PERMANENTS OF POSITIVE SEMIDEFINITE HERMITIAN MATRICES

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Abstract

In this project, we are interested in approximating permanents of positive semidefinite Hermitian matrices. Specifically, we find conditions on positive semidefinite Hermitian matrices such that we can generalize the algorithm described in Sections 3.6 - 3.7 of [1] to matrices satisfying these conditions.

1 Introduction

1.1 Permanent

Definition 1.1. *Let $A = (a_{ij})$ be an $n \times n$ real or complex matrix. We define the* permanent *of A by*

$$per A = \sum_{\sigma \in S_n} \prod_{i=1}^{n} a_{i\sigma(i)},$$

where the sum is taken over the symmetric group S_n of all permutations $\sigma : \{1, \cdots, n\} \to \{1, \cdots, n\}$.

In our REU project, we consider only positive semidefinite Hermitian matrices. In that case, it can be shown that perA is a real number and, moreover, per A can be approximated. Hermitian means for all i, j, $a_{i,j} = \overline{a_{j,i}}$ and positive semi-definite, means for a hermitian matrix that for all complex vectors Z, $\sum_{1 \leq i,j \leq n} a_{i,j} z_i \overline{z_j} \geq 0$. In general the best known algorithm to compute a Permanent exactly runs in $2^n \cdot n^2$ time, which is why we are interested in approximating the Permanent efficiently. The Permanent of these types of matrices is of use in quantum physics and quantum computations.

1.2 Professor Barvinok's Approximation Algorithm

Given an $n \times n$ Hermitian Positive Semi-Definite Matrix A, we shall consider the polynomial $g(z) = per(I + z(A - I))$, where I is the $n \times n$ identity matrix. Note that

$$g(0) = perI = 1, g(1) = perA \tag{1}$$

Hence the quantity we are interested in approximating is $g(1)$.
Let β be a number such that for all $z \leq \beta$, $g(z) \neq 0$
Now define

$$f(z) = ln(g(z)) \tag{2}$$

(Choose a continuous branch) and let

$$T_m(z) = f(0) + \sum_{k=1}^{m} \frac{f^{(k)}(0)}{k!} z^k \tag{3}$$

be the m^{th} degree taylor polynomial of f centered at 0. Then

$$|f(1) - T_m(1)| \leq \frac{n}{(\beta - 1)\beta^m (m+1)} \tag{4}$$

see Lemma 2.2.1 in [Ba16] or Lemma 7.1 in [Ba17]. Note that the error of this approximation goes down exponentially fast if $\beta \geq 1$ and to achieve an error $\leq \epsilon$ we can choose

$$m = \mathcal{O}(ln\frac{n}{\epsilon}) \tag{5}$$

with m from equation 3. Computing

$$f(0), f^{(1)}(0), \cdots, f^{(m)}(0) \tag{6}$$

reduces to computing

$$g(0), g^{(1)}(0), \cdots, g^{(m)}(0) \tag{7}$$

reference in Section 2.2.2 of [Ba16] or section 7.1 of [Ba17]. Recall $G(0) = 1$ and denoting $\delta_{i,j} = 1$ if $i = j$ and 0 else.
Now for $k > 0$ we get

$$g^{(k)}(0) = \frac{d^k}{dz^k} \sum_{\sigma \in S_n} \prod_{i=1}^{n} (\delta_{i\sigma(i)} + z(a_{i\sigma(i)} - \delta_{i\sigma(i)})|_{z=0} \tag{8}$$

$$= \sum_{i_1, \cdots i_k} \sum_{\sigma \in S_n s.t. \sigma(i) = i for i \neq i_1, \cdots, i_k} (a_{i_1\sigma(i_1)} - \delta_{i_1\sigma(i_1)}) \cdots (a_{i_k\sigma(i_k)} - \delta_{i_k\sigma(i_k)}) \tag{9}$$

Another way to calculate these are if we let $B = A - I$ and then for any subset $I \subset (1, \cdots, n)$ and let B_I denote the principal sub matrix determined by I such that $b_{i,j}$ has $i, j \in I$. Now we can write

$$g^{(k)}(0) = k! \sum_{I \subset (1, \cdots, n): |I| = k} per(B_I) \tag{10}$$

Rysers method runs in $n^2 \cdot 2^n$ and computing $g^{(k)}(0)$ by (10) gives us $\binom{n}{k} k^2 2^k$ complexity. This gives us a quasi-polynomial complexity algorithm for approximating per A if we use $k \sim \mathcal{O}(\ln n)$. If we indeed have that all the roots of $g(z)$ are outside the unit disc, we obtain an efficient (though more complicated) algorithm for approximating per A.

1.3 Approach to $g(z)$ (suggested by Prof. Barvinok)

Instead of considering $g(z)$, we consider another related polynomial

$$h(z) = h_A(z) = per(I + zA), \tag{11}$$

which satisfies

$$g(z) = (1 - z)^n h(\frac{z}{1 - z}) \tag{12}$$

and

$$g(\frac{z}{1 + z}) = \frac{1}{(1 - z)^n} h(z). \tag{13}$$

It can be shown that the map $z \to \frac{z}{1+z}$ takes $B((0,0), r) \to B((-\frac{r^2}{1-r^2}, 0), \frac{r}{1-r^2})$ for $r \leq 1$, so determining where h is zero free can imply where g is zero free. For example, if we can show that $h(z)$ is zero free inside $|z| = 0.5$, then we know that $g(z)$ is zero free inside $|z| = \frac{1}{3}$. Therefore, we are trying to find a lower bound on the magnitude of the roots of $h(z)$.
Looking back to $h(z)$, we can write

$$h(z) = \sum_{k=0}^{n} h_k z^k, \tag{14}$$

where $h_0 = 1$ and $h_k = h_k(A)$ is the sum of all $k \times k$ principal subpermanents of A (there are $\binom{n}{k}$ of them):

$$h_k(A) = \sum_{\substack{I \subset 1, \cdots n \\ |I| = k}} per A_I, \tag{15}$$

where A_I is the $k \times k$ submatrix of A consisting of the entries in the rows and columns indexed by $i \in I$. Since A_I are positive semidefinite Hermitian, we conclude that $h_k(A)$ are non-negative real. We see that compared to $g(z)$, the

coefficients of $h(z)$ have a nice interpretation.
Prof. Barvinok introduces a nice integral representation in Section 3.1.4 of [2]. We follow his representation here: given an $n \times n$ positive definite Hermitian matrix $A = (a_{ij})$, we can find linear functions $f_1, \cdots, f_n : \mathsf{C}^n \to \mathsf{C}$ such that

$$a_{ij} = \int_{\mathsf{C}^n} f_i \bar{f}_j \, d\mu_n, \tag{16}$$

where μ_n is the standard Gaussian measure in C^n with density

$$\frac{1}{\pi^n} e^{-\|z\|^2} \text{ where } \|z\|^2 = |z_1|^2 + \cdots + |z_n|^2 \text{ for } z = (z_1, \cdots, z_n).$$

The measure is normalized in such a way that

$$\mathbf{E}\|z_i\|^2 = 1 \text{ for } i = 1, \cdots, n \text{ and } \mathbf{E} z_i \bar{z_j} = 0 \text{ for } i \neq j.$$

We can pick linear functions $f_1, \cdots, f_j$ in such a way: given A positive definite Hermitian and rank n, we can write $A = BB^*$ for some matrix $n \times n$ matrix B. Therefore, we have that $a_{ij} = \sum_{k=1}^{n} b_{ik} \bar{b_{jk}}$, then we can pick $f_j = \sum_{k=1}^{n} b_{jk} z_k$. If we use this integral representation, we have nice representations for both the per A and $h_k(A)$:

$$per A = \int_{\mathsf{C}^n} |f_1|^2 \cdots |f_n|^2 \, d\mu_n \tag{17}$$

$$h_k(A) = \int_{\mathsf{C}^n} e_k(|f_1|^2, \cdots, |f_n|^2) \, d\mu_n, \tag{18}$$

where

$$e_k(x_1, \cdots, x_n) = \sum_{1 \le i_1 < \cdots < i_k \le n} x_{i_1} \ldots x_{i_k}$$

is the k-th elementary symmetric polynomial in $x_1, \cdots, x_n$.
Note that e_k is a homogeneous polynomial of degree k, the integral (18) can be reduced to

$$h_k(A) = \frac{(k+n-1)!}{(n-1)!} \int_{\mathsf{S}^{2n-1}} e_k(|f_1|^2, \cdots, |f_n|^2) \, d\nu, \tag{19}$$

where S^{2n-1} is the unit sphere in R^{2n} and ν is the rotationally invariant probability (Haar) measure on S^{2n-1}.

2 Theoretical Results

2.1 2 by 2 Case

Proposition 2.1. *Given an 2×2 Hermitian positive semidefinite matrix A such that the Frobenius norm of A is less that $\sqrt{2}$, then all the roots of $G(z)$ are outside unit disc.*

Proof. For the proof of this proposition, we can directly work with g_z.

We write $A = \begin{bmatrix} \gamma & \alpha - \beta i \\ \alpha + \beta i & \delta \end{bmatrix}$, with $\alpha, \beta, \gamma, \delta$ real numbers. By Sylvester criterion and the restriction on the Frobenius norm, we have that

$$
\begin{aligned}
2\alpha^2 + 2\beta^2 + \gamma^2 + \delta^2 &< 2 &\quad (20)\\
\gamma &> 0 &\quad (21)\\
\gamma\delta - \alpha^2 - \beta^2 &> 0 &\quad (22)
\end{aligned}
$$

From (21) and (22), we can easily see that $\delta > 0$. Now we calculate $g(z)$. We have that

$$
\begin{aligned}
g(z) &= (\gamma z - z + 1)(\delta z - z + 1) + (\alpha z + \beta i z)(\alpha z - \beta i z) \\
&= [(\gamma - 1)(\delta - 1) + \alpha^2 + \beta^2]z^2 + (\gamma + \delta - 2)z + 1. \quad (23)
\end{aligned}
$$

Let λ_1, λ_2 be two roots of $g(z)$ (counting multiplicities), then we have

$$\lambda_1 \lambda_2 = \frac{1}{(\gamma - 1)(\delta - 1) + \alpha^2 + \beta^2} \quad (24)$$

We want $|\lambda_1| > 1$, $|\lambda_2| > 1$. Since $\lambda_1 = \bar{\lambda_2}$, we have $|\lambda_1| = |\lambda_2|$, so it is equivalent to

$$|\lambda_1 \lambda_2| > 1,$$

i.e.,

$$\alpha^2 + \beta^2 + (\gamma - 1)(\delta - 1) < 1$$

equivalently,

$$\gamma\delta + \alpha^2 + \beta^2 < \gamma + \delta \quad (25)$$

By (20), we have that $2\gamma\delta < 2$, which implies $\gamma\delta < 1$. So,

$$
\begin{aligned}
\gamma\delta + \alpha^2 + \beta^2 &< 2\gamma\delta \\
&< 2\sqrt{\gamma\delta} \\
&\leq \gamma + \delta
\end{aligned}
$$

□

From this proposition, we can see that $\sqrt{2}$ is the sharp bound on the Frobenius norm.

2.2 Rank 1 Case

Proposition 2.2. *Given an $n \times n$ rank 1 positive semidefinite Hermitian matrix, A, such that the Trace of $A \leq 1$ then all the roots of $h(z)$ are outside the unit disc.*

Proof. Given these properties of A, we can write $A = BB^*$ for a complex vector B. From (16) we know we can find linear functions $f_1, \cdots, f_n : \mathsf{C}^n \to \mathsf{C}$ such that $a_{ij} = \int_{\mathsf{C}^n} f_i \bar{f}_j \, d\mu_n$. However since A is rank 1, we can do better and find linear functions from $\mathsf{C} \to \mathsf{C}$ with the same properties except now we integrate over C. One can check that the functions

$$f_i = B_i \cdot z, \ \forall i \tag{26}$$

satisfy the desired property. Now if we consider the Eneström - Kakeya Theorem, see Chapter 8 of [4], which states that the roots of a complex polynomial $P = \sum_{i=0}^{n} a_i * z^i$ lie outside the disc $z = \alpha$ where $\alpha = max(\frac{a_{i+1}}{a_i})$, we will be interested in the ratios of $(\frac{a_{i+1}}{a_i})$. Recalling formula (19) we can rewrite this ratio as

$$\frac{\frac{(k+n)!}{(n-1)!} \int_{\mathsf{S}^{2n-1}} e_{k+1}(|f_1|^2, \cdots, |f_n|^2) \, d\nu}{\frac{(k+n-1)!}{(n-1)!} \int_{\mathsf{S}^{2n-1}} e_k(|f_1|^2, \cdots, |f_n|^2) \, d\nu} \tag{27}$$

$$= \frac{(k+n) \int_{\mathsf{S}^{2n-1}} e_{k+1}(|f_1|^2, \cdots, |f_n|^2) \, d\nu}{\int_{\mathsf{S}^{2n-1}} e_k(|f_1|^2, \cdots, |f_n|^2) \, d\nu} \tag{28}$$

Now using the below inequality and monotonicity of the integral we get $e_{k+1}(x_1, \cdots, x_n) \leq \frac{x_1 + \cdots + x_n}{k+1} e_k(x_1, \cdots, x_n)$

$$\leq \frac{sup\{|f_1|^2 + \cdots + |f_n|^2\}(k+n)}{(k+1)} \tag{29}$$

So if we have

$$sup\{|f_1|^2 + \cdots + |f_n|^2\} \leq \frac{c}{n} \tag{30}$$

for some c we get that h is zero free outside the disc of radius c. Now in the rank 1 case, since we are integrating over C rather than C^n, $n = 1$ so we need $sup\{|f_1|^2 + \cdots + |f_n|^2\} \leq c$ over the unit disc.

$$\sum_{i=1}^{n} |f_i|^2 = \sum_{i=1}^{n} |B_i \cdot z|^2 = \sum_{i=1}^{n} |B_i|^2 = Trace(A) \tag{31}$$

where the 3rd inequality comes from the fact we are integrating over the disc. Hence, if $Trace(A) \leq c$ we get h is zero free in the disc $|z| = c$ □

Proposition 2.3. *If we are given a rank 1, positive semidefinite Hermitian matrix, A, such that $Trace(A) < r$ for some $r < 1$ then $g(z)$ is zero free in the ball $B((-\frac{r^2}{1-r^2}, 0), \frac{r}{1-r^2})$*

Proof. This is an immediate consequence of Proposition 2.2 and the previously mentioned fact that the map $z \to \frac{z}{1+z}$ takes $B((0,0), r) \to B((-\frac{r^2}{1-r^2}, 0), \frac{r}{1-r^2})$ for $r \leq 1$ □

2.3 General Case

Proposition 2.4. *Given an $n \times n$ Hermitian positive semidefinite matrix such that $Trace(A) \leq \frac{1}{4}$ then all the roots of $G(z)$ are inside the ball $B((\frac{4}{3}, 0), \frac{2}{3})$, which implies that $G(z)$ is zero free inside $|z| = \frac{2}{3}$.*

2.3.1 Set Up

Let $L(z) = per(Iz + A)$ and note that this is a polynomial in terms of z. Hence,

$$L(z) = \sum_{k=0}^{n} L_k * z^k \tag{32}$$

One can see that L_k is the sum of all $(n-k) \times (n-k)$ principal sub permanents. Using the fact that $Per(cA) = c^n Per(A)$ where n is the dimmension of A we can rewrite

$$G(\frac{1}{1+z}) = (\frac{1}{z+1})^n \cdot L(z) \tag{33}$$

The fujiwara theorem [3] says all the roots of a polynomial, $P(z) = \sum_{k=0}^{n} a_k \cdot z^k$ lie inside the disc of radius $2 \cdot max\{\frac{a_{n\ 1}}{a_n}, (\frac{a_{n\ 2}}{a_n})^{\frac{1}{2}}, (\frac{a_{n\ 3}}{a_n})^{\frac{1}{3}}, ..., (\frac{a_0}{2 \cdot a_n})^{\frac{1}{n}}\}$. Now since we are working with L, $a_n = L_n =$ the constant term in $L(z)$ which is 1. This simplifies this formula to $2 * max\{a_{n-1}, (a_{n-2})^{\frac{1}{2}}, (a_{n-3})^{\frac{1}{3}}, \cdots, \frac{a_0}{2}^{\frac{1}{n}}\}$, where a_i is the sum of all (n-i)x(n-i) subpermanents.

2.4 Maximum Value of Coefficients

To find the maximum value of the subpermanents we may consider only real valued matrices, since if given a matrix with complex numbers, we can just take the norms of all of the entries and the permanent will increase. Next, since the matrix is positive semi definite we know that

$$|a_{i,j}| \leq \sqrt{a_{i,i} \cdot a_{j,j}} \tag{34}$$

Since we are maximizing and all the values are positive, increasing the values just increases the permanent, so let the above inequality be an equality.

Now consider one $k \times k$ principal submatrix, call this B.

$$Per(b) = \sum_{\sigma \in S_k} \prod_{i=1}^{k} b_{i,\sigma(i)} \tag{35}$$

now plug in $b_{i,j} = \sqrt{b_{i,i} \cdot b_{j,j}}$ and we get

$$= \sum_{\sigma \in S_k} \prod_{i=1}^{k} \sqrt{b_{i,i} \cdot b_{\sigma(i),\sigma(i)}} = \sum_{\sigma \in S_k} \sqrt{\prod_{i=1}^{k} b_{i,i} \cdot b_{\sigma(i),\sigma(i)}} \tag{36}$$

Now since it's a permutation map every $b_{i,i}$ appears exactly twice in the product, so this is equal to

$$\sum_{\sigma\in S_k}\prod_{i=1}^{k} b_{i,i} = k!\prod_{i=1}^{k} b_{i,i}. \tag{37}$$

Now we sum this up for all possible principal submatrices. This yields the sum of all subpermanents is $e_k(a_{1,1},...,a_{n,n})$, now we want to maximize this subject to $Tr(A)\leq .25$ to find an upper bound.
Using the Lagrange multiplier method we get

$$\nabla e_k(a_{1,1},...,a_{n,n}) = \lambda\cdot\nabla(\sum_{i=1}^{n} a_{i,i} - .25)\&\sum_{i=1}^{n} a_{i,i} = .25 \tag{38}$$

so setting the partials equal for all i, we get:

$$e_{k-1}(a_{1,1},..,\overline{a_{i,i}},...,a_{n,n}) = \lambda,\ \forall i \tag{39}$$

Where the bar in the e_k means that term is missing. This implies for all i,j

$$e_{k-1}(a_{1,1},..,\overline{a_{i,i}},...,a_{n,n}) = e_{k-1}(a_{1,1},..,\overline{a_{j,j}},...,a_{n,n}) \tag{40}$$

.
The L.H.S. of this is the same as the R.H.S. except anything on the L.H.S. that has a j is replaced with an i on the R.H.S.. Now when we set these equal, cancel all terms on both sides that have neither an i or j. We will be left with

$$c\cdot a_{i,i} = c\cdot a_{j,j} \tag{41}$$

where the c is some products of the diagonal elements. If all diagonal elements are non zero, we get c is nonzero and hence $a_{i,i} = a_{j,j}$.

If we do get c equal to zero, there is an α such that $a_{\alpha,\alpha} = 0$.
Since our constrained optimization problem is symmetric with respect to the variables, assume it is $a_{n,n}$ and now we want to maximize $e_k(a_{1,1},...,a_{n-1,n-1})$ subject to $\sum_{i=1}^{n-1} a_{i,i} = 1$.
Repeat this argument until we get all nonzero terms(note once we get to just one variable, it has to be .25 since the trace is .25).

So we get our solution must be of the form

$$a_{1,1} = a_{2,2} = ... = a_{m,m} = \frac{.25}{m}\&a_{m+1,m+1} = a_{m+2,m+2} = ... = a_{n,n} = 0 \tag{42}$$

This is optimized for $m = n$ since if $k > m$ then the sum of all k sub permanent is zero while its always nonzero for $m = n$, now if $k < m < n$, the value of e_k is $\binom{m}{k} \cdot (\frac{1}{m})^k$.
and writing

$$\binom{m}{k} \cdot (\frac{.25}{m})^k \overset{?}{\leq} \binom{n}{k} \cdot (\frac{.25}{n})^k \tag{43}$$

$$\iff \frac{m!}{(m-k)! \cdot k! m^k} \overset{?}{\leq} \frac{n!}{(n-k)! \cdot k! n^k} \tag{44}$$

$$\iff \frac{m}{m} \cdot \frac{m}{m-1} \cdots \frac{m}{m-k+1} \overset{?}{\leq} \frac{n}{n} \cdot \frac{n}{n-1} \cdots \frac{n}{-k+1} \tag{45}$$

And term by term the R.H.S. is bigger, so it is maximized with $m = n$.
So now we see the max value of these subpermanents is when the matrix has all its entries $= \frac{1}{n}$. The sum of all kxk subpermanents of this matrix is $\binom{n}{k}$ times the value of each subpermanent which is $k! \cdot (\frac{.25}{n})^k$ which becomes $\frac{n!}{(n-k)! n^k 4^k}$ and this is less than $(\frac{1}{4})^k$ for all k from 1 to n

2.4.1 Actual Bound

Plugging back into the Fujiwara bound, we see that all the roots of $L(z)$ are in a disc of radius $\frac{1}{2}$. Now recalling that

$$G(\frac{1}{1+z}) = (\frac{1}{z+1})^n \cdot L(z) \tag{46}$$

So if L is zero free in the disc of radius $\frac{1}{2}$, since the map $\frac{1}{1+z}$ is conformal it sends the circle $|z| = \frac{1}{2}$ to $B((\frac{4}{3}, 0), \frac{2}{3})$. So all the zero's of G must be inside this ball.

3 Empirical Results

The following are plots for the roots of $G(z)$ for random P.S.D. Hermitian Matrices where $Tr(A) = n^\alpha$
Dimension = 7: