SHARP BOUNDS FOR SUMS ASSOCIATED TO GRAPHS OF MATRICES

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Abstract. We provide a simple algorithm for finding the optimal upper bound for sums of products of matrix entries of the form

\[ S_\pi(N) := \sum_{j_1, \ldots, j_{2m} = 1 \atop \ker j \geq \pi} N \prod_{k=1}^{m} t^{(k)}_{j_{2k-1}j_{2k}} \]

where some of the summation indices are constrained to be equal.

The upper bound is easily obtained from a graph \( G_\pi \) associated to the constraints, \( \pi \), in the sum.

1. Introduction

We want to consider sums of the form

\[ S_\pi(N) := \sum_{j_1, \ldots, j_{2m} = 1 \atop \ker j \geq \pi} N \prod_{k=1}^{m} t^{(k)}_{j_{2k-1}j_{2k}}, \]

where \( T_k = (t^{(k)}_{ij})_{i,j=1}^N \) are given matrices and \( \pi \) is a partition of \( \{1, 2, \ldots, 2m\} \) which constrains some of the indices \( j_1, \ldots, j_{2m} \) to be the same.

The formal definition of this is given in the following notation.

Notation 1. 1) A partition \( \pi = \{V_1, \ldots, V_r\} \) of \( \{1, \ldots, k\} \) is a decomposition of \( \{1, \ldots, k\} \) into disjoint non-empty subsets \( V_i \); the \( V_i \) are called the blocks of \( \pi \). The set of all partitions of \( \{1, \ldots, k\} \) is denoted by \( \mathcal{P}(k) \).

2) For \( \pi, \sigma \in \mathcal{P}(k) \), we write \( \pi \geq \sigma \) if each block of \( \pi \) is a union of some blocks of \( \sigma \).

3) For a multi-index \( \mathbf{j} = (j_1, \ldots, j_k) \) we denote by \( \ker \mathbf{j} \in \mathcal{P}(k) \) that partition where \( p \) and \( q \) are in the same block if and only if \( j_p = j_q \).

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Thus, for a given partition \( \pi \in \mathcal{P}(k) \), the constraint \( \ker j \geq \pi \in (1) \) means that two indices \( j_q \) and \( j_p \) have to agree, whenever \( q \) and \( p \) are in the same block of \( \pi \). Note that we do not exclude that more indices might agree.

The problem which we want to address is the optimal bound of the sum (1). One expects a bound of the form

\[
|S_\pi(N)| \leq N^{\tau(\pi)} \prod_{k=1}^{m} \|T_k\|,
\]

for some exponent \( \tau(\pi) \), where \( \|T\| \) denotes the operator norm of the matrix \( T \). The question is: what is the optimal choice of this exponent?

Our interest in sums of the form \( S_\pi(N) \) was aroused by investigations on random matrices where such sums show up quite canonically, see [3]. Indeed, when one considers the asymptotic properties of products of random and deterministic matrices, one has to find efficient bounds for the sums, \( S_\pi(N) \), of products of entries of the deterministic matrices in order to determine their contribution to the limiting distribution. Yin and Krishnaiah [4], working on the product of random matrices, already faced this problem and obtained the first results for some special cases; a more systematic approach was given by Bai [1]. Our investigations are inspired by the presentation in the book of Bai and Silverstein [2].

A first upper bound comes from the trivial observations that we have in \( S_\pi(N) \) one free summation index for each block of \( \pi \) and that \( |\ell^{(k)}_{ij}| \leq \|T_k\| \) for all \( i, j \), and thus one clearly has (2) with \( \tau(\pi) = |\pi| \), where \( |\pi| \) the number of blocks of \( \pi \). However, this is far from optimal.

The main reason for a reduction of the exponent comes from the fact that some of the indices which appear are actually used up for matrix multiplication and thus do not contribute a factor of \( N \). For example, for \( \sigma = \{(2,3), (4,5), \cdots, (2m,1)\} \) one has

\[
S_\sigma(N) = \sum_{j_1,\ldots,j_{2m}=1}^{N} \ell^{(1)}_{j_1j_2} \ell^{(2)}_{j_2j_3} \cdots \ell^{(m)}_{j_{2m-1}j_{2m}}
\]

\[
= \sum_{i_1,\ldots,i_m=1}^{N} \ell^{(1)}_{i_1i_2} \ell^{(2)}_{i_2i_3} \cdots \ell^{(m)}_{i_{m}i_1}
\]

\[
= \text{Tr}(T_1 \cdots T_m),
\]

thus

\[
|S_\sigma(N)| \leq N\|T_1 \cdots T_m\| \leq N \prod_{k=1}^{m} \|T_k\|.
\]
Hence the trivial estimate \( r(\sigma) = m \) can here actually be improved to \( r(\sigma) = 1 \).

Other cases, however, might not be so clear. For example, what would one expect for

\[
(3) \quad \tau = \{(1), (2, 4, 11), (3, 5, 10), (6, 7, 8), (9, 12, 14, 16, 20), (13, 15, 17, 18), (19, 22, 24), (21, 23)\}.
\]

The corresponding sum

\[
S_\tau = \sum_{j_1, \ldots, j_{24} = 1}^N t_{j_1 j_2}^{(1)} t_{j_3 j_4}^{(2)} t_{j_5 j_6}^{(3)} t_{j_7 j_8}^{(4)} t_{j_9 j_{10}}^{(5)} t_{j_{11} j_{12}}^{(6)} t_{j_{13} j_{14}}^{(7)} t_{j_{15} j_{16}}^{(8)} t_{j_{17} j_{18}}^{(9)} t_{j_{19} j_{20}}^{(10)} t_{j_{21} j_{22}}^{(11)} t_{j_{23} j_{24}}^{(12)}
\]

subject to the constraints

\[
\begin{align*}
    j_2 &= j_4 = j_{11}, \\
    j_3 &= j_5 = j_{10}, \\
    j_6 &= j_7 = j_8, \\
    j_9 &= j_{12} = j_{14} = j_{16} = j_{20}, \\
    j_{13} &= j_{15} = j_{17} = j_{18}, \\
    j_{19} &= j_{22} = j_{24}, \\
    j_{21} &= j_{23}
\end{align*}
\]

or, in terms of unrestricted summation indices:

\[
S_\tau = \sum_{i_1, i_2, \ldots, i_{8} = 1}^N t_{i_1 i_2}^{(1)} t_{i_3 i_4}^{(2)} t_{i_5 i_6}^{(3)} t_{i_7 i_8}^{(4)} t_{i_9 i_{10}}^{(5)} t_{i_{11} i_{12}}^{(6)} t_{i_{13} i_{14}}^{(7)} t_{i_{15} i_{16}}^{(8)} t_{i_{17} i_{18}}^{(9)} t_{i_{19} i_{20}}^{(10)} t_{i_{21} i_{22}}^{(11)} t_{i_{23} i_{24}}^{(12)}
\]

The trivial estimate here is of order \( N^8 \), but it might not be obvious at all that in fact the optimal choice is \( r(\tau) = 3/2 \). The non-integer value in this case shows that the problem does not just come down to a counting problem of relevant indices.

We will show that there is an easy and beautiful algorithm for determining the optimal exponent \( r(\pi) \) for any \( \pi \). Actually, it turns out that \( r(\pi) \) is most easily determined in terms of a graph \( G_\pi \) which is associated to \( \pi \) as follows. We start from the directed graph \( G_{02m} \) with \( 2m \) vertices \( 1, 2, \ldots, 2m \) and directed edges \( (2, 1), (4, 3), \ldots, (2m, 2m - 1) \). (This is the graph which corresponds to unrestricted summation, i.e., to \( \pi = 0_{2m} \), where \( 0_{2m} \) is the minimal partition in \( P(2m) \) with \( 2m \) blocks, each consisting of one element. The reason that we orient our edges in the apparently wrong direction will be addressed in Remark \[2\]) Given a \( \pi \in P(2m) \) we obtain the directed graph \( G_\pi \) by identifying in \( G_{02m} \) the vertices which belong to the same blocks of \( \pi \). We will not
identify the edges (actually, the direction of two edges between identified vertices might be incompatible) so that $G_\pi$ will in general have multiple edges, as well as loops.

For example, the graph $G_\tau$ for $\tau$ from Equation (3) is given in Figure 1. It should be clear how one can read off the graph $G_\tau$ directly from Equation (4).

The optimal exponent $r(\pi)$ is then determined by the structure of the graph $G_\pi$. Before we explain how this works, let us rewrite the sum (1) more intrinsically in terms of the graph $G = G_\pi$ as

$$S_G(N) := \sum_{i : V \rightarrow [N]} \prod_{e \in E} t_{i(s(e)),i(t(e))}^{(e)}.$$  

We sum over all functions $i : V \rightarrow [N]$ where $N = \{1, 2, 3, \ldots, N\}$, $V$ is the set of vertices of $G$, $E$ the set of edges, and $s(e)$ and $t(e)$ denote the source vertex and the target vertex of $e$ respectively. Note that we keep all edges through the identification according to $\pi$, thus the $m$ matrices $T_1, \ldots, T_m$ in (1) show up in (5) as the various $T_e$ for the $m$ edges of $G_\pi$.

**Remark 2.** Note that a factor of $t_{i_s,i_s}^{(l)}$ in the sum in (5) produces an edge labelled $T_l$ starting at a vertex labelled $i_s$ and ending at a vertex labelled $i_r$. 

**Figure 1.** The graph $G_\tau$ for the sum (4).
This reversing of the indices is an artifact of the usual convention of writing $TS$ for the operator where one first applies $S$ and then $T$.

Clearly $\pi$ and $G_\pi$ contain the same information about our problem; however, since the bound on $S_G(N)$ is easily expressed in terms of $G_\pi$, we will in the following forget about $\pi$ and consider the problem of bounding the graph sum $S_G(N)$ in terms of $N$ for an arbitrary graph $G$ with attached matrices. We will call a picture as in Figure 1 a graph of matrices; for a precise definition, see Definition 8.

Example 3. In the figures below we give four directed graphs and below each graph the corresponding graph sum. One can see that if the graph is a circuit then the graph sum is a trace of the product of the matrices. However for more general graphs the graph sum cannot easily be written in terms of traces. Nevertheless, as Theorem 6 will show, there is a simple way to understand the dependence of the graph sum on $N$, the size of the matrices.

\[
\text{Tr}(T) = \sum_i t_{ii} \quad \quad \quad \quad \sum_{i,j} t_{ij}
\]

\[
\text{Tr}(T_1T_2T_3) = \sum_{i,j,k} t_{ij}^{(1)} t_{jk}^{(2)} t_{ki}^{(3)} \quad \quad \quad \sum_{i,j,k,l} t_{ij}^{(1)} t_{jk}^{(2)} t_{kl}^{(3)}
\]

The relevant feature of the graph is the structure of its two-edge connected components.

Notation 4. 1) A cutting edge of a connected graph is an edge whose removal would result in two disconnected subgraphs. A connected graph is two-edge connected if it does not contain a cutting edge, i.e., if it cannot be cut into disjoint subgraphs by removing one edge. A two-edge connected component of a graph is a subgraph which is two-edge connected and cannot be enlarged to a bigger two-edge connected subgraph.

2) A forest is a graph without cycles. A tree is a component of a forest, i.e., a connected graph without cycles. A tree is trivial if it
consists of only one vertex. A leaf of a non-trivial tree is a vertex which meets only one edge. The sole vertex of a trivial tree will also be called a trivial leaf.

It is clear that if one takes the quotient of a graph with respect to the two-edge connectedness relation (i.e., one shrinks each two-edge connected component of a graph to a vertex and just keeps the cutting edges), then one does not have cycles any more, thus the quotient is a forest.

**Notation 5.** For a graph $G$ we denote by $\mathcal{F}(G)$ its *forest of two-edge connected components*: the vertices of $\mathcal{F}(G)$ consist of the two-edge connected components of $G$ and two distinct vertices of $\mathcal{F}(G)$ are connected by an edge if there is a cutting edge between vertices from the two corresponding components in $G$.

For the graph from Figure 1 the corresponding forest $\mathcal{F}(G_\tau)$ is drawn in Figure 2.

Now we can present our main theorem on bounds for sums of the form (5). In the special case of a two-edge connected graph we obtain the same bound as appears in the book of Bai and Silverstein [2]. In the general case, however, our bound is less than that of [2].

**Theorem 6.** 1) Let $G$ be a directed graph, possibly with multiple edges and loops. Let for each edge $e$ of $G$ be given an $N \times N$ matrix $T_e = \left( t_{ij}^{(e)} \right)_{i,j=1}^N$. Let $E$ and $V$, respectively, be the edges and vertices of $G$ and

$$S_G(N) := \sum_{i:V \rightarrow [N]} \prod_{e \in E} t_{i(s(e)),i(t(e))}^{(e)}$$

**Figure 2.** The quotient graph $\mathcal{F}(G_\tau)$ of Figure 1; the forest here consists of just one tree.
Figure 3. Putting the non-cutting edge matrices equal to the identity matrix reduces the problem for $G_{\tau}$ of Figure 1 to this one.

where the sum runs over all functions $i : V \rightarrow [N]$. Then

$$|S_G(N)| \leq N^{\tau(G)} \cdot \prod_{e \in E} \|T_e\|,$$

where $\tau(G)$ is determined as follows from the structure of the forest $\mathcal{F}(G)$ of two-edge connected components of $G$:

$$\tau(G) = \sum_{l \text{ leaf of } \mathcal{F}(G)} \tau(l)$$

where

$$\tau(l) := \begin{cases} 1, & \text{if } l \text{ is a trivial leaf} \\ \frac{1}{2}, & \text{if } l \text{ is a leaf of a non-trivial tree} \end{cases}$$

2) The bound in Equation (7) is optimal in the following sense. For each graph $G$ and each $N \in \mathbb{N}$ there exist $N \times N$ matrices $T_e$ with $\|T_e\| = 1$ for all $e \in E$ such that

$$S_G(N) = N^{\tau(G)}.$$

Example 7. Consider again our example $S_{\tau}$ from (4). Its forest $\mathcal{F}(G_{\tau})$, given in Figure 2, consists of one tree with three leaves; thus Theorem 6 predicts an order of $N^{3/2}$ for the sum (4). In order to see that this can actually show up (and thus give the main idea for the proof of optimality), put all the matrices in Figure 1 for the non-cutting edges equal to the identity matrix; then the problem collapses to the corresponding problem on the tree, where we are just left with the four indices $i_1, i_2, i_4, i_7$ and the three matrices $T_1, T_3, T_{10}$. See Figure 3.

The corresponding sum is

$$S = \sum_{i_1, i_2, i_4, i_7 = 1}^N t_{(1)}^{(1)} t_{(3)}^{(3)} t_{(10)}^{(10)} t_{i_1 i_2} t_{i_2 i_4} t_{i_4 i_7} t_{i_7 i_2}$$
Let $V$ now be the matrix

$$V = \frac{1}{\sqrt{N}} \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 1 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 0 & \cdots & 0 \end{pmatrix};$$

and put $T_3 = V^t$, $T_1 = T_{10} = V$. Then $\|T_1\| = \|T_3\| = \|T_{10}\| = 1$ and we have for this case

$$S = \frac{1}{N^{3/2}} \sum_{i_1, i_2, i_1, i_7 = 1}^{N} \delta_{i_1} \delta_{i_2} \delta_{i_2} = \frac{1}{N^{3/2}} N^3 = N^{3/2}.$$

Note that each tree of the forest $\mathcal{F}(G)$ makes a contribution of at least 1 in $v(G)$, because a non-trivial tree has at least two leaves. One can also make the above description more uniform by having a factor $1/2$ for each leaf, but counting a trivial leaf as actually two leaves. (The reason for this special role of trivial leaves will become apparent in the proof of Theorem 6 in the next section.) Note also that the direction of the edges plays no role in the estimate above. The direction of an edge is only important in order to define the contribution of an edge to the graph sum. One direction corresponds to the matrix $T_e$, the other direction corresponds to the transpose $T_e^t$. Since the norm of a matrix is the same as the norm of its transpose, the estimate is the same for all graph sums which correspond to the same undirected graph.

Finally, we want to give an idea of our strategy for the proof of Theorem 6. One of the main steps consists in modifying the given graph of matrices (by reversing some orientations, and by splitting some vertices into two) in such a way that the corresponding sum $S_G(N)$ is not changed and such that the modified graph has the structure of an input-output graph. By the latter we mean that we have a consistent orientation of the graph from some input vertices to some output vertices, see Definition 10.

For example, a suitable modification of the graph $G_\tau$ is presented in Figure 4. We have reversed the orientation of two edges (but compensated this by taking the adjoint of the attached matrices) and also split each of the vertices $i_4$, $i_5$, $i_6$ into two copies. To take care of the fact that in the summation we must have $i_4 = i'_4$ we have added an additional edge between $i_4$ and $i'_4$ with the identity matrix attached and similarly for $i_5$ and $i'_5$ and $i_6$ and $i'_6$. So in order to obtain a bound for $S_\tau$ it suffices to obtain a bound for the graph $G$ from Figure 4. But this has now a kind of linear structure, with $i_4$ as input vertex and $i_1$ and $i_8$ as output vertices. This structure allows us to associate to the
A modification of the graph $G_\tau$ from Figure 1 in input-output form. Note that the input vertex $i_4$ and the output vertices $i_1$ and $i_8$ are chosen from the leaves of $\mathfrak{F}(G_\tau)$.

Graph $G$ an operator $T_G$, which is described in terms of tensor products of the maps $T_e$ and partial isometries describing the splittings at the internal vertices. $T_G$ maps from the vector space associated to $i_4$ to the tensor product of the vector spaces associated to $i_1$ and $i_8$. It is then fairly easy to see that the norm of $T_G$ is dominated by the product of the norms of the involved operators $T_e$; and the estimate for the sum $S_G(N)$ is finally just an application of the Cauchy-Schwarz inequality, where each of the input and output vertices gives a factor $N^{1/2}$.

The rest of the paper is organized as follows. In Section 2 we formulate a slight generalization of our theorem to rectangular matrices and introduce abstractly the notion of a graph of matrices. Section 3 deals with input-output graphs and the norm estimates for their associated operators. In Section 4 we address the general case by showing
how one can modify a general graph of matrices to become an input-output graph. Finally, in Section 5 we generalize the considerations from Example 7 to show the optimality of our choice for \(r(G)\).

### 2. Generalization to Rectangular Matrices

Let us first formalize the input information for Theorem 6. We will deal here with the more general situation of rectangular instead of square matrices. In order for the graph sum to make sense we require that for a given vertex \(v\) all the matrices associated with an incoming edge have the same number of rows, \(N_v\) and likewise all the matrices associated with an outgoing edge have the same number of columns \(N_v\). Moreover we shall find it advantageous to treat the matrices as linear operators between finite dimensional Hilbert spaces. So for each vertex \(v\) let \(H_v = \mathbb{C}^{N_v}\) have the standard inner product and let \(\{\xi_1, \ldots, \xi_{N_v}\}\) be the standard orthonormal basis of \(\mathbb{C}^{N_v}\). Note that we use the convention that inner products \((x, y) \mapsto \langle x, y \rangle\) are linear in the second variable and we shall use Dirac’s bra-ket notation for rank one operators; \(|\xi\rangle\langle\eta| (\mu) = \langle\eta, \mu\rangle_\xi\).

**Definition 8.** A graph of matrices consists of a triple \(\mathcal{G} = (G, (H_v)_{v \in V}, (T_e)_{e \in E})\) in which

1. \(G = (V, E)\) is a directed graph (possibly with multiple edges and loops),
2. \(H_v\) is a finite dimensional Hilbert space equal to \(\mathbb{C}^{N_v}\) and
3. \(T_e : H_{s(e)} \to H_{t(e)}\) is a linear operator.

(This is also known as a representation of a quiver, but we shall not need this terminology.)

Here is the generalization of Theorem 6 to the case of a rectangular matrices.

**Theorem 9.** Let \(\mathcal{G} = (G, (H_v)_{v \in V}, (T_e)_{e \in E})\) be a graph of matrices. Let

\[
S(\mathcal{G}) := \sum_{i : V \to \mathbb{N}} \prod_{e \in E} \langle \xi_{i(t(e))}, T_e \xi_{i(s(e))} \rangle.
\]

where the sum runs over all functions \(i : V \to \mathbb{N}\) such that for each \(v \in V\) we have \(1 \leq i(v) \leq N_v\).

Let \(\mathcal{F} = \mathcal{F}(G)\) be the forest of two-edge connected components of \(G\). Then

\[
|S(\mathcal{G})| \leq \prod_{\text{leaf } l \text{ of } \mathcal{F}} \left( \max_{v \in l} \dim H_v \right)^{r(l)} \cdot \prod_{e \in E} \|T_e\|,
\]
where, for a leaf \( l \), \( v \) runs over all vertices in the two edge connected component of \( G \) corresponding to \( l \), and where
\[
\tau(l) := \begin{cases} 
1, & \text{if } l \text{ is a trivial leaf}, \\
\frac{1}{2}, & \text{if } l \text{ is a leaf of a non-trivial tree}.
\end{cases}
\]

3. ESTIMATE FOR INPUT-OUTPUT GRAPHS

The main idea for proving the estimate (10) for a graph of matrices is to first suppose that there is a flow from some vertices designated input vertices, \( V_{\text{in}} \), to some other vertices designated output vertices, \( V_{\text{out}} \), and then to show that every graph can be modified to have such a flow. All the remaining vertices, which are neither input nor output vertices, will be called internal vertices.

**Definition 10.** Let \( G \) be a directed graph (possibly with multiple edges). We say that \( G \) is an input-output graph if there exists two disjoint non-empty subsets, \( V_{\text{in}} \) and \( V_{\text{out}} \), of the set of vertices of \( G \) such that the following properties are satisfied.

- \( G \) does not contain a directed cycle. (Recall that a cycle is a closed path and that a path is directed if all the edges are oriented in the same direction.)
- Each vertex of \( G \) lies on a directed path from some vertex in \( V_{\text{in}} \) to some vertex in \( V_{\text{out}} \).
- Every internal vertex has at least one incoming edge and at least one outgoing edge.
- Every input vertex has only outgoing edges and every output vertex has only ingoing edges.

Recall that \( \{\xi_i\}_{i=1}^{N_v} \) is an orthonormal basis for \( \mathcal{H}_v \). Let \( V_0 \subset V \) be a subset, suppose that we have a function \( i : V_0 \to \mathbb{N} \) such that \( i(v) \leq N_v \) then for each \( v \in V_0 \), \( \xi_{i_v} \) is an element of our orthonormal basis of \( \mathcal{H}_v \). Thus an element of our orthonormal basis of \( \bigotimes_{v \in V_0} \mathcal{H}_v \) is specified by a function \( i : V_0 \to \mathbb{N} \) such that \( i(v) \leq N_v \) for each \( v \) in \( V_0 \). When it is clear from the context we shall just say that a basis element of \( \bigotimes_{v \in V_0} \mathcal{H}_v \) is specified by a function \( i : V_0 \to \mathbb{N} \), but it should always be understood that \( i(v) \leq N_v \).

Hence if we form \( \{\bigotimes_{v \in V_0} \xi_{i_v}\}_i \) where \( i \) runs over all functions \( i : V_0 \to \mathbb{N} \), we obtain an orthonormal basis of \( \bigotimes_{v \in V_0} \mathcal{H}_v \). Thus an operator \( T_{\mathcal{E}} : \bigotimes_{v \in V_{\text{in}}} \mathcal{H}_v \to \bigotimes_{w \in V_{\text{out}}} \mathcal{H}_w \) can be specified by giving
\[
\langle \bigotimes_{w \in V_{\text{out}}} \xi_{j_w}, T_{\mathcal{E}}(\bigotimes_{v \in V_{\text{in}}} \xi_{i_v}) \rangle
\]
for each basis vector $i : V_{in} \to \mathbb{N}$ and $j : V_{out} \to \mathbb{N}$. In the theorem below we shall show that a certain kind of graph sum can be written in terms of a vector state applied to an operator defined by the inner product above. This is the first of two key steps in proving Theorem 9.

**Theorem 11.** Let $G = (G, (H_v)_{v \in V}, (T_e)_{e \in E})$ be a graph of matrices and assume that $G$ is an input-output graph with input vertices $V_{in}$ and output vertices $V_{out}$.

1) We define $T_G : \bigotimes_{v \in V_{in}} H_v \to \bigotimes_{w \in V_{out}} H_w$ by

$$\langle \bigotimes_{w \in V_{out}} \xi_w, T_G( \bigotimes_{v \in V_{in}} \xi_v) \rangle = \sum_{k : V \to \mathbb{N}} \prod_{e \in E} \langle \xi_{k(e)} T_e \xi_{k(e)} \rangle,$$

where $i : V_{in} \to \mathbb{N}$, $j : V_{out} \to \mathbb{N}$ and $k$ runs over all maps $k : V \to \mathbb{N}$ such that $k|_{V_{in}} = i$ and $k|_{V_{out}} = j$.

Then we have

$$\|T_G\| \leq \prod_{e \in E} \|T_e\|.$$

2) For the graph sum \([9]\) we have

$$S(G) = \langle \bigotimes_{w \in V_{out}} \xi_w', T_G \bigotimes_{v \in V_{in}} \xi_v' \rangle,$$

where $\xi' = \xi_1 + \cdots + \xi_{N_v} \in H_v$, and we have the estimate

$$|S(G)| \leq \prod_{w \in V_{in} \cup V_{out}} \dim(H_v)^{1/2} \cdot \prod_{e \in E} \|T_e\|.$$

**Proof.** The key point is to observe that we can write the operator $T_G$ as a composition of tensor products of the edge operators $T_e$ and isometries corresponding to the internal vertices. Every internal vertex has, by the definition of an input-output graph, some incoming edges and some outgoing edges, let’s say $t$ incoming and $s$ outgoing (with $t,s \geq 1$). Then the summation over the orthonormal basis of $H_v$ for this internal vertex corresponds to an application of the mapping $L_v : H_v^{\otimes t} \to H_v^{\otimes s}$ given by

$$L_v = \sum_{i=1}^{N_v} |\xi_{i}^{\otimes s}\rangle \langle \xi_{i}^{\otimes t}|.$$

In terms of our basis we have for all $1 \leq i_1, \ldots, i_t \leq N_v$

$$L_v(\xi_{i_1} \otimes \cdots \otimes \xi_{i_t}) = \begin{cases} (\xi_{i_1}^{\otimes s} \otimes \cdots \otimes \xi_{i_t}^{\otimes s}) & \text{if } i_1 = \cdots = i_t \\ 0 & \text{otherwise}. \end{cases}$$

The mapping $L_v$ is, for all internal vertices $v$, a partial isometry, and thus has norm equal to 1.
It remains to put all the edge operators and the vertex isometries together in a consistent way. For this, we have to make sure that we can order the application of all these operators in a linear way so that their composition corresponds to the operator defined by $\prod$. However, this is guaranteed by the input-output structure of our graph. We can think of our graph as an algorithm, where we are feeding input vectors into the input vertices and then operate them through the graph, each edge doing some calculation, and each vertex acting like a logic gate, doing some compatibility checks. The main problem is the timing of the various operations, in particular, how long one has to wait at a vertex, before applying an operator on an outgoing edge. In algorithmic terms, it is clear that one has to wait until all the input information is processed; i.e. one has to wait for information to arrive along the longest path from an input vertex to the given vertex.

To formalize this, let us define a distance function $d : V \to \{0, 1, 2, \ldots \}$ on our graph $G$ which measures the maximal distance from a vertex to a input vertex,

$$d(v) := \max \left\{ k \left| \begin{array}{c} \text{there exists a directed path of length} \\ k \text{ from some input vertex to } v \end{array} \right. \right\}.$$ 

The length of a path is the number of edges it uses. Note that since an input vertex has no incoming edges, we have $d(v) = 0$ for all input vertices. The number $d(v)$ tells us how long we should wait before we apply the isometry corresponding to $v$; after $d(v)$ steps all information from the input vertices has arrived at $v$. Let $r$ be the maximal distance (which is achieved for one of the output vertices). The distance function $d$ gives us a decomposition of the vertices $V$ of our graph into disjoint level sets

$$V_k := \{ v \in V \mid d(v) = k \}, \quad V = \bigcup_{k=0}^{r} V_k.$$ 

Note that, for any edge $e$, we have $d(t(e)) \geq d(s(e)) + 1$. In order to have a clearer notation it is preferable if our edges connect only vertices which differ in $d$ exactly by 1. This can easily be achieved by adding vertices on edges for which this difference is bigger than 1. The new vertices have one incoming edge and one outgoing edge. We have of course also to attach matrices to those edges, and we do this in such a way that all incoming edges of the new vertices get the identity matrix, the original matrix $T_e$ is reserved for the last piece of our decomposition. These new vertices will not change the operator $T_\emptyset$ nor the graph sum $S(\emptyset)$. In the same way we can insert some new vertices for all incoming edges of the output vertices and thus arrange that every output vertex
$v$ has maximal possible distance $d(v) = r$. (Note that there cannot be a directed path from one output vertex to another output vertex, because an output vertex has no outgoing edges.)

Thus we can assume without loss of generality that we have $d(t(e)) = d(s(e)) + 1$ for all edges $e \in E$ and that $d(v) = r$ for all $v \in V_{\text{out}}$. We have now also a decomposition of $E$ into a disjoint union of level sets,

$$E_k := \{ e \in E \mid d(t(e)) = k \}, \quad E = \bigcup_{k=1}^r E_k.$$ 

Edges from $E_k$ are connecting vertices from $V_{k-1}$ to vertices from $V_k$.

Note that our Hilbert spaces correspond on one side to the vertices, but on the other side also to the edges as source and target Hilbert spaces; to make the latter clearer, let us also write

$$T_e : \mathcal{H}_e^\triangleright \to \mathcal{H}_e^\lt, \quad T_e : \mathcal{H}_e^\lt \to \mathcal{H}_e^\triangleright,$$

where of course $\mathcal{H}_e^\triangleright$ is the same as $\mathcal{H}_{s(e)}$ and $\mathcal{H}_e^\lt$ is the same as $\mathcal{H}_{t(e)}$.

We can now write

$$T_\varnothing = L_r \cdot T_r \cdot L_{r-1} \cdot T_{r-1} \cdots L_1 \cdot T_1 \cdot L_0,$$

where $L_k$ is the tensor product of all partial isometries corresponding to the vertices on level $k$, and $T_k$ is the tensor product of all edge operators corresponding to the edges on level $k$. More precisely,

$$T_k : \bigotimes_{e \in E_k} \mathcal{H}_e^\triangleright \to \bigotimes_{e \in E_k} \mathcal{H}_e^\lt$$

is defined as

$$T_k := \bigotimes_{e \in E_k} T_e;$$

whereas

$$L_k := \bigotimes_{v \in V_k} L_v,$$

with the vertex partial isometry

$$L_v : \bigotimes_{e \in E \atop t(e) = v} \mathcal{H}_e^\triangleright \to \bigotimes_{f \in E \atop s(f) = v} \mathcal{H}_f^\lt$$

given by

$$L_v = \sum_{i=1}^{N_v} \langle \xi_i^\otimes s | \xi_i^\otimes t \rangle,$$

where $s$ and $t$ are the number of edges which have $v$ as their source and target, respectively.
Since we do not have incoming edges for \( v \in V_{in} \) nor outgoing edges for \( v \in V_{out} \), one has to interpret \( L_0 \) and \( L_r \) in the right way. Namely, for \( v \in V_{in} \), the operator \( L_v \) acts on

\[
L_v : \mathcal{H}_v \rightarrow \bigotimes_{e \in E \atop s(e) = v} \mathcal{H}_e
\]

given by

\[
L_v = \sum_{i=1}^{N_v} |\xi_i \otimes s_i \rangle \langle \xi_i |
\]

and similarly for \( v \in V_{out} \). (Formally, one can include this also in the general formalism by adding one incoming half-edge to each input vertex and one outgoing half-edge to each output vertex.) With this convention, the product given in (14) is an operator from \( \bigotimes_{v \in V_{in}} \mathcal{H}_v \) to \( \bigotimes_{w \in V_{out}} \mathcal{H}_w \). It is clear that (14) gives the same operator as (11).

Now the factorization (14) and the fact that all \( L_v \) and thus all \( L_k \) are partial isometries yield

\[
\| T_{G} \| \leq \prod_{k=0}^{r} \| L_k \| \cdot \prod_{k=1}^{r} \| T_k \| = \prod_{k=1}^{r} \| T_k \| = \prod_{e \in E} \| T_e \|.
\]

This is the norm estimate (12) claimed for the operator \( T_{G} \).

In order to get the estimate for the graph sum \( S(G) \) we have to note the difference between \( T_{G} \) and \( S(G) \): for \( T_{G} \) we sum only over the internal vertices and thus remain with a matrix, indexed by the input and output vertices; for \( S(G) \) we also have to sum over these input and output vertices. If we denote by

\[
\xi^v := \sum_{i=1}^{N_v} \xi_i \in \mathcal{H}_v
\]

the sum over the vectors from our orthonormal basis of \( \mathcal{H}_v \), then we have

\[
S(G) = \langle \bigotimes_{w \in V_{out}} \xi^w, T_{G} \bigotimes_{v \in V_{in}} \xi^v \rangle.
\]

An application of the Cauchy-Schwartz inequality yields then

\[
|S(G)| \leq \| T_{G} \| \cdot \prod_{v \in V_{in}} \| \xi^v \| \cdot \prod_{w \in V_{out}} \| \xi^w \|.
\]

Since the norm of \( \xi^v \) is, by Pythagoras’s theorem, given by \((\dim \mathcal{H}_v)^{1/2}\), we get the graph sum estimate (13). \( \square \)
4. Proof of the General Case

Let us now consider a graph of matrices as in Theorem 9. The problem is that the underlying graph $G$ might not be an input-output graph. However, we have some freedom in modifying $G$ without changing the associated graph sum. First of all, we can choose the directions of the edges arbitrarily, because reversing the direction corresponds to replacing $T_e$ by its transpose $T_e^t$. Since the norm of $T_e$ is the same as the norm of $T_e^t$, the estimate for the modified graph will be the same as the one for the old graph. More serious is that, in order to apply Theorem 11 we should also remove directed cycles in $G$. This cannot, in general, be achieved by just reversing some directions. (As can clearly be seen in the case of a loop.) The key observation for taking care of this is that we can split a vertex $v$ into $v$ and $v'$ and redistribute at will the incoming and outgoing edges from $v$ between $v$ and $v'$. We put one new edge $f$ between $v$ and $v'$ with the corresponding operator $T_f$ being the identity matrix. The constraint from $T_f$ in the graph sum will be that after the splitting, the basis vector for the vertex $v$ has to agree with the basis vector for the vertex $v'$, so summation over them yields the same result as summation over the basis of $H_v$ before the splitting. Thus this splitting does not change the given graph sum. Since the norm of the identity matrix is 1, this modification will also not affect the wanted norm estimate.

One should of course also make sure that the forest structure of the two-edge connected components is not changed by such modifications. For the case of reversing arrows this is clear; in the case of splitting vertices the only problem might be that the new edge between $v$ and $v'$ is a cutting edge. This can actually happen, but only in the case where $v$ constitutes a two-edge connected component by itself. In that case, we do the splitting as before but add two new edges between $v$ and $v'$, both with the same orientation and both with the identity operator.

This motivates the following definition of the modification of a graph of matrices.

**Definition 12.** We say that $\hat{G} = (\hat{G}, (\hat{H}_v)_{v \in \hat{V}}, (\hat{T}_e)_{e \in \hat{E}})$ is a modification of $G = (G, (H_v)_{v \in V}, (T_e)_{e \in E})$, if the former can be obtained from the latter by finitely many applications of the following operations:

- change the direction of the arrow of an edge $e$ and replace $T_e : H_{s(e)} \rightarrow H_{t(e)}$ by its transpose $T_e^t : H_{t(e)} \rightarrow H_{s(e)}$
- split a vertex $v$ into two vertices $v$ and $v'$, redistribute in some way the incoming and outgoing edges for $v$ together with their matrices to $v$ and $v'$ and add a new edge between $v$ and $v'$ with arbitrary direction for this edge and the identity matrix
attached to it; should \( v \) be a two-edge connected component, then we add two edges between \( v \) and \( v' \), both with the same orientation, and both having the identity matrix attached to them.

Our discussion from above can then be summarized in the following proposition.

**Proposition 13.** Let \( \hat{\mathfrak{G}} = (\hat{G}, (\hat{H}_w)_{w \in \hat{V}}, (\hat{T}_f)_{f \in \hat{E}}) \) be a modification of \( \mathfrak{G} = (G, (H_v)_{v \in V}, (T_e)_{e \in E}) \). Then we have:

- the graph sums are the same,
  \[ S(\mathfrak{G}) = S(\hat{\mathfrak{G}}); \]
- the forests of two-edge connected components are the same,
  \[ \mathfrak{F}(G) = \mathfrak{F}(\hat{G}); \]
- the product of the norm of the edge operators is the same,
  \[ \prod_{e \in E} \|T_e\| = \prod_{f \in \hat{E}} \|\hat{T}_f\|. \]

Thus, in order to show the graph sum estimate (10) for \( \mathfrak{G} \) it is enough to prove this estimate for some modification \( \hat{\mathfrak{G}} \).

So the crucial step for the proof of Theorem 9 is now to modify a given graph \( G \) to an input-output graph \( \hat{G} \) with the right number of input and output vertices.

**Proposition 14.** Let \( \mathfrak{G} \) be a graph of matrices. Then there exists a modification \( \hat{\mathfrak{G}} \) such that the underlying graph \( \hat{G} \) of the modification is an input-output graph.

Furthermore, the input and output vertices can be chosen such that:
for each non-trivial tree of the forest \( \mathfrak{F}(G)(= \mathfrak{F}(\hat{G})) \) we have one leaf as input leaf and all the other leaves as output leaves. For a trivial tree, the trivial leaf is considered both as input and output leaf. The input vertices of \( \hat{G} \) shall consist of one vertex from each input leaf, and the output vertices shall consist of one vertex from each output leaf.

**Proof.** Clearly we can assume that the underlying graph \( G \) of \( \mathfrak{G} \) is connected, because otherwise we do the following algorithm separately for each connected component.

For such a connected \( G \), consider the tree of its two-edge connected components. Declare arbitrarily one leaf as *input leaf*, all the other leaves as *output leaves*; if the tree is trivial, we declare its only leaf both as input and output leaf. Furthermore, we choose an arbitrary
For each two-edge connected component we define now one input vertex and one output vertex. For the input leaf we have already chosen the input vertex; its output vertex is the source vertex of one (arbitrarily chosen) of the outgoing cutting edges. For the output leaves we have already chosen their output vertices; as input vertex we take the target vertex of the (unique) incoming cutting edge. For all the other, non-leaf, components we choose the target vertex of the (unique) incoming cutting edge as input vertex and the source vertex of one (arbitrarily chosen) of the outgoing cutting edges as the output vertex. We want all those input and output vertices to be different, which can be achieved by splitting, if necessary, some of them into two.

So now each two-edge connected component has one input vertex and one output vertex. If we are able to modify each two edge connected component in such a way that it is an input-output graph with respect to its input and output vertex, then by putting the two-edge connected components together and declaring all input vertices but the one from the input leaf and all output vertices but the ones from the output leaves as internal indices, we get the modification $\hat{G}$ with the claimed properties. It only remains to do the modification of the two-edge connected components. This will be dealt with in the next lemma. □

Lemma 15. Let $\mathfrak{G}$ be a graph of matrices and assume that the underlying graph $G$ is two-edge connected. Let $v$ and $w$ be two disjoint vertices from $G$. Then there exists a modification $\hat{\mathfrak{G}}$ of $\mathfrak{G}$, such that the underlying graph $\hat{G}$ of the modification is an input-output graph, with input vertex $v$ and output vertex $w$.

Proof. The proof of this can be found in [2 Ch. 11]. Let us recall the main steps. One builds a sequence $G_k$ of input-output graphs (all with $v$ as input vertex and $w$ as output vertex) such that each step is manageable and that the last graph is the wanted one. For this construction we ignore the given orientation of the edges of $G$, but will just use the information from $G$ as undirected graph; then we will choose convenient orientations for the edges when constructing the sequence $G_k$.

First, we choose a simple path (i.e., a path without cycles), in our graph $G$ from $v$ to $w$. We direct all edges on this path from $v$ to $w$. 
This path with this orientation of edges is our first input-output graph $G_1$.

Assume now we have constructed an input-output graph $G_k$. If this is not yet the whole graph, then we can choose an edge $e$ which is not part of $G_k$ and which has one of its vertices, say $x$, on $G_k$. Let us denote the other vertex of $e$ by $z$. Then one can find a simple path in $G$ which connects $z$ with $G_k$ and does not use $e$. (This is possible, because otherwise $e$ would be a cutting edge.) Denote the end point of this path (lying on $G_k$) by $y$. (Note that $y$ might be the same as $z$.) We have now to direct this path between $x$ and $y$. If $x \neq y$, then there was:

- i) either a directed path from $x$ to $y$ in $G_k$, in which case we direct the new path also from $x$ and $y$;
- ii) or a directed path from $y$ to $x$ in $G_k$, in which case we direct the new path also from $y$ and $x$;
- iii) or there was no such path in $G_k$, in which case we can choose any of the two orientations for the new path between $x$ and $y$.

(Note that the first and second case cannot occur simultaneously, because otherwise we would have had a directed cycle in $G_k$.)

The only problematic case is when $x = y$, i.e., when the new path is actually a cycle. In this case we split the vertex $x = y$ into two different vertices, $x$ and $y$; $x$ gets all the incoming edges from $G_k$ and $y$ gets all the outgoing edges from $G_k$, and the new edge is directed from $x$ to $y$. Furthermore, the new cycle becomes now a directed path from $x$ to $y$.

Our new graph $G_{k+1}$ is now given by $G_k$ (possibly modified by the splitting of $x$ into $x$ and $y$) together with the new path from $x$ to $y$. It is quite easy to see that $G_{k+1}$ is again an input-output graph, with the same input vertex and output vertex as $G_k$.

We repeat this adjoining of edges until we have exhausted our original graph $G$, in which case our last input-output graph is the wanted modification. \[\Box\]

5. Proof of Optimality

In order to show the second part of Theorem 6 that our exponent $r(G)$ is optimal, we just have to adapt the corresponding considerations in Example 7 to the general case. For a given graph we attach to each non-cutting edge the identity matrix; thus all indices in a two-edge connected component of $G$ get identified and we reduce the problem to the case that $G$ is a forest. Since it suffices to look on the components separately, we can thus assume that $G$ is a tree. If this tree is trivial, then we have no cutting edges left and we clearly get a factor $N$.\


Otherwise, we put an orientation on our tree by declaring one leaf as input leaf and all the other leaves as output leaves. Then we attach the following matrices to the edges of this tree

\[
T_e = \begin{cases} 
V^t, & \text{if } e \text{ joins the input leaf with an internal vertex} \\
V, & \text{if } e \text{ joins an output leaf with an internal vertex} \\
1, & \text{otherwise}
\end{cases}
\]

where \( V \) is the matrix given in \([8]\). Again, it is straightforward to see that this choice forces every index corresponding to an internal vertex to be equal to 1, whereas there is no restriction for the indices corresponding to the leaves; taking into account also the \( 1/\sqrt{N} \) factors from the operators \( V \), we will get in the end \( N\#\text{leaves}/2 \) for the sum.

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