NONNEGATIVITY FOR HAFNIANS OF CERTAIN MATRICES

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ABSTRACT. We show that a complex symmetric matrix of the form $A(Y,B) = \begin{bmatrix} Y & B \\ B^\top & \overline{Y} \end{bmatrix}$, 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 $\operatorname{haf} A(Y,L) \geq \operatorname{haf} A(Y,B)$ if $L \succeq B$.

1. INTRODUCTION

Let $A = [a_{ij}]$ be a $2n \times 2n$ symmetric matrix with entries in $\mathbb{C}$. The hafnian 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 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 $A = [a_{ij}] \in \mathrm{S}_{2n}$.

Then the hafnian of A is defined as follows [7]:

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

For various properties of the hafnian see, e. g., [4].

In particular we consider A of the form

$$(1.1) \qquad A(Y,B) = \begin{bmatrix} Y & B \\ B^\top & \overline{Y} \end{bmatrix},$$

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

Theorem 1.1. *Assume that $A(Y,B)$ is of the form* (1.1), *where Y is complex symmetric and B positive semidefinite Hermitian. Then* haf $A(Y,B) \geq$

0. *If B has no zero row then* haf $A(Y, B) > 0$. *Furthermore, if $L \succeq B$ i.e., $L - B$ is positive semidefinite Hermitian then* haf $A(Y, L) \geq$ haf $A(Y, B)$.

The inequality haf $A(Y, B) \geq 0$ for $B \succeq 0$ can be deduced from the physical arguments stated in [6]. 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 σ 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 per $B \geq 0$. This is a corollary of Schur's theorem [11] that for a positive semidefinite B we have the inequality per $B \geq \det B$. The latter is nonnegative (being the product of the eigenvalues of B). See also [3]. Moreover, per $B = 0$ if and only if B has a zero row [10, Theorem 3]. Theorem 1.1 yields that per $L \geq$ per B if $L \succeq B \succeq 0$. 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 [1]. 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 $Q^\top$ and Q^*, respectively. The r-th induced matrix $P_r(Q)$ is defined as follows [9, 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 α. For $\alpha \in G_{k,m}, \beta \in G_{l,n}$ we set $Q[\alpha, \beta] \overset{\text{df}}{=} (q_{\alpha_s \beta_t})_{\substack{s=1\ldots k \\ t=1\ldots l}}$ to be the $k \times l$ submatrix of Q with the rows and columns in α and β, respectively. Now $P_r(Q)$ is the $\binom{m+r-1}{r} \times \binom{n+r-1}{r}$ matrix whose entries are per $Q[\alpha, \beta]/\sqrt{\mu(\alpha)\mu(\beta)}$ arranged lexicographically in $\alpha = (\alpha_1, \ldots, \alpha_r) \in G_{r,m}, \beta = (\beta_1, \ldots, \beta_r) \in G_{r,n}$. Recall that $P_r(Q^*) = P_r(Q)^*$ and if S is an $n \times p$ matrix then $P_r(QS) = P_r(Q)P_r(S)$ [9].

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

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

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. 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 $\binom{m+r-1}{r}$ 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 $n + \beta, \beta \subset [n]$ 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 α and β is

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

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, $0 \le k \le \lfloor n/2 \rfloor$, is

$$(2.1) \qquad \sum_{\alpha:|\alpha|=2k} \sum_{\beta:|\beta|=2k} \mathrm{haf}(Y[\alpha, \alpha]) \, \mathrm{per}(B([n] \setminus \alpha, [n] \setminus \beta)) \, \overline{\mathrm{haf}(Y[\beta, \beta])}.$$

Note that the matrix $F_{n-2k}(B)$ whose entries are per $B[\gamma, \delta]$ for γ, δ 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 (2.1) is real and nonnegative if $B \succeq 0$. This shows that haf $A(Y, B) \ge 0$. Recall [10, Theorem 3] that per $B > 0$ if B has no zero row. Hence haf $A(Y, B) > 0$ if B has now zero row.

Assume now that $L \succeq B \succeq 0$. We claim that $P_r(L) \succeq P_r(B) \succeq 0$. (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 $L_1 \stackrel{\mathrm{df}}{=} R^{-1}LR^{-1} \succeq \mathbb{I}_n$, 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 ≥ 1. Recall that $P_r(\mathbb{I}_n) = \mathbb{I}_{\binom{n+r-1}{r}}$ [9, 2.12.5]. Thus

$$P_r(L_1) = P_r(UDU^*) = P_r(U)P_r(D)P_r(U)^*,$$
$$\mathbb{I}_{\binom{n+r-1}{r}} = P_r(\mathbb{I}_n) = P_r(UU^*) = P_r(U)P_r(U)^*.$$

As each diagonal entry of D is at least 1 we deduce that $P_r(D) \succeq P_r(\mathbb{I}_m) = \mathbb{I}_{\binom{n+r-1}{r}}$. Thus, each eigenvalue of $P_r(L_1)$ is at least 1. Hence $P_r(L_1) \succeq \mathbb{I}_{\binom{n+r-1}{r}}$. Observe next

$$P_r(L_1) = P_r(R^{-1}LR^{-1}) = P_r(R)^{-1}P_r(L)P_r(R)^{-1} \succeq \mathbb{I}_{\binom{n+r-1}{r}}.$$

Use the previous observation to deduce that $P_r(L) \succeq P_r(R)P_r(R) = P_r(R^2) = P_r(B)$. This concludes the proof in the case that B is nonsingular. For the general case, we note that haf $A(Y, L + \epsilon\mathbb{I}_n) \ge$ 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).

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Appendix A. 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 was put forward in [8] and further explored in [6]. Ref. [8] introduced a Gaussian boson sampler (GBS) as a generalization of the boson sampler [2] 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 [6]).

The complex covariance matrix describing the input to the interferometer has dimension $2M \times 2M$ and encodes the covariances of the canonical

operators $\boldsymbol{\xi} = (a_1, \ldots, a_M, a_1^\dagger, \ldots, a_M^\dagger)$:

$$(A.1) \qquad\qquad \sigma_{ij} = \tfrac{1}{2}\langle \xi_i \xi_j + \xi_j \xi_i \rangle - \langle \xi_i \rangle \langle \xi_j \rangle.$$

The symbol $\dagger$ denotes Hermitian conjugation and $\langle . \rangle$ denotes the operator expectation value. The physical covariance matrix is Hermitian, positive semidefinite and its symplectic eigenvalues are greater than $1/2$ [12]. The authors of [8] did not offer the most general form of A leading to a physical covariance matrix. Instead, they use $A = \begin{bmatrix} Y & B \\ B^\top & \overline{Y} \end{bmatrix}$ 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 [5]. In [8] the canonical form $A = Y \oplus \overline{Y}$ was used, as this always leads to a physical covariance matrix. However, this comes at the expense of 'doubling' the adjacency matrix [5], leading to lower detection probabilities.

We claim that Corollary 3 of [6] 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* σ *such that*

$$(A.2) \qquad\qquad cR = X_{2M}[\mathbb{I}_{2M} - (\sigma + \frac{1}{2}\mathbb{I}_{2M})^{-1}],$$

where

$$X_{2M} = \begin{bmatrix} 0 & \mathbb{I}_M \\ \mathbb{I}_M & 0 \end{bmatrix}$$

if and only if:

    (1) $R_{11} = \overline{R}_{22}$ *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 (1.1). Let $F = cX_{2M}R$ for some $c > 0$. Then equality (A.2) shows that $X_{2M}R$ is Hermitian. Therefore B is Hermitian and $R_{22} = \overline{Y}$. Set $F = cR$ and use Lemma 2 in [6]. $\qquad\square$

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