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Numerical methods of calculating projection to positive eigenspace[*1]

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Abstract

Recently, Sakashita and Nagaoka presented their research on numerical simulation of asymptotic methods in quantum statistics. Their method heavily depends on accurate calculation of all the eigenvalues and eigenvectors of a huge Hermitian matrix. However, only a projection operator to the eigenspace corresponding to positive eigenvalues is necessary. We propose two different numerical methods, both of which avoid numerical diagonalization.

1 Basic Motivation

Recently, Sakashita and Nagaoka [9] has worked for numerical simulation of asymptotic methods in quantum statistics. Their method heavily depends on accurate calculation of all the eigenvalues and eigenvectors of

$$\{\rho_1^{\otimes n} - k\rho_2^{\otimes n} > 0\}, \tag{1}$$

where n is sufficiently large integer, k is a real constant, and ρ_1 and ρ_2 are density matrices in the two-dimensional Hilbert space. The notation $\{X > 0\}$ for a given Hermitian matrix X is defined by

$$\{X > 0\} := \sum_{a:\ \lambda_a \in \sigma(X),\ \lambda_a > 0} E_a,$$

where $\sigma(X)$ denotes the set of eigenvalues (spectrum) of X and E_a is a projection operator corresponding to the eigenvalue λ_a. Other projection operators, $\{X < 0\}, \{X =$

[*1] This research is a joint work with Dr. Sakashita.

0} are also defined in the same manner.

The above projection operator (1) is indeed the quantum Neyman-Pearson test [4] for $\rho_1^{\otimes n}$ vs $\rho_2^{\otimes n}$ (k is determined according to the significance level.). Asymptotic behavior of some quantities derived from (1) has theoretical importance [6, 3, 5]. However, our proposed methods are very general and the author believes that they are important apart from quantum statistical significance.

Efficient computation of all the eigenvalues and eigenvectors of a huge but structured Hermitian matrix X is the essence of the previous result [9]. However, a general-purpose method (diagonalization of a matrix) was applied to numerical computation of the projection operator $\{X > 0\}$ while not eigenvalues themselves but their signs are necessary. Thus, a basic question arises: *Is there any other numerical method comparable to the previous approach?* Since the workshop, some discussions with Sakashita have continued and finally we obtain two numerical methods of calculating $\{X > 0\}$. Both methods avoid the numerical diagonalization of a Hermitian matrix to compute the projection operator.

2 Problem Setting

Suppose that a Hermitian matrix X in a d-dimensional complex vector space is given. (d is assumed to be very large, say, $d = 10^6$.) Our purpose here is to propose a numerical method of computing projection operators *without* numerical diagonalization.

$$\{X > 0\}, \{X < 0\}, \{X = 0\}.$$

We obtain two methods in the present article.

(i) Monte Carlo Optimization

(ii) Topological Method

Monte Carlo Optimization is one of the most common optimization methods (See, e.g., Robert and Casella [8]). Topological Method uses the stability of some points in a discrete-time dynamical system (See, e.g., Guckenheimer and Holmes [1] for dynamical systems). The latter method is developed by the author in order to deal with our problem.

3 Monte Carlo Optimization

The first method applies the well-known optimization technique to our specific problem. The basic idea is very simple. We construct the objective function so that its maximizer is the desired projection $\{X > 0\}$. Our method uses some results in classical and quantum hypothesis testing for simple hypotheses (See, e.g., Hayashi [2] for basic notations and terminology).

Definition 1. Let $\mathbf{M} := \{M_x\}_{x\in\mathcal{X}}$ denote a finite-valued POVM ($|\mathcal{X}| < \infty$). The set of test with $\mathbf{M}$ is defined by

$$\mathcal{P}_{\mathbf{M}} := \{T = \sum_x \phi(x) M_x : \ 0 \le \phi(x) \le 1, \ \forall x \in \mathcal{X}\}$$

and the whole set of test is defined by

$$\mathcal{P}_{full} := \{T : \ 0 \le T \le I\}.$$

(By definition $\mathcal{P}_{\mathbf{M}} \subset \mathcal{P}_{full}$.)

It is easy to see that both $\mathcal{P}_{\mathbf{M}}$ and $\mathcal{P}_{full}$ are closed (compact) and convex. We give a slightly general form of our algorithm.

Algorithm

First we pick a standard PVM,

$$\mathbf{E} := \{E_1 = |1\rangle\langle 1|, \ldots, E_d = |d\rangle\langle d|\},$$

where $|1\rangle, \ldots, |d\rangle$ are orthonormal basis. We set an initial value $M^{(0)} \in \mathcal{P}_{\mathbf{E}}$ (e.g., the identity I). Then update M as follows.

1. Generate a d-dimensional unitary matrix

$$U \sim \mu(U),$$

where $\mu(U)$ is a probability distribution of unitary matrices (e.g., Haar measure).

2. Calculate M_{prop}.

$$Ind := \{j : \mathrm{Tr} X U E_j U^* > 0\},$$
$$M_{prop} := \sum_{j \in Ind} U E_j U^*.$$

3. If $\mathrm{Tr} X M_{prop} > \mathrm{Tr} X M^{(n)}$, then update $M^{(n+1)} = M_{prop}$. Otherwise $M^{(n+1)} = M^{(n)}$.

For general algorithm, we can select the candidate distribution $\mu(U)$ to be independent of the current $M^{(n)}$. Practically speaking, it is inefficient and it would be faster to generate U according to the current $M^{(n)}$ if we assume some conditions on X.

It is easily seen that $\sup\{\mathrm{Tr} TX : T \in \mathcal{P}\}$ is achieved when the subset $\mathcal{P} \subseteq \mathcal{P}_{full}$ is compact. In order to understand the above algorithm, we need three lemmas (those are easy to prove, thus, proofs are omitted.).

Lemma 1. Let X be a Hermitian matrix and $\mathbf{M} = \{M_x\}_{x \in \mathcal{X}}$ be a POVM. Then

$$\tilde{M} := \sum_{x : \mathrm{Tr} X M_x > 0} M_x$$

achieves the following maximum.

$$\max\{\mathrm{Tr} TX : T \in \mathcal{P}_{\mathbf{M}}\}.$$

The above result is another form of the result in classical Bayesian hypothesis testing (See, e.g., Chap.5 in Robert [7] for Bayesian testing).

Now we define

$$\mathbf{E}_U := \{UE_1U^*, \ldots, UE_dU^*\},$$
$$\tilde{E}_U := \arg\max\{\mathrm{Tr}TX : T \in \mathcal{P}_{\mathbf{E}_U}\}$$

for every unitary matrix $U \in \mathcal{U}$. In particular, the following holds.

Lemma 2. For a standard PVM $\mathbf{E}$ fixed,

$$\mathcal{P}_{full} = \overline{\mathrm{co}\{\mathcal{P}_{\mathbf{E}_U} : U \in \mathcal{U}\}},$$

where $\overline{\mathrm{co}\{A\}}$ denotes the closed convex hull of a subset $A \subset \mathcal{P}_{full}$ and $\mathcal{U}$ denotes the whole set of unitary matrices.

For a pair of subsets satisfying $\mathcal{P}_1 \subseteq \mathcal{P}_2$,

$$\max\{\mathrm{Tr}TX : T \in \mathcal{P}_1\} \leq \max\{\mathrm{Tr}TX : T \in \mathcal{P}_2\}$$

holds. Using this monotonicity and the above Lemma 1 and Lemma 2, we easily obtain the following lemma, which is essential to our algorithm.

Lemma 3. For a standard PVM $\mathbf{E}$ fixed, the following holds.

$$\begin{aligned}\{X > 0\} &= \max\{\mathrm{Tr}TX : T \in \mathcal{P}_{full}\} \\ &= \max\{\max\{\mathrm{Tr}TX : T \in \mathcal{P}_{\mathbf{E}_U}\} : U \in \mathcal{U}\} \\ &= \max\{\mathrm{Tr}\tilde{E}_U X : U \in \mathcal{U}\}\end{aligned}$$

Clearly the last equality in Lemma 3 assures the validity of our algorithm. For a sufficiently large n, $M^{(n)} \approx \{X > 0\}$. The projection to negative eigenspace $\{X < 0\}$ is also obtained in the same manner.

4 Topological Method

First we deal with exceptional cases where $\mathrm{rank}X = 1$. In numerical calculation we do not have this information on X. (Again, we emphasize that X is a huge matrix.) Without diagonalization and knowing eigenvalues, we can decide whether $\mathrm{rank}X$ is equal to one or not by calculating $\mathrm{Tr}X^2$ and $(\mathrm{Tr}X)^2$. When X is a Hermitian matrix, $\mathrm{Tr}X^2 \geq (\mathrm{Tr}X)^2$ holds. In particular, $\mathrm{rank}X = 1$ if and only if $\mathrm{Tr}X^2 = (\mathrm{Tr}X)^2$ and $X \neq 0$.

If we know $\mathrm{rank}X = 1$, then dividing X by the scalar $\mathrm{Tr}X$ yields

$$\{X > 0\} = \begin{cases} \frac{1}{\mathrm{Tr}X}X, & X > 0, \\ 0, & X < 0, \end{cases}$$

$$\{X < 0\} = \begin{cases} 0, & X > 0, \\ \frac{1}{\mathrm{Tr}X}X, & X < 0, \end{cases}$$

$$\{X = 0\} = I - \{X > 0\} - \{X < 0\}.$$

Now we assume that $\mathrm{rank}X \geq 2$ and present our main result. In this case, we may consider the maximum of the absolute eigenvalue is smaller than one for simplicity. Indeed $\|X\|_2 := \sqrt{\mathrm{Tr}X^2} > \|X\|_\infty$ when $\mathrm{rank}X \geq 2$ and if we take $Y := X/\|X\|_2$ then $\{Y > 0\} = \{X > 0\}$ holds.

Our main result is due to the following elementary result in a discrete-time dynamical system.

Lemma 4. There exist two positive constants $b > 0$ and $c > 0$ and a third order polynomial $h(x)$ satisfying the following. For the initial value $x_0 \in (-c, c)$, we recursively define

$$x_{n+1} := h(x_n), \ n = 0, 1, 2, \ldots,$$

and the sequence converges to three values depending on the initial value, i.e.,

$$\lim_{n\to\infty} x_n = \begin{cases} b, & 0 < x_0 < c \\ 0, & x_0 = 0, \\ -b, & -c < x_0 < 0 \end{cases} \tag{2}$$

One example is $b = c = \sqrt{3}/2$ and $h(x) = -x^3 + 7/4x$ (c could be larger). Fig. 1 shows the graph of x_1, x_3, x_5, x_{10} as a function of the initial value x_0. We see that x_{10} is nearly a step function taking three values $-\sqrt{3}/2, 0, \sqrt{3}/2$ according to the initial value x_0. It implies that 10 times repetition of the calculation of $h(x)$ is enough except when x_0 is very close to 0.0.

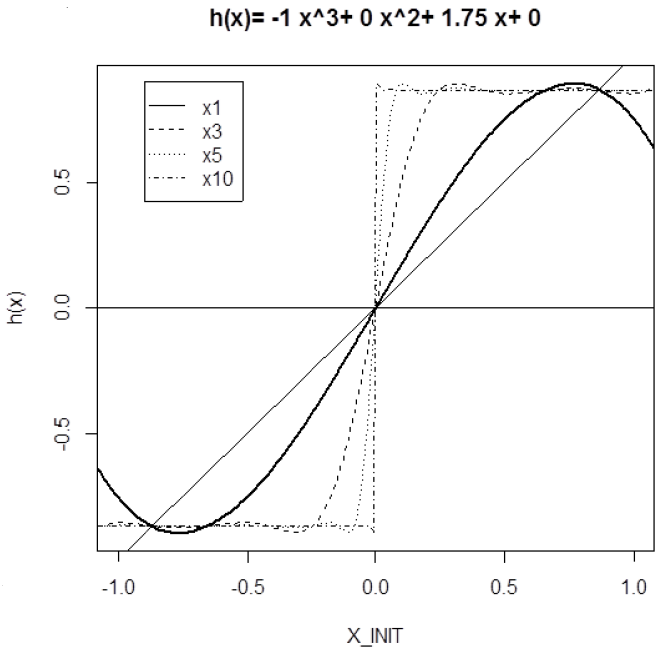

Fig. 1: Example of $h(x) = -x^3 + 7/4x$.

Remark 1. The smallest degree of a polynomial satisfying the condition (2) is three.

4.1 Our Algorithm

When the maximum absolute eigenvalue of Y is smaller than one, the following formula is used.

$$\lim_{n\to\infty}(I-Y^2)^n = \{Y=0\}.$$

Thus, the projection to the nonzero eigenspace,

$$\{Y\neq 0\} = \{Y>0\}+\{Y<0\} = I-\{Y=0\}$$

is easily obtained by numerical computation. If we can compute $\{Y>0\}-\{Y<0\}$ as above, then we obtain a numerical method of computing $\{Y>0\}$.

If we do not impose any condition, then we could use the following analytical formula, generally intractable in numerical computation. Take a sequence of real-valued analytical functions $\{f_n\}$ satisfying

$$\lim_{n\to\infty} f_n(x) = \begin{cases} 1, & x>0, \\ 0, & x=0, \\ -1, & x<0. \end{cases}$$

Then, for a Hermitian matrix Y we obtain

$$\lim_{n\to\infty} f_n(Y) = \{Y>0\}-\{Y<0\}.$$

$f_n(x)=\tanh(nx)$ is a typical example. There are too many candidates other than this function. However, for example, numerical computation of $\tanh(nY)$ is troublesome. The matrix function e^{nY} is intractable as $n\to\infty$ in numerical computation. Even if we use the Taylor expansion of $\tanh(x)$, the higher order is more essential as $n\to\infty$.

Thus, we impose some conditions on our numerical method.

(i) Not solving any eigenvalue problem or linear equation

(ii) Not using numerically unstable calculations such as matrix inverse or matrix determinant

Under these conditions, we find a simple method due to the last lemma.

Theorem 1. We fix a Hermitian matrix Y with maximum absolute eigenvalue smaller than one. We take positive constants $b > 0, c > 0$ and $h(x)$ satisfying the condition (2). Let us define $Z_0 := Y/c$ and $Z_{n+1} := h(Z_n),\ n = 0, 1, 2, \ldots$ recursively. Then,

$$\frac{1}{b} \lim_{n\to\infty} Z_n = \{Y > 0\} - \{Y < 0\}$$

holds.

Its proof is also elementary due to Lemma 4.

The main point here is that we derive a recursive way of obtaining $\{Y > 0\} - \{Y < 0\}$ by using only matrix multiplication and summation. As an illustrative example, we give an explicit form.

$$\begin{aligned}
Z_0 &= \frac{2}{\sqrt{3}} Y, \\
Z_1 &= h(Z_0) = -(Z_0)^3 + 7/4 Z_0, \\
Z_2 &= h(Z_1) = -\{-(Z_0)^3 + 7/4 Z_0\}^3 + 7/4\{-(Z_0)^3 + 7/4 Z_0\}, \ldots
\end{aligned}$$

For a sufficiently large n, we obtain $\frac{\sqrt{3}}{2} Z_n \approx \{Y > 0\} - \{Y < 0\}$.

5 Concluding Remarks

In the present article, we proposed two numerical methods to compute $\{X > 0\}$ without numerical diagonalization. We showed the result of the numerical experiment of the latter method for real scalar values. In addition, we tried to perform numerical computation of the latter one for 2×2 matrices, which will be reported later. It was surprisingly easy to implement and converges well. Numerical experiment for huge matrices, which was the original motivation, and detailed comparison with the previous result from the viewpoint of efficiency, robustness to numerical errors are left for future study.

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