Nonnegativity for hafnians of certain matrices

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ABSTRACT

We show that a complex symmetric matrix of the form $A(Y, B) = \begin{bmatrix} Y & B \\ B^\top & Y \end{bmatrix}$, where $B$ is Hermitian positive semidefinite, has a nonnegative hafnian. Some positive scalar multiples of matrices $A(Y, B)$ are encodable in a Gaussian boson sampler. Further, the hafnian of this matrix is non-decreasing in $B$ in the sense that $\text{haf}(A(Y, L)) \geq \text{haf}(A(Y, B))$ if $L \succeq B$.

1. Introduction

Let $A = [a_{ij}]$ be a $2n \times 2n$ symmetric matrix with entries in $\mathbb{C}$. The hafnian $\text{haf} A$ is defined as the sum of $\prod_{k=1}^{n} a_{i_k j_k}$ over all perfect matchings $(i_1, j_1), \ldots, (i_n, j_n)$ of the complete graph $K_{2n}$. The pairs $(i, j)$ for which $i \neq j$ and $a_{ij} \neq 0$ form the edges of a graph $G$ with vertex set $[2n]$; we can consider $A$ (with diagonal entries ignored) as a weighted adjacency matrix of $G$, and $\text{haf} A$ is a weighted sum over the perfect matchings of $G$.

Assume that $m = 2n$ and $K_{2n} = ([2n], E_{2n})$ is a complete graph on $[2n]$ vertices. Recall that $M \subset E_{2n}$ is a perfect match of $K_{2n}$ if $([2n], M)$ is a 1-regular spanning subgraph of $K_{2n}$. So $M = \bigcup_{k \in [n]} \{(i_k, j_k)\}$, where $[2n] = \bigcup_{k \in [n]} \{i_k, j_k\}$. Let $\mathcal{M}_{2n}$ be the set of perfect matchings in $K_{2n}$. Assume that $A = [a_{ij}] \in S_{2n}$.

Then, the hafnian of $A$ is defined as follows [1]:

$$\text{haf} A = \sum_{M=\bigcup_{k \in [n]} \{(i_k, j_k)\} \in \mathcal{M}_{2n}} \prod_{k=1}^{n} a_{i_k j_k}.$$  

For various properties of the hafnian; see, e.g. [2].

In particular, we consider $A$ of the form

$$A(Y, B) = \begin{bmatrix} Y & B \\ B^\top & Y \end{bmatrix},$$  

(1)
where $Y$ is a (complex) symmetric matrix and $B$ is a hermitian positive semidefinite matrix. The main result of this paper is the following theorem.

**Theorem 1.1:** Assume that $A(Y, B)$ is of the form (1), where $Y$ is complex symmetric and $B$ positive semidefinite Hermitian. Then $\text{haf} A(Y, B) \geq 0$. If $B$ has no zero row, then $\text{haf} A(Y, B) > 0$. Furthermore, if $L \geq B$ i.e. $L - B$ is positive semidefinite Hermitian, then $\text{haf} A(Y, L) \geq \text{haf} A(Y, B)$.

The inequality $\text{haf} A(Y, B) \geq 0$ for $B \succeq 0$ can be deduced from the physical arguments stated in [3]; see Appendix.

Observe that $A(0, B)$ for any $B \in \mathbb{C}^{n \times n}$ is a weighted adjacency matrix of the complete bipartite graph $K_{n,n}$, where the first part is $[n]$ and the second part is $[n+1, \ldots, 2n]$. Permutations of $[n]$ correspond to perfect matchings of $K_{n,n}$, so that the permutation $\sigma$ corresponds to the matching consisting of pairs $(j, n + \sigma(j))$. Hence

$$\text{haf} A(0, B) = \text{per} B = \sum_{\sigma \in \Sigma_n} \prod_{k=1}^n b_{k\sigma(k)}.$$ 

Assume that $B$ is positive semidefinite. It is well known that $\text{per} B \geq 0$. This is a corollary of Schur’s theorem [4] that for a positive semidefinite $B$, we have the inequality $\text{per} B \geq \text{det} B$. The latter is nonnegative (being the product of the eigenvalues of $B$); see also [5]. Moreover, $\text{per} B = 0$ if and only if $B$ has a zero row [6, Theorem 3]. Theorem 1.1 yields that $\text{per} L \geq \text{per} B$ if $L \geq B \succeq 0$. This inequality may be known, but we did not find it in the literature.

**Remark 1.2:** Note that the problem of computing the sign of the permanent is in general hard [7]. Hence a similar result holds for the hafnian.

### 2. Proof of the main theorem

Let $Q = (q_{st})$ be an $m \times n$ complex-valued matrix and denote the transpose and the conjugate transpose as $Q^T$ and $Q^*$, respectively. The $r$th induced matrix $P_r(Q)$ is defined as follows [8, p. 20]. Denote by $G_{k,n}$ the totality of nondecreasing sequences of $k$ integers chosen from $[n] = \{1, \ldots, n\}$. Let $\alpha \in G_{k,n}$. Then $\mu(\alpha)$ is defined to be the product of the factorials of the multiplicities of the distinct integers appearing in the sequence $\alpha$. For $\alpha \in G_{k,m}, \beta \in G_{l,n}$, we set $Q[\alpha, \beta] \overset{\text{df}}{=} (q_{\alpha,\beta, s})_{s=1 \ldots k}^{t=1 \ldots l}$ to be the $k \times l$ submatrix of $Q$ with the rows and columns in $\alpha$ and $\beta$, respectively. Now, $P_r(Q)$ is the $\binom{m+r-1}{r} \times \binom{n+r-1}{r}$ matrix whose entries are $\text{per} Q[\alpha, \beta]/\sqrt{\mu(\alpha)\mu(\beta)}$ arranged lexicographically in $\alpha = (\alpha_1, \ldots, \alpha_r) \in G_{m,r}, \beta = (\beta_1, \ldots, \beta_r) \in G_{n,r}$. Recall that $P_r(Q^*) = P_r(Q)^*$ and if $S$ is an $n \times p$ matrix then $P_r(QS) = P_r(Q)P_r(S)$ [8].

Assume that $B$ is an $m \times m$ Hermitian matrix. Then, the spectral decomposition of $B$ is $UDU^*$ where $D$ is a real diagonal matrix. Then

$$P_r(UDU^*) = P_r(U)P_r(D)P_r(U^*) = P_r(U)P_r(D)P_r(U^*) = P_r(U)P_r(D)P_r(U)^*.$$

Clearly, if $D$ is a real diagonal matrix, then $P_r(D)$ is also a diagonal matrix with real entries. Hence $P_r(B)$ is Hermitian. Assume that $B$ is positive semidefinite. Hence $D$ is a nonnegative diagonal matrix. It is straightforward to show that $P_r(D)$ is also a nonnegative diagonal matrix.
matrix. Hence, if $B$ is an $m \times m$ positive semidefinite Hermitian matrix, then $P_r(B)$ is positive semidefinite. Let $H$ be a diagonal matrix of order $(m + r - 1)$ whose diagonal entries are $\sqrt{\mu(\alpha)}$. If $B$ is positive semidefinite, then the matrix $C_r(B) = HP_r(B)H$ is also positive semidefinite. Note that the entries of $C_r(B)$ are per $B[\alpha, \beta]$.

We now consider the hafnian of $A = A(Y, B)$, where $Y$ is complex symmetric and $B$ Hermitian. A perfect matching of $[2n]$ will match some $\alpha \subseteq [n]$ with itself, while a subset $n + \beta, \beta \subseteq [n]$ of $n + [n] = \{n + 1, \ldots, 2n\}$ of equal cardinality is matched to itself, and the remaining members $[n] \setminus \alpha$ of $[n]$ are matched to $n + ([n] \setminus \beta)$. The contribution to haf $A(Y, B)$ of such matchings for a particular $\alpha$ and $\beta$ is

\[
\text{haf}(Y[\alpha, \alpha]) \text{per}(B([n] \setminus \alpha, [n] \setminus \beta)) \overline{\text{haf}(Y[\beta, \beta])},
\]

where we take the hafnian or permanent of an empty matrix to be 1. The total contribution of all of these for a given $k, 0 \leq k \leq \lfloor n/2 \rfloor$, is

\[
\sum_{\alpha:|\alpha|=2k} \sum_{\beta:|\beta|=2k} \text{haf}(Y[\alpha, \alpha]) \text{per}(B([n] \setminus \alpha, [n] \setminus \beta)) \overline{\text{haf}(Y[\beta, \beta])}. \tag{2}
\]

Note that the matrix $F_{n-2k}(B)$ whose entries are per $B[\gamma, \delta]$ for $\gamma, \delta$ all $n-2k$-subsets of $[n]$ is a principal submatrix of $C_{n-2k}(B)$, hence Hermitian, and positive semidefinite if $B \succeq 0$. Hence the sum (2) is real and nonnegative if $B \succeq 0$. This shows that haf $A(Y, B) \geq 0$. Recall [6, Theorem 3] that per $B > 0$ if $B$ has no zero row. Hence haf $A(Y, B) > 0$ if $B$ has no zero row.

Assume now that $L \succeq B \succeq 0$. We claim that $P_r(L) \geq P_r(B) \geq 0$. (The last inequality was established above.) Assume first that det $B > 0$, i.e. $B$ is positive definite. Then $B$ has a unique positive definite square root $R$, and $L \succeq B$ is equivalent to $L_1 \overset{\text{def}}{=} R^{-1}LR^{-1} \succeq \mathbb{I}_n$, where $\mathbb{I}_n$ is the identity matrix of order $n$. Thus we can diagonalize $L_1 = UDU^*$, where $U$ is unitary and $D$ is diagonal with diagonal entries and the eigenvalues of $L_1$ are all $\geq 1$. Recall that $P_r(\mathbb{I}_n) = \mathbb{I}_{\lfloor n/r \rfloor}$ [8, 2.12.5]. Thus

\[
P_r(L_1) = P_r(UDU^*) = P_r(U)P_r(D)P_r(U)^*,
\]

\[
\mathbb{I}_{\lfloor n/r \rfloor} = P_r(\mathbb{I}_n) = P_r(UU^*) = P_r(U)P_r(U)^*.
\]

As each diagonal entry of $D$ is at least 1 we deduce that $P_r(D) \geq P_r(\mathbb{I}_m) = \mathbb{I}_{\lfloor m/r \rfloor}$. Thus, each eigenvalue of $P_r(L_1)$ is at least 1. Hence $P_r(L_1) \geq \mathbb{I}_{\lfloor n/r \rfloor}$. Observe next

\[
P_r(L_1) = P_r(R^{-1}LR^{-1}) = P_r(R)^{-1}P_r(L)P_r(R)^{-1} \geq \mathbb{I}_{\lfloor n/r \rfloor}.
\]

Use the previous observation to deduce that $P_r(L) \geq P_r(R)P_r(R) = P_r(R^2) = P_r(B)$. This concludes the proof in the case that $B$ is nonsingular. For the general case, we note that haf $A(Y, L + \epsilon \mathbb{I}_n) \geq \text{haf} A(Y, B + \epsilon \mathbb{I}_n)$ for $\epsilon > 0$ and take the limit as $\epsilon \to 0^+$ (the hafnian being a continuous function).

**Disclosure statement**

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Appendix. Gaussian Boson sampling

In this appendix, we discuss the connection of our results to Gaussian Boson Sampling. To keep this section aligned with the notation of the physics literature, we replace the integer $n$ by the integer $M$.

A link between hafnians of certain matrices and covariance matrices of quantum-optical Gaussian states were put forward in [9] and further explored in [3]. Hamilton et al. [9] introduced a Gaussian boson sampler (GBS) as a generalization of the boson sampler [10] where an $M$-mode linear interferometer is fed by a product of $M$ single-mode squeezed states and its output is sampled by an array of $M$ photon number-resolving detectors. It turns out that the probability of detecting exactly one photon in each output detector is proportional to the hafnian of a certain matrix $A$ (for a generalization to all possible multiphoton events see [3]).

The complex covariance matrix describing the input to the interferometer has dimension $2M \times 2M$ and encodes the covariances of the canonical operators $\xi = (a_1, \ldots, a_M, a_1^\dagger, \ldots, a_M^\dagger)$:

$$
\sigma_{ij} = \frac{1}{2} \langle \xi_i \xi_j + \xi_j \xi_i \rangle - \langle \xi_i \rangle \langle \xi_j \rangle .
$$

(A1)

The symbol $\dagger$ denotes Hermitian conjugation and $\langle \cdot \rangle$ denotes the operator expectation value. The physical covariance matrix is Hermitian, positive semidefinite and its symplectic eigenvalues are greater than 1/2 [11]. The authors of [9] did not offer the most general form of $A$ leading to a physical covariance matrix. Instead, they use $A = \left[ \begin{array}{cc} Y & B \\ B^\dagger & Y \end{array} \right]$ for an arbitrary complex $B$ and complex symmetric $Y$; however, the corresponding covariance matrix may be non-physical. The physical relevance of knowing what $A$ can be encoded in the GBS device is related to the question of which weighted undirected graphs can have their hafnians sampled by a GBS device [12]. In [9], the canonical form $A = Y \oplus \bar{Y}$ was used, as this always leads to a physical covariance matrix. However, this comes at the expense of ‘doubling’ the adjacency matrix [12], leading to lower detection probabilities.

We claim that Corollary 3 of [3] holds for complex matrices as well:
Lemma A.1: Let \( R = \begin{bmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{bmatrix} \) be a \( 2M \times 2M \) complex symmetric matrix. Then there exists a Gaussian covariance matrix \( \sigma \) such that

\[
cR = X_{2M} [I_{2M} - (\sigma + \frac{1}{2}\|I_{2M}\|^{-1})], \quad (A2)
\]

where

\[
X_{2M} = \begin{bmatrix} 0 & I_M \\ I_M & 0 \end{bmatrix}
\]

if and only if:

1. \( R_{11} = R_{22} \) and \( R_{12} = R_{21}^\top \).
2. \( R_{12} \) is Hermitian and positive semidefinite.
3. \( c \in (0, 1/\|R\|_2) \)

Proof: Since \( R \) is complex symmetric, we must have that \( R_{11}, R_{22} \) are complex symmetric and \( R_{21} = R_{12}^\top \). Set \( Y = R_{11}, B = R_{12} \) in (1). Let \( F = cX_{2M}R \) for some \( c > 0 \). Then equality (A2) shows that \( X_{2M}R \) is Hermitian. Therefore \( B \) is Hermitian and \( R_{22} = \overline{Y} \). Set \( F = cR \) and use Lemma 2 in [3]. \( \blacksquare \)