_Γ is such that all operators N_j, $j \in V$, defined by (13), are nonnegative and invertible, then B_Γ is an abstract Gram operator if and only if so is the operator $B^0_{\Gamma_0} = (B^0_{ij})_{i,j\in V_0}$, defined by (14).*

Proof. The nonnegativity and invertibility of the operators N_j, $j \in V$, imply that all of them are well-defined by (13), and $B^0_{\Gamma_0}$ is well-defined by (14). This also ensures that $B^0_{\Gamma_0}$ is a reduction of B_Γ on Γ_0. Thus, we can apply Corollary 4.5. □

In general, the nonnegativity of the operator B_Γ does not imply the invertibility of the operator $N_k(B_\Gamma, \mathcal{V})$ associated with the induced star subgraph $\Gamma_\star(k, \mathcal{V})$. For example, consider the star $\Gamma = (V = \{1, 2, 3, 4\}, E = \{\gamma_{12}, \gamma_{23}, \gamma_{24}\})$ and its induced star subgraph $\Gamma_\star = (V_\star = \{2, 3, 4\}, E_\star = \{\gamma_{23}, \gamma_{24}\})$.



Let

$$B_\Gamma = \left(\begin{array}{c|cc|c|c} 1 & 0 & \sqrt{0.3} & 0 & 0 \\ \hline 0 & 1 & 0 & \sqrt{0.4} & \sqrt{0.6} \\ \sqrt{0.3} & 0 & 1 & 0 & 0 \\ \hline 0 & \sqrt{0.4} & 0 & 1 & 0 \\ \hline 0 & \sqrt{0.6} & 0 & 0 & 1 \end{array}\right).$$

Then, the operator

$$N_2(B_\Gamma, \{3,4\}) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \begin{pmatrix} 0.4 & 0 \\ 0 & 0 \end{pmatrix} - \begin{pmatrix} 0.6 & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

is nonnegative but not invertible. On the other hand, B_Γ is nonnegative, as the operator

$$N_2(B_\Gamma, \{1,3,4\}) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \begin{pmatrix} 0 & 0 \\ 0 & 0.3 \end{pmatrix} - \begin{pmatrix} 0.4 & 0 \\ 0 & 0 \end{pmatrix} - \begin{pmatrix} 0.6 & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0.7 \end{pmatrix}$$

is nonnegative.

Lemma 6.2. *Let $\Gamma = (\Gamma_0; \{\Gamma_r\}_{r \in V_0})$. Suppose the operator B_Γ is an abstract Gram operator, and for each vertex $j \in V_+$, the star $\Gamma_\star^j$ can be extended by some vertices $\check{\mathcal{V}}_j$, such that the operator $S_j = S_j(B_\Gamma, \check{\mathcal{V}}_j)$ is invertible. Then the operators N_j, $j \in V$, defined by (13), are nonnegative and invertible.*

We prove this lemma by induction on the number of elements in the set V_+ (see Appendix D). Combining it with Propositions 6.1 we get the following criterion.

Theorem 6.3. *Let $\Gamma = (\Gamma_0; \{\Gamma_r\}_{r \in V_0})$. If for each vertex $j \in V_+$ the star $\Gamma_\star^j$ can be extended by vertices $\check{\mathcal{V}}_j$ such that operator $S_j = S_j(B_\Gamma, \check{\mathcal{V}}_j)$ is invertible, then B_Γ is an abstract Gram operator if, and only if,*

(i) *all operators N_j, $j \in V$, defined by (13), are nonnegative and invertible;*
(ii) *the operator $B^0_{\Gamma_0} = (B^0_{ij})_{i,j \in V_0}$, defined by (14), is an abstract Gram operator.*

Now consider the case where the operator B_Γ is such that, for each pair of vertices $j \in V_+$ and $i \in \mathcal{V}_j$, there exists a number $\tau_{ij} \in (0,1)$ so that $\tau_{ij}^{-1} B_{ij}$ is a unitary operator. Suppose B_Γ can be reduced on Γ_0. If $N_i = \nu_i I$, $\nu_i > 0$, for any vertex i from some layer $\mathcal{L}_q$, $0 < q \le d$, then, by (13), the operators N_j are scalar for all $j \in \mathcal{L}_{q-1}$ as well, i.e., $N_j = \nu_j I$ for some numbers $\nu_j \ge 0$. But by Propositions 4.2, ν_j can only be zero if $q = 1$ and $V_0 = \{j\}$. Taking into account that $N_i = I$ for all $i \in \mathcal{L}_d$, we obtain that $N_j = \nu_j I$ for $j \in V$,

$$B^0_{ij} = \frac{B_{ij}}{\sqrt{\nu_i \nu_j}}, \quad \gamma_{ij} \in E_0, \tag{15}$$

where

$$\nu_j = 1 - \sum_{i \in \mathcal{V}_j} \frac{\tau_{ij}^2}{\nu_i}, \quad j \in V, \tag{16}$$

and the following lemma holds.

Lemma 6.4. *Let $\Gamma = (\Gamma_0; \{\Gamma_r\}_{r \in V_0})$ and $|V_0| \ge 2$. Suppose the operator B_Γ is such that, for each edge $\gamma_{ij} \in E \setminus E_0$, a number $\tau_{ij} \in (0,1)$ is specified, and the operator $\tau_{ij}^{-1} B_{ij}$ is unitary. If B_Γ is an abstract Gram operator then the numbers ν_j, $j \in V$, defined by (16), are positive.*

Combining this lemma with Proposition 6.1, we obtain the following theorem (see also [10], Theorem 1).

Theorem 6.5. *Let* $\Gamma = (\Gamma_0; \{\Gamma_r\}_{r\in V_0})$ *and* $|V_0| \geq 2$. *Suppose the operator* B_Γ *is such that, for each edge* $\gamma_{ij} \in E \setminus E_0$, *a number* $\tau_{ij} \in (0,1)$ *is specified, and the operator* $\tau_{ij}^{-1} B_{ij}$ *is unitary. Then,* B_Γ *is an abstract Gram operator if and only if*

(i) *the numbers* ν_j, $j \in V$, *defined by* (16), *are positive;*
(ii) *the operator* $B^0_{\Gamma_0}$, *defined by* (15), *is an abstract Gram operator.*

Appendix A.

In this appendix, we prove several elementary but useful propositions. In the following statements, H, H_1 and H_2 are arbitrary Hilbert spaces.

Proposition A.1. *For any* $x, y \in H$,

(i) $\operatorname{Im}\langle x, y\rangle = \operatorname{Re}\langle x, iy\rangle$,
(ii) $\operatorname{Re}\langle x, y\rangle = -\operatorname{Im}\langle x, iy\rangle$,
(iii) $\langle x, y\rangle = \operatorname{Re}\langle x, y\rangle + i\operatorname{Re}\langle x, iy\rangle = -\operatorname{Im}\langle x, iy\rangle + i\operatorname{Im}\langle x, y\rangle$.

Proof. Let $\langle x, y\rangle = a + ib$, where $a, b \in \mathbb{R}$. Then $\langle x, iy\rangle = -i\langle x, y\rangle = b - ia$. □

As a corollary, we get the following statements.

Proposition A.2. *Let* $A : H_1 \to H_2$ *be an operator. If*

$$\operatorname{Re}\langle Ax, y\rangle = 0 \qquad \textit{or} \qquad \operatorname{Im}\langle Ax, y\rangle = 0$$

for any $x \in H_1$ *and* $y \in H_2$, *then* $A = 0$.

Proposition A.3. *Let* $A : H_1 \to H_2$ *and* $B : H_2 \to H_1$ *be operators. If*

$$\langle Ax, y\rangle + \langle By, x\rangle = 0$$

for any $x \in H_1$, $y \in H_2$, *then* $A = B^* = 0$.

Proof. For any $x \in H_1$, $y \in H_2$, we have

$$0 = \operatorname{Re}(\langle Ax, y\rangle + \langle By, x\rangle) = \operatorname{Re}\langle (A + B^*)x, y\rangle,$$
$$0 = \operatorname{Im}(\langle Ax, y\rangle + \langle By, x\rangle) = \operatorname{Im}\langle (A - B^*)x, y\rangle,$$

so by Proposition A.2, we get $A + B^* = 0$ and $A - B^* = 0$. □

Proposition A.4. *Let* $A : H_1 \to H_2$ *and* $B : H_2 \to H_1$ *be operators. If*

$$\langle Ax, y\rangle + \langle By, x\rangle = \operatorname{Re}\langle (A + B^*)x, y\rangle$$

for any $x \in H_1$, $y \in H_2$, *then* $A = B^*$.

Proof. We have

$$0 = \langle Ax, y\rangle + \langle By, x\rangle - \operatorname{Re}\langle (A + B^*)x, y\rangle = i\operatorname{Im}(\langle Ax, y\rangle + \langle By, x\rangle).$$

So $\operatorname{Im}\langle (A - B^*)x, y\rangle = 0$. Thus by Proposition A.2, we get $A = B^*$. □

Appendix B.

Proof of Lemma 4.4. (⇒) Suppose that B_Γ can be reduced on Γ_0. From (5), for $z = (T_i^* x_i)_{i\in V_0}$, we get

$$\langle B^0_{\Gamma_0} z, z\rangle = \sum_{i\in V_0} \|T_i^* x_i\|^2 + 2 \sum_{\gamma_{ij}\in E_0} \operatorname{Re}\langle B^0_{ij} T_j^* x_j, T_i^* x_i\rangle.$$

Taking into account that $E \setminus E_0 = \{\gamma_{ij} : j \in V_+, i \in \mathcal{V}_j\}$ and applying (9), (10), and (11), we find from (5) that

$$\langle B_\Gamma x, x\rangle = \sum_{j\in V} \|x_j\|^2 + 2 \sum_{\gamma_{ij}\in E} \operatorname{Re}\langle B_{ij}x_j, x_i\rangle = \sum_{j\in V} \big(\|T_j^* x_j\|^2 + \sum_{i\in\mathcal{V}_j} \|D_{ij}x_j\|^2\big)$$
$$+ 2 \sum_{\gamma_{ij}\in E_0} \operatorname{Re}\langle B_{ij}^0 T_j^* x_j, T_i^* x_i\rangle + 2 \sum_{j\in V_+} \sum_{i\in\mathcal{V}_j} \operatorname{Re}\langle D_{ij}x_j, T_i^* x_i\rangle.$$

Since $V \setminus V_0 = \bigsqcup_{j\in V_+} \mathcal{V}_j$ and $V_+ = \{j \in V : \mathcal{V}_j \neq \varnothing\}$,

$$\langle B_\Gamma x, x\rangle - \langle B_{\Gamma_0}^0 z, z\rangle = \sum_{j\in V_+} \sum_{i\in\mathcal{V}_j} \left(\|T_i^* x_i\|^2 + 2\operatorname{Re}\langle D_{ij}x_j, T_i^* x_i\rangle + \|D_{ij}x_j\|^2\right).$$

Thus, we conclude equality (12).

(⇐) Now let (12) hold for some objects introduced by items (a), (b), and (c) of Definition 4.1.

For a vertex $k \in V$ consider $x = (x_i)_{i\in V}$ such that $x_i = 0$ for all vertices $i \neq k$ and x_k is an arbitrary vector from H_k. Then, equality (12) takes the form

$$\|x_k\|^2 = \|T_k^* x_k\|^2 + \sum_{i\in\mathcal{V}_k} \|D_{ik}x_k\|^2. \tag{17}$$

The last one is equivalent to (11).

For a pair of vertices $j \in V_+$ and $k \in \mathcal{V}_j$, consider $x = (x_i)_{i\in V}$ such that $x_i = 0$ for all $i \notin \{j, k\}$, and x_j, x_k are arbitrary vectors from H_j, H_k, respectively. Then, equality (12) takes the form

$$\|x_j\|^2 + \|x_k\|^2 + 2\operatorname{Re}\langle B_{kj}x_j, x_k\rangle$$
$$= \|T_j^* x_j\|^2 + \sum_{i\in\mathcal{V}_j\setminus\{k\}} \|D_{ij}x_j\|^2 + \|T_k^* x_k + D_{kj}x_j\|^2 + \sum_{i\in\mathcal{V}_k} \|D_{ik}x_k\|^2$$

Taking into account that equality (17) holds for k and j we get

$$2\mathrm{Re}\,\langle B_{kj}x_j, x_k\rangle = \|T_k^* x_k + D_{kj}x_j\|^2 - \|T_k^* x_k\|^2 - \|D_{kj}x_j\|^2 = 2\mathrm{Re}\,\langle D_{kj}x_j, T_k^* x_k\rangle.$$

Thus by Proposition A.2, we conclude equality (9).

For a pair of vertices $k, j \in V_0$, $k \neq j$, consider $x = (x_i)_{i\in V}$ such that $x_i = 0$ for all $i \notin \{k, j\}$, and x_j, x_k are arbitrary vectors from H_j, H_k, respectively. Then, equality (12) takes the form

$$\|x_j\|^2 + \|x_k\|^2 + 2\operatorname{Re}\langle B_{kj}x_j, x_k\rangle$$
$$= \|T_j^* x_j\|^2 + \|T_k^* x_k\|^2 + 2\operatorname{Re}\langle B_{kj}^0 T_j^* x_j, T_k^* x_k\rangle + \sum_{i\in\mathcal{V}_k} \|D_{ik}x_k\|^2 + \sum_{i\in\mathcal{V}_j} \|D_{ij}x_j\|^2.$$

After applying equality (17) for k and j, we get $\operatorname{Re}\langle B_{kj}x_j, x_k\rangle = \operatorname{Re}\langle B_{kj}^0 T_j^* x_j, T_k^* x_k\rangle$. Hence by Proposition A.2, equality (10) follows immediately. □

Appendix C.

Proof of Lemma 4.6. We fix the root subgraph Γ_0 and prove the lemma by induction on the number of elements $m = m(\Gamma)$ in the set $V_+ = V_+(\Gamma)$. The case $m = 0$ is trivial, so we assume that $m > 0$.

The base case. The case $m = 1$ has been proved in Corollary 5.4.

The induction step. Suppose $m > 1$. Fix a vertex $k \in \mathcal{L}_{d-1} \cap V_+$, and define $\tilde{\Gamma} = \tilde{\Gamma}(k)$ by (7) and $\hat{\Gamma} = \hat{\Gamma}(k)$ by (8).

By Corollary 5.4, the operator $B_{\hat{\Gamma}}$—which is B_Γ—can be reduced on $\tilde{\Gamma}$. Thus, taking into account statement (i) of Proposition 3.1, there exist (a) spaces $\tilde{H}_i$ and injective operators $\hat{T}_i : \tilde{H}_i \to H_i$, $i \in V$; (b) operators $\hat{D}_{ik} : H_k \to \tilde{H}_i$, $i \in \mathcal{V}_k$; and (c) the operator $\tilde{B}_{\tilde{\Gamma}} = (\tilde{B}_{ij})_{i,j\in\tilde{V}}$, $\tilde{B}_{ij} : \tilde{H}_j \to \tilde{H}_i$; such that

$$
\begin{aligned}
B_{ik} &= \hat{T}_i \hat{D}_{ik}, && i \in \mathcal{V}_k,\\
B_{ij} &= \hat{T}_i \tilde{B}_{ij} \hat{T}_j^*, && \gamma_{ij} \in \tilde{E},\\
I_{H_j} &= \hat{T}_j \hat{T}_j^* + \sum_{i\in\hat{\mathcal{V}}_j} \hat{D}_{ij}^* \hat{D}_{ij}, && j \in V.
\end{aligned}
$$

Then, by Corollary 4.5, $\tilde{B}_{\tilde{\Gamma}}$ is nonnegative. By statement (ii) of Proposition 3.1, $m(\tilde{\Gamma}) = m - 1$, so the operator $\tilde{B}_{\tilde{\Gamma}}$ can be reduced on Γ_0 based on the inductive assumption. Thus, there exist (a) spaces H_i^0 and injective operators $\tilde{T}_i : H_i^0 \to \tilde{H}_i$, $i \in \tilde{V}$; (b) operators $\tilde{D}_{ij} : \tilde{H}_j \to H_i^0$, $j \in \tilde{V}_+$ and $i \in \mathcal{V}_j$; and (c) the operator $B_{\Gamma_0}^0 = (B_{ij}^0)_{i,j\in V_0}$, $B_{ij}^0 : H_j^0 \to H_i^0$; such that

$$
\begin{aligned}
\tilde{B}_{ij} &= \tilde{T}_i \tilde{D}_{ij}, && j \in \tilde{V}_+,\, i \in \mathcal{V}_j,\\
\tilde{B}_{ij} &= \tilde{T}_i B_{ij}^0 \tilde{T}_j^*, && \gamma_{ij} \in E_0,\\
I_{\tilde{H}_j} &= \tilde{T}_j \tilde{T}_j^* + \sum_{i\in\tilde{\mathcal{V}}_j} \tilde{D}_{ij}^* \tilde{D}_{ij}, && j \in \tilde{V}.
\end{aligned}
$$

The spaces H_i^0 are defined for $i \in \tilde{V} = V \setminus \mathcal{V}_k$. For $i \in \mathcal{V}_k$, we set $H_i^0 = \tilde{H}_i$, and then define the operators T_i and D_{ij} as follows:

$$
T_i = \begin{cases} \hat{T}_i, & i \in \mathcal{V}_k,\\ \hat{T}_i \tilde{T}_i, & i \in \tilde{V}, \end{cases} \qquad D_{ij} = \begin{cases} \hat{D}_{ik}, & j = k,\, i \in \mathcal{V}_k,\\ \tilde{D}_{ij} \hat{T}_j^*, & j \in \tilde{V}_+,\, i \in \mathcal{V}_j. \end{cases}
$$

For $j \in V_+$ and $i \in \mathcal{V}_j$, we obtain

$$
T_i D_{ij} = \begin{cases} \hat{T}_i \hat{D}_{ik} = B_{ik}, & j = k,\, i \in \mathcal{V}_k,\\ \hat{T}_i \tilde{T}_i \tilde{D}_{ij} \hat{T}_j^* = \hat{T}_i \tilde{B}_{ij} \hat{T}_j^* = B_{ij}, & j \in \tilde{V}_+,\, i \in \mathcal{V}_j. \end{cases}
$$

Thus, we have proved equality (9).

Since $V_0 \subset \tilde{V}$, for adjacent vertices i and j from V_0, we get

$$
T_i B_{ij}^0 T_j^* = \hat{T}_i \tilde{T}_i B_{ij}^0 \tilde{T}_j^* \hat{T}_j^* = \hat{T}_i \tilde{B}_{ij} \hat{T}_j^* = B_{ij}.
$$

This proves equality (10).

For $j \in \mathcal{V}_k$, we have $\hat{\mathcal{V}}_j = \mathcal{V}_j = \varnothing$, and therefore, $I_{H_j} = \hat{T}_j \hat{T}_j^* = T_j T_j^*$. Let $j = k$. In this case, $\tilde{\mathcal{V}}_k = \varnothing$, so $I_{\tilde{H}_k} = \tilde{T}_k \tilde{T}_k^*$, and therefore, $\hat{T}_k \hat{T}_k^* = \hat{T}_k \tilde{T}_k \tilde{T}_k^* \hat{T}_k^* = T_k T_k^*$. Since $\hat{\mathcal{V}}_k = \mathcal{V}_k$, it follows that

$$
I_{H_k} = \hat{T}_k \hat{T}_k^* + \sum_{i\in\hat{\mathcal{V}}_k} \hat{D}_{ik}^* \hat{D}_{ik} = T_k T_k^* + \sum_{i\in\mathcal{V}_k} D_{ik}^* D_{ik}.
$$

The last case is $j \in \tilde{V} \setminus \{k\}$. In this case, $\hat{\mathcal{V}}_j = \varnothing$ and $\tilde{\mathcal{V}}_j = \mathcal{V}_j$, so

$$
I_{H_j} = \hat{T}_j \hat{T}_j^* = \hat{T}_j I_{\tilde{H}_j} \hat{T}_j^* = \hat{T}_j \Big(\tilde{T}_j \tilde{T}_j^* + \sum_{i\in\tilde{\mathcal{V}}_j} \tilde{D}_{ij}^* \tilde{D}_{ij} \Big) \hat{T}_j^* = T_j T_j^* + \sum_{i\in\mathcal{V}_j} D_{ij}^* D_{ij}
$$

Thus, in all three possible cases, condition (11) is fulfilled. □

Appendix D.

Proof of Lemma 6.2. We prove the proposition by induction on the number of elements $m = m(\Gamma)$ in the set $V_+ = V_+(\Gamma)$. Case $m = 0$ is trivial, so assume that $m > 0$.

The base case. In the case where $m = 1$, Corollary 2.6 establishes the nonnegativity of the operators N_j, and Corollary 2.8 proves their invertibility.

The induction step. Suppose $m > 1$, fix $k \in \mathcal{L}_{d-1} \cap V_+$, and define $\tilde{\Gamma} = \tilde{\Gamma}(k)$ by (7) and $\hat{\Gamma} = \hat{\Gamma}(k)$ by (8).

By statement (i) of Proposition 3.1, $\hat{V}_+ = \{k\}$, so $\hat{N}_j = I$ for $j \in V \setminus \{k\}$, and

$$\hat{N}_k = I - \sum_{i \in \hat{\mathcal{V}}_k} B_{ki} \hat{N}_i^{-1} B_{ik} = I - \sum_{i \in \mathcal{V}_k} B_{ki} B_{ik} = N_k$$

is nonnegative by Corollary 2.6 and invertible by Corollary 2.8. Then, by Proposition 6.1, the operator $\tilde{B}_{\tilde{\Gamma}} = (\tilde{B}_{ij})_{i,j \in \tilde{V}}$,

$$\tilde{B}_{ij} = \begin{cases} N_k^{-1/2} B_{kj}, & i = k, \\ B_{ik} N_k^{-1/2}, & j = k, \\ B_{ij}, & \text{otherwise}, \end{cases} \qquad \gamma_{ij} \in \tilde{E},$$

is an abstract Gram operator, as B_Γ is assumed to be one.

By statement (ii) of Proposition 3.1, $\tilde{V}_+ = V_+ \setminus \{k\}$ and $\tilde{\mathcal{V}}_j = \mathcal{V}_j$ for $j \in \tilde{V}_+$. Thus, for any $j \in V_+ \setminus \{k\}$, the star $\tilde{\Gamma}^j_\star = \Gamma_\star(j, \tilde{\mathcal{V}}_j)$ coincides with $\Gamma^j_\star$ and can be extended by $\check{\mathcal{V}}_j$ as an induced subgraph of $\tilde{\Gamma}$. Let us show that the operators $\tilde{S}_j = S_j(\tilde{B}_{\tilde{\Gamma}}, \check{\mathcal{V}}_j)$ are invertible. It is clear that $\tilde{S}_j = S_j$ if $k \notin \check{\mathcal{V}}_j$. Let $k \in \check{\mathcal{V}}_j$. Taking into account the inequality

$$\|B_{kj} x\|^2 \le \|N_k\| \|N_k^{-1/2} B_{kj} x\|^2 \le \|\tilde{B}_{kj} x\|^2$$

we get that $S_j \le \tilde{S}_j$. So, all operators $\tilde{S}_j$, $j \in \tilde{V}_+$, are invertible and operators $\tilde{N}_j$, $j \in \tilde{V}$, are nonnegative and invertible by the inductive assumption.

To finish the proof, we need to show that $\tilde{N}_j = N_j$ for all $j \in \tilde{V}_+$. It holds for $j \in \mathcal{L}_{d-1} \cap \tilde{V}_+$ because $\tilde{N}_i = I = N_i$ and $\tilde{B}_{ij} = B_{ij}$ for any $i \in \mathcal{V}_j$. Suppose that for some $0 < q \le d$, the equality holds for all $j \in \mathcal{L}_q \cap \tilde{V}_+$. Let $j \in \mathcal{L}_{q-1} \cap \tilde{V}_+$, then for vertex $i \in \mathcal{V}_j$ there are three possibilities: (i) $i \in \mathcal{L}_q \cap \tilde{V}_+$, (ii) $i \in \mathcal{L}_q \setminus V_+$, and (iii) $q = d-1$, $i = k$. In the first case, $\tilde{N}_i = N_i$ by the inductive assumption; in the second one, $\tilde{N}_i = N_i = I$; and in both these cases, $\tilde{B}_{ij} = B_{ij}$, so

$$\tilde{B}_{ji} \tilde{N}_i^{-1} \tilde{B}_{ij} = B_{ji} N_i^{-1} B_{ij}, \quad i \in \mathcal{V}_j \setminus \{k\}.$$

In the last case,

$$\tilde{B}_{jk} \tilde{N}_k^{-1} \tilde{B}_{kj} = (B_{jk} N_k^{-1/2}) \cdot I \cdot (N_k^{-1/2} B_{kj}) = B_{jk} N_k^{-1} B_{kj}.$$

Thus, $\tilde{N}_j = N_j$ in all three possible cases. □

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