Nonpositive-transpose entanglement and bound entanglement: From distillability sets to inequalities and multivariable insights

Si-Yuan Qi,[1,2] Geni Gupur,[3,*] Yu-Chun Wu,[1,2,4,†] and Guo-Ping Guo[1,2,4,5]

[1]CAS Key Laboratory of Quantum Information, University of Science and Technology of China, Hefei, Anhui 230026, People's Republic of China

[2]CAS Center for Excellence in Quantum Information and Quantum Physics, University of Science and Technology of China, Hefei, Anhui 230026, People's Republic of China

[3]College of Mathematics and Systems Science, Xinjiang University, Urumqi, Xinjiang 830017, People's Republic of China

[4]Institute of Artificial Intelligence, Hefei Comprehensive National Science Center, Hefei, Anhui 230088, People's Republic of China

[5]Origin Quantum Computing Hefei, Anhui 230026, People's Republic of China

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Equivalence between positive partial transpose (PPT) entanglement and bound entanglement is a long-standing open problem in quantum information theory. Limited progress has been made so far, even on the seemingly simple case of the bound entanglement of Werner states. The primary challenge is to give a concise mathematical representation of undistillability. To this end, we propose a decomposition of the N-undistillability verification into $\log(N)$ repeated steps of 1-undistillability verification. For Werner states' N-undistillability verification, a parameter interval for N-undistillability is given, which is independent of the dimensionality of Werner states. Equivalent forms of inequalities for both rank 1 and 2 matrices are presented, before transforming the 2-undistillability case into a matrix analysis problem. A new perspective is also attempted by seeing it as a nonconvex multivariable function, proving its critical points and conjecturing Hessian positivity, which would make them local minimums.

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I. INTRODUCTION

Entanglement [1] is what distinguishes the quantum world from classical worlds. Unfortunately, our understanding of it remains quite limited to this day. Entanglement exhibits varying degrees of strength, the highest of which falls into a subclass called "maximal entanglement." The Bell state is one such example. No consensus has yet been reached about what qualifies as a "weak entanglement." Quantum states with small Schmidt numbers are generally seen as weakly entangled, since quantum states with Schmidt number 1 are separable. Undistillable entanglement is another kind of widely accepted weak entanglement. Relationships between these two kinds of weak entanglements are discussed in [2].

Entanglement distillation [3] is the process of obtaining pure Bell states only by local operations and classical communication (LOCC) from multiple copies of an entangled bipartite state. If N copies of a given entangled bipartite state can be transformed into pure Bell states through LOCC, then the entangled bipartite state is referred to as N-distillable. If not, then it is N-undistillable. If a particular entangled bipartite state is N-undistillable for arbitrary N, it is considered undistillable and is also referred to as a bound entangled state.

Another property we are concerned with here is "positive partial transpose" (PPT), which refers to a bipartite quantum state whose partial transpose is positive semidefinite. It is established in [4] that PPT entanglement implies bound entanglement, and therefore weakly entangled in terms of distillability. However, the question of whether the converse is true remains an open problem, which is usually referred to as the nonpositive partial transpose (NPT) bound problem, or the distillability problem [5]. The popular conjecture regarding this problem is that the converse is not true, and that NPT bound entanglement exists. A number of special circumstances have been worked out in [6–10]. Indirect approaches to this problem include expansion of distillation operations to k-extendible operations [11], catalysis-assisted distillation [12], and dually nonentangling and PPT-preserving channels [13]; linking the problem with squashed entanglement [14] and linear preserver [15]; studying the transformation of bound entangled states under certain dynamic process [16]; or considering the problem in a broader scenario such as hyperquantum states [17].

In three separate attempts to directly tackle the distillability problem [6,18,19], they each had a subset of quantum states singled out, and they proved that for any finite number of copies N, there exist undistillable states in this subset. However, as N approaches infinity, the subset shrinks to emptiness. It has been shown in [20] that N-undistillability does not imply $(N+1)$-undistillability by demonstrating a set of states that are distillable only by an arbitrarily large number of copies, thus ruling out the easy route of concentrating on distillation of only a few copies.

For the Werner states [21], a family of single-parameter states, the existence of NPT bound states implies the existence of NPT bound Werner states [22]. Therefore, it is sufficient

*Contact author: genigupur@vip.163.com

†Contact author: wuyuchun@ustc.edu.cn

to study Werner states only. Due to the inherent complexity of addressing N-distillability of Werner states, over the past decade direct attempts to solve the problem have been focused primarily on the seemingly straightforward problem of 2-distillability of Werner states, but so far only limited progress has been made. In an attempt to attack the 2-distillability of the Werner-states problem, the special case of 4×4 bipartite states is considered in [23]. In that special case, the distillability condition can be reduced to a convenient form of a "half-property," and subsequently the distillability problem can be reformulated into a matrix analysis problem. For a special case in which the matrices are normal, a proof was given.

In [24] the problem is reformulated, and it was established that for $d \times d$ bipartite Werner states, the 2-undistillability is equivalent to a certain $2d^2 \times 2d^2$ matrix being positive semidefinite. Positive definiteness of the block matrices in the upper-left and lower-right corners has been proven.

In this work, we introduce a method that decomposes N-undistillability verification into repeated steps of 1-undistillability verification before giving a new parameter interval for N-undistillability that is independent of quantum state dimensions d, and therefore different from that given in [6,18,19]. However, similar to the problem encountered in [6,18,19], our set of N-undistillable states also shrinks to emptiness for $N \to \infty$. Also, an equivalent matrix analysis inequality form is presented, which is applicable to all finite dimensionalities, as opposed to the case in [23] where only the $d = 4$ case is considered. Another equivalent version of inequalities regarding only rank-1 matrices is also included, which takes on a form reminiscent of Cauchy-Schwartz inequality. Finally, we take on a brand new perspective of considering it as a multivariable function problem, finding critical points, proving nonconvexity, and conjecturing Hessian positivity.

We will be using $\mathcal{H}_A$ and $\mathcal{H}_B$ to denote Hilbert spaces pertaining to A and B subsystems, and X_i to denote matrices with rank less than or equal to i. Throughout the paper, we will be considering multipartite quantum states with identical dimensions, i.e., quantum states on $\mathcal{H}_A \otimes \mathcal{H}_B$, where $\dim(\mathcal{H}_A) = \dim(\mathcal{H}_B) = d$. This is justified by noticing that any quantum state of $d_1 \times d_2$ can be equivalently transformed into a quantum state of identical dimensions $\max\{d_1, d_2\} \times \max\{d_1, d_2\}$, with all unnecessary elements set to zero.

The structure of this paper is as follows: In Sec. II, we introduce a matrix transformation that takes the N-distillability problem into a higher-dimensional 1-distillability problem. In Sec. III, the process of N-undistillability verification is transformed into $\log(N)$ repeated steps of 1-undistillability verification. In Sec. IV, parameter intervals on N-undistillability are given, yielding a result similar to that of [6,18,19], effectively finding shrinking families of N-undistillable quantum states. In Sec. V, equivalent partial trace inequalities are presented before turning them into a matrix analysis problem. The rank-2 matrix analysis problem is also reduced to a rank-1 matrix analysis problem, resulting in a Cauchy-Schwartz inequality look-alike. The inequalities can be generalized to infinite matrix inequalities in an infinite-dimensional Hilbert space, all of which remain unsolved in mathematics. In Sec. VI, we take on a new perspective by treating the problem as a multivariable function, proving critical points, nonconvexity, and conjecturing positive-semidefinite Hessians.

II. STATEMENT OF THE DISTILLABILITY PROBLEM

Since NPT is a sufficient condition for entanglement [25], the open problem of equivalence between PPT entanglement and bound entanglement can be resolved by finding bound entangled states with NPT. Compared to ascertaining positive semidefiniteness of a certain matrix, the major difficulty usually lies in finding a concise mathematical interpretation for undistillability, and asserting it for two types of arbitrariness: arbitrary LOCC operation and an arbitrarily finite number of copies of the entangled state. This will be the main focus of this section, and the analysis of mathematical structure will eventually lead to a transformation that reduces N-undistillability verification to 1-undistillability verification of a transformed state.

Let us recall the concept of Schmidt decomposition, Schmidt coefficients, and Schmidt rank [26]. Schmidt decomposition of a pure state $|\psi\rangle$ in $\mathcal{H}_A \otimes \mathcal{H}_B$ is

$$|\psi\rangle = \sum_{i=1}^{d} \alpha_i |u_i v_i\rangle, \tag{1}$$

where $\mathcal{H}_A$ and $\mathcal{H}_B$ are both d-dimensional Hilbert spaces, with $\{|u_1\rangle, \dots, |u_d\rangle\}$ and $\{|v_1\rangle, \dots, |v_d\rangle\}$ as their respective orthonormal bases. Schmidt coefficients α_i are real, nonnegative, and unique up to reordering. The number of nonzero Schmidt coefficients is called a Schmidt rank of pure state $|\psi\rangle$, denoted by $\mathrm{SR}(|\psi\rangle)$.

A bipartite quantum state is called N-distillable if pure Bell states can be obtained using LOCC from N copies of the state. It has been proven in [27] that all entangled 2×2 bipartite quantum states are distillable, therefore all we need to do is transform the original quantum state into a 2×2 entangled state by LOCC. This is demonstrated in the following result: A bipartite quantum state ρ on $\mathcal{H}_A \otimes \mathcal{H}_B$ is N-undistillable iff for any $d^N \times d^N$ bipartite pure state $|\psi^{\mathrm{SR}\leqslant 2}\rangle$ on $\mathcal{H}_A^{\otimes N} \otimes \mathcal{H}_B^{\otimes N}$ with Schmidt rank $\leqslant 2$ the following holds:

$$\langle \psi^{\mathrm{SR}\leqslant 2} | (\rho^{T_A})^{\otimes N} | \psi^{\mathrm{SR}\leqslant 2} \rangle \geqslant 0, \tag{2}$$

where $\rho^{T_A} = (T \otimes I)\rho$ is the partial transpose of ρ, with T being the transpose operator. The above expression overlooks the pairing between different subsystems, and so an additional operator M_N from $(\mathcal{H}_A \otimes \mathcal{H}_B)^{\otimes N}$ to $\mathcal{H}_A^{\otimes N} \otimes \mathcal{H}_B^{\otimes N}$ is introduced to make it meaningful:

Definition II.1. Operator $M_N : (\mathcal{H}_A \otimes \mathcal{H}_B)^{\otimes N} \to \mathcal{H}_A^{\otimes N} \otimes \mathcal{H}_B^{\otimes N}$ is defined as

$$M_N = \sum \left| i_{A_1} \cdots i_{A_N} i_{B_1} \cdots i_{B_N} \right\rangle \! \left\langle i_{A_1} i_{B_1} \cdots i_{A_N} i_{B_N} \right|, \tag{3}$$

where $\mathcal{H}_A^{\otimes N} = \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \otimes \cdots \otimes \mathcal{H}_{A_N}$, $\mathcal{H}_B^{\otimes N} = \mathcal{H}_{B_1} \otimes \mathcal{H}_{B_2} \otimes \cdots \otimes \mathcal{H}_{B_N}$, and i_{A_j}, i_{B_j} stands for the index corresponding to system A_j, B_j. The sum is taken over all indexes $i_{A_j}, i_{B_k}, j, k \in \{1, \dots, N\}$, with each index in the range $\{0, \dots, d-1\}$.

Operator M_N then takes the $A_1B_1A_2B_2 \cdots A_NB_N$ structure of $(\rho^{T_A})^{\otimes N}$ and merges the A-subsystems and B-subsystems, resulting in a structure of $A_1A_2 \cdots A_NB_1B_2 \cdots B_N$ that suits the pure quantum state, thus explicitly demonstrating the process of system pairing, which is essential to any further calculations derived from this representation of undistillability.

For a better representation of undistillability and further use in following sections, we use a certain state-operator isomorphism introduced in [23]. We notice that it is in essence a Choi-Jamiolkowski isomorphism followed by a transposition on the resulting matrix.

Definition II.2. State-operator isomorphism [23]. A state-operator isomorphism Ψ is one that takes a pure bipartite state $|\psi\rangle$ of

$$|\psi\rangle = \sum_{i,j=0}^{d-1} \alpha_{ij}|ij\rangle \tag{4}$$

to a matrix form of

$$\Psi(|\psi\rangle) = \begin{pmatrix} \alpha_{00} & \alpha_{01} & \cdots & \alpha_{0,d-1} \\ \alpha_{10} & \alpha_{11} & \cdots & \alpha_{1,d-1} \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_{d-1,0} & \alpha_{d-1,1} & \cdots & \alpha_{d-1,d-1} \end{pmatrix}. \tag{5}$$

Note that Schmidt decomposition of a pure quantum state $|\psi\rangle$ is related to the singular value decomposition of $\Psi(|\psi\rangle)$ through state-operator isomorphism. In fact, Schmidt coefficients of $|\psi\rangle$ are the same as the singular values of $\Psi(|\psi\rangle)$, and a Schmidt rank of $|\psi\rangle$ is equal to the rank of $\Psi(|\psi\rangle)$ [26].

The following is a more concise mathematical representation of N-undistillability: A bipartite quantum state ρ is N-undistillable iff

$$[\Psi^{-1}(X_2)]^\dagger M_N (\rho^{T_A})^{\otimes N} M_N^\dagger \Psi^{-1}(X_2) \geqslant 0, \tag{6}$$

where X_2 is any $d^N \times d^N$ matrix with rank $\leqslant 2$. Note that $\Psi^{-1}(X_2)$ is equivalent to $|\psi^{\mathrm{SR}\leqslant 2}\rangle$, a pure bipartite quantum state with a Schmidt rank no larger than 2. For the case of $N = 1$, 1-undistillability is

$$[\Psi^{-1}(X_2)]^\dagger \rho^{T_A} \Psi^{-1}(X_2) = \langle\psi^{\mathrm{SR}\leqslant 2}|\rho^{T_A}|\psi^{\mathrm{SR}\leqslant 2}\rangle \geqslant 0. \tag{7}$$

Effectively, the problem of ρ being N-undistillable is equivalent to the problem of $M_N(\rho^{\otimes N})M_N^\dagger$ being 1-undistillable, but on a Hilbert space with higher dimensions $\mathcal{H}'_A \otimes \mathcal{H}'_B$, $\dim(\mathcal{H}'_A) = \dim(\mathcal{H}'_B) = d^N$.

Since discussions of the 1-distillability problem rarely involve specification of finite-dimensional Hilbert space dimensionality, and most of the theorems and methods are applicable to arbitrary dimensions, this transformation poses an advantage. In the next section, a specific symmetry of M_{2^N} transformations is utilized for decomposing the increasingly complicated structure of M_{2^N} into identical steps repeated N times. In fact, verification of 2^N-undistillability, as N approaches infinity, is enough to assert bound entanglement.

III. N-UNDISTILLABILITY PROBLEM AS REPEATED STEPS

From the observation that $(N+1)$-undistillability implies N-undistillability, we can get the following result, which relaxes the N-undistillability requirement for all N to only an infinite sequence of N diverging to infinity:

Proposition III.1. $\{g_i\}$ is a sequence of positive real numbers diverging to infinity. A bipartite entangled quantum state is g_i-undistillable for arbitrary i iff the state is bound entangled.

In the 2-copy case, M_2 transformation is simply

$$E = M_2 = \sum |i_{A_1} i_{A_2} i_{B_1} i_{B_2}\rangle\langle i_{A_1} i_{B_1} i_{A_2} i_{B_2}|, \tag{8}$$

which is merely an exchange of the second and third parts of B_1 and A_2. The sum is taken over all indexes $i_{A_1}, i_{A_2}, i_{B_1}, i_{B_2}$, with each index ranging in $\{0, \ldots, d-1\}$. From now on we will always refer to the 2-copy case of M_2 as E, emphasizing that it is only a simple exchange as opposed to complicated M_N of a larger number of copies.

According to Eq. (6), the quantum state ρ is 2-undistillable iff $E(\rho \otimes \rho)E^\dagger$ is 1-undistillable.

In the 4-copy case, M_4 can actually be decomposed into two steps:

$$\begin{aligned} A_1B_1A_2B_2A_3B_3A_4B_4 &\to A_1A_2B_1B_2A_3A_4B_3B_4 \\ &\to A_1A_2A_3A_4B_1B_2B_3B_4. \end{aligned} \tag{9}$$

Step 1: Do the 2-copy exchange on subsystems 1,2 ($A_1B_1A_2B_2 \to A_1A_2B_1B_2$) and subsystems 3,4 ($A_3B_3A_4B_4 \to A_3A_4B_3B_4$). This step is no different from in the 2-copy case, except that it is done on two systems simultaneously. Group every neighboring 2 subsystem (in terms of A, B), so that the eight parts are now seen as four parts (A_1A_2, B_1B_2, A_3A_4, B_3B_4 to $ABAB$). To separate this newly obtained four-part state from 2-copy Werner states, we denote this state as $\rho(e) \otimes \rho(e)$, where $\rho(e) = E(\rho \otimes \rho)E^\dagger$.

Step 2: Do the 2-copy exchange E again, obtaining $\rho(e^2) = E(\rho(e) \otimes \rho(e))E^\dagger$, where E is taken with regard to the "merged" parts. This step takes once-transformed Werner states into twice-transformed Werner states.

The above steps are equivalent to doing the M_4 translations directly. The original state ρ is 4-undistillable iff $\rho(e^2)$ is 1-undistillable.

Similarly, in the 2^N-copy case, M_{2^N} is decomposed into N steps, with each step taking state $\rho(e^{i-1}) \otimes \rho(e^{i-1})$, producing a state $\rho(e^i) = E(\rho(e^{i-1}) \otimes \rho(e^{i-1}))E^\dagger$, verifying its positivity on Schmidt rank $\leqslant 2$ states and effectively ascertaining 2^i-undistillability, before passing two copies of this state on, as a starting state for the next step. The following theorem demonstrates the process.

Theorem III.2. Defining $\rho(e^0) = \rho$ to be the initial state, and

$$\rho(e^k) = E(\rho(e^{k-1}) \otimes \rho(e^{k-1}))E^\dagger, \tag{10}$$

then $\rho(e^k)$ being 1-undistillable is equivalent to ρ being 2^k-undistillable.

In other words, we are essentially searching for an infinite sequence of points connected by the operation E, with the first point being $\rho = \rho(e^0)$, the second point being $\rho(e^1) = E(\rho(e^0) \otimes \rho(e^0))E^\dagger$, and the $(i+2)$th point being $\rho(e^{i+1}) = E(\rho(e^i) \otimes \rho(e^i))E^\dagger$. If points of this infinite sequence always fall within the set of 1-undistillability, then we can safely say that the starting point ρ is N-undistillable for arbitrary N, or that it is a bound state.

IV. PARAMETER INTERVALS FOR N-UNDISTILLABLE WERNER STATES

A. 1-undistillability and NPT condition for Werner states

It has been shown in [22] that it is sufficient to consider Werner states for an NPT bound problem only, namely if an NPT bound state exists, there must be an NPT bound state within the family of Werner states. In this section, we obtain necessary and sufficient conditions of Werner states' 1-undistillability and partial transpose negativity.

We first introduce a lemma that would assist further attempts concerning inner products with Schmidt rank $\leqslant 2$ pure states:

Lemma IV.1. Let $|\psi\rangle$ be an arbitrary pure quantum state, and s_j are the Schmidt coefficients of $|\psi\rangle$ arranged in descending order. Then

$$\sum_{j=1}^{k} s_j^2 = \max_{|\phi^{\mathrm{SR}\leqslant k}\rangle} |\langle\psi|\phi^{\mathrm{SR}\leqslant k}\rangle|^2, \tag{11}$$

where $|\phi^{\mathrm{SR}\leqslant k}\rangle$ is an arbitrary quantum pure state with Schmidt rank being less than k, namely $\mathrm{SR}(|\phi^{\mathrm{SR}\leqslant k}\rangle) \leqslant k$.

Proof of this lemma is provided in Appendix A.

A Werner state is as follows:

$$\rho_w = \frac{1}{d^2+\beta d}(I+\beta F), \tag{12}$$

where $F = \sum_{i,j=0}^{d-1} |ij\rangle\langle ji|$, I is the unnormalized identity matrix, d denotes the dimensionality of both parts of the system, and β is a parameter characterizing the "portion" of swap operator F, ranging in $-1 \leqslant \beta \leqslant 1$.

Its partial transpose is

$$\rho_w^{T_A} = \frac{1}{d^2+\beta d}(I+\beta G), \tag{13}$$

where $G = \sum_{i,j=0}^{d-1} |ii\rangle\langle jj|$, which is in fact the unnormalized density matrix of a pure maximally entangle state $|\Phi\rangle$, namely

$$G = d|\Phi\rangle\langle\Phi|, \quad |\Phi\rangle = \sum_{i=0}^{d-1} \frac{1}{\sqrt{d}}|ii\rangle. \tag{14}$$

When $\beta > 0$, $\rho_w^{T_A}$ is always positive semidefinite, hence we consider the $\beta < 0$ case only. Combining Eqs. (6) and (11), we obtain

$$\langle\psi^{\mathrm{SR}\leqslant 2}|\rho_w^{T_A}|\psi^{\mathrm{SR}\leqslant 2}\rangle = \frac{1}{d^2+\beta d}[1+\beta d|\langle\Phi|\psi^{\mathrm{SR}\leqslant 2}\rangle|^2] \overset{L.IV.1}{\geqslant} \frac{1+2\beta}{d^2+\beta d}. \tag{15}$$

A Werner state ρ_w is 1-undistillable iff $\langle\psi^{\mathrm{SR}\leqslant 2}|\rho_w^{T_A}|\psi^{\mathrm{SR}\leqslant 2}\rangle \geqslant 0$ for any $|\psi^{\mathrm{SR}\leqslant 2}\rangle$ pure bipartite quantum state of Schmidt rank no larger than 2. Therefore, a Werner state is 1-undistillable iff $\beta \geqslant -\frac{1}{2}$.

Furthermore, for arbitrary quantum state $|\psi\rangle$, we have

$$\langle\psi|\rho_w^{T_A}|\psi\rangle = \frac{1}{d^2+\beta d}[1+\beta d|\langle\Phi|\psi\rangle|^2] \geqslant \frac{1+\beta d}{d^2+\beta d}, \tag{16}$$

with the equality achieved when $|\psi\rangle = |\Phi\rangle$. Therefore, a Werner state is NPT iff $\beta < -\frac{1}{d}$. Any NPT 1-undistillable Werner states can therefore only be found within the parameter range of $-\frac{1}{2} \leqslant \beta < -\frac{1}{d}$, provided $d > 2$.

B. Sufficient conditions for N-undistillable Werner states

We derive new parameter intervals for N-undistillable Werner states in this section. As a result, for any finite N, a set of N-undistillable states can be found, but similar to the circumstances encountered in [6,18,19], the set of N-undistillable states shrinks to emptiness as N approaches infinity.

In the previous section, it has been established that the N-undistillability of Werner states is equivalent to

$$\langle\psi^{\mathrm{SR}\leqslant 2}|M_N\big(\rho_w^{T_A}\big)^{\otimes N}M_N^\dagger|\psi^{\mathrm{SR}\leqslant 2}\rangle \geqslant 0, \tag{17}$$

where $|\psi^{\mathrm{SR}\leqslant 2}\rangle$ is an arbitrary quantum pure state with Schmidt rank being no larger than 2.

Take the 2-copy case as an example, recalling operation E defined in Eq. (8):

$$\begin{aligned} &E\big(\rho_w^{T_A}\otimes\rho_w^{T_A}\big)E^\dagger \\ &= \left(\frac{1}{d^2+\beta d}\right)^2\{E(I\otimes I)E^\dagger + \beta[E(I\otimes G)E^\dagger \\ &\quad + E(G\otimes I)E^\dagger] + \beta^2 E(G\otimes G)E^\dagger\}. \end{aligned} \tag{18}$$

The normalization factor of $(\frac{1}{d^2+\beta d})^2$ can be ignored since it does not affect positivity. The first and last terms remain unchanged in the sense that

$$\begin{aligned} E(I\otimes I)E^\dagger &= E\left(\sum_{i,j,k,l=0}^{d-1}|ijkl\rangle\langle ijkl|\right)E^\dagger \\ &= \sum_{i,j,k,l=0}^{d-1}|ikjl\rangle\langle ikjl| = I(e), \end{aligned} \tag{19}$$

with $I(e)$ still being the identity matrix, only it exists on a higher dimensionality of $d^4\times d^4$. Similarly,

$$\begin{aligned} E(G\otimes G)E^\dagger &= E\left(\sum_{i,j,k,l=0}^{d-1}|iikk\rangle\langle jjll|\right)E^\dagger \\ &= \sum_{i,j,k,l=0}^{d-1}|ikik\rangle\langle jljl| = G(e), \end{aligned} \tag{20}$$

with $G(e) = |\Phi(e)\rangle\langle\Phi(e)|$ still being the pure state density matrix of unnormalized $|\Phi(e)\rangle = \sum_{i,j=0}^{d-1}|ijij\rangle$, only it exists on a higher dimensionality of $d^4\times d^4$.

Regarding the positivity of the middle part $E(I\otimes G)E^\dagger + E(G\otimes I)E^\dagger$ on $|\psi^{\mathrm{SR}\leqslant 2}\rangle$,

$$E(I\otimes G)E^\dagger = E\left(\sum_{i,j,k,l=0}^{d-1}|ijkk\rangle\langle ijll|\right)$$
$$E^\dagger = \sum_{i,j,k,l=0}^{d-1}|ikjk\rangle\langle iljl|$$
$$= d\big(\big|\psi_{00}^{s_2=s_4}\big\rangle\big\langle\psi_{00}^{s_2=s_4}\big| + \cdots + \big|\psi_{d-1,d-1}^{s_2=s_4}\big\rangle$$
$$\times\ \big\langle\psi_{d-1,d-1}^{s_2=s_4}\big|\big)$$
$$= d\sum_{i,j=0}^{d-1}\big|\psi_{ij}^{s_2=s_4}\big\rangle\big\langle\psi_{ij}^{s_2=s_4}\big|, \tag{21}$$

where $|\psi_{ij}^{s_2=s_4}\rangle = \frac{1}{\sqrt{d}}\sum_{k=0}^{d-1}|ikjk\rangle$ is the superposition of all multipartite states with identical states on the second and fourth subsystems, while their first and third subsystems are of states i and j, respectively. $|\psi_{ij}^{s_2=s_4}\rangle$ is a normalized pure state of Schmidt rank d, and all Schmidt coefficients are $\frac{1}{\sqrt{d}}$. Do a decomposition of $|\psi^{\mathrm{SR}\leqslant 2}\rangle$ in the following way:

$$|\psi^{\mathrm{SR}\leqslant 2}\rangle = \sum_{i,j=0}^{d-1}p_{ij}\big|\psi_{ij}^{\mathrm{SR}\leqslant 2}\big\rangle, \tag{22}$$

where $|\psi_{ij}^{\mathrm{SR}\leqslant 2}\rangle$ represents the normalized extraction of all $|i-j-\rangle$ terms from the state of $|\psi^{\mathrm{SR}\leqslant 2}\rangle$. More specifically, for a state $|\psi^{\mathrm{SR}\leqslant 2}\rangle$ of

$$|\psi^{\mathrm{SR}\leqslant 2}\rangle = \sum_{a,b,c,d=0}^{d-1}p_{abcd}|abcd\rangle, \tag{23}$$

the corresponding $|\psi_{ij}^{\mathrm{SR}\leqslant 2}\rangle$ is

$$\big|\psi_{ij}^{\mathrm{SR}\leqslant 2}\big\rangle = \frac{1}{N_p}\sum_{a,b=0}^{d-1}p_{iajb}|iajb\rangle, \tag{24}$$

where $N_p = \sqrt{\sum_{a,b=0}^{d-1}|p_{iajb}|^2}$.

It can be proven that the normalized extraction of all $|ixjy\rangle$ terms must also have Schmidt rank $\leqslant 2$. Consider the state-operator isomorphism in Def. II.2; the Schmidt rank of $|\psi\rangle$ is equivalent to the rank of the matrix $\Psi(|\psi\rangle)$. The normalized extraction of all $|i-j-\rangle$ terms composes a new state of $|\psi_{ij}^{\mathrm{SR}\leqslant 2}\rangle$, therefore its corresponding matrix is a submatrix of $\Psi(|\psi^{\mathrm{SR}\leqslant 2}\rangle)$, composed of rows $i\times d+x$ and columns $j\times d+y$, with x, y taking values from $\{0,\dots,d-1\}$. Since the rank of a submatrix is never larger than the rank of the whole matrix, $|\psi_{ij}^{\mathrm{SR}\leqslant 2}\rangle$ must have a Schmidt rank less than or equal to that of $|\psi^{\mathrm{SR}\leqslant 2}\rangle$.

Using Lem. IV.1 again, it is then clear that

$$\big|\big\langle\psi_{ij}^{\mathrm{SR}\leqslant 2}\big|\psi_{pq}^{s_2=s_4}\big\rangle\big|^2 = \big|\big\langle\psi_{ij}^{\mathrm{SR}\leqslant 2}\big|\psi_{ij}^{s_2=s_4}\big\rangle\big|^2\delta_{ip}\delta_{jq} \overset{L.IV.1}{\leqslant} \frac{2}{d}\delta_{ip}\delta_{jq}. \tag{25}$$

It follows that

$$\langle\psi^{\mathrm{SR}\leqslant 2}|E(I\otimes G)E^\dagger|\psi^{\mathrm{SR}\leqslant 2}\rangle$$
$$= d\sum_{i,j=0}^{d-1}|p_{ij}|^2\big|\big\langle\psi_{ij}^{\mathrm{SR}\leqslant 2}\big|\psi_{ij}^{s_2=s_4}\big\rangle\big|^2$$
$$\leqslant 2\sum_{i,j=0}^{d-1}|p_{ij}|^2 = 2. \tag{26}$$

A similar analysis is applied to $E(G\otimes I)E^\dagger$, getting

$$\langle\psi^{\mathrm{SR}\leqslant 2}|E(G\otimes I)E^\dagger|\psi^{\mathrm{SR}\leqslant 2}\rangle$$
$$= d\sum_{i,j=0}^{d-1}|q_{ij}|^2\big|\big\langle\phi_{ij}^{\mathrm{SR}\leqslant 2}\big|\psi_{ij}^{s_1=s_3}\big\rangle\big|^2$$
$$\leqslant 2\sum_{i,j=0}^{d-1}|q_{ij}|^2 = 2. \tag{27}$$

A sufficient condition for the 2-undistillability of Werner states is

$$\langle\psi^{\mathrm{SR}\leqslant 2}|I(e) + \beta^2G(e) + \beta E(I\otimes G + G\otimes I)E^\dagger|\psi^{\mathrm{SR}\leqslant 2}\rangle$$
$$\geqslant 1 + \beta^2|\langle\Psi(e)|\psi^{\mathrm{SR}\leqslant 2}\rangle|^2 + 4\beta \geqslant 1 + 4\beta \geqslant 0. \tag{28}$$

Therefore, we can conclude that when $\beta \geqslant -\frac{1}{4}$, ρ_w must be 2-undistillable.

A similar process is followed in the arbitrary N case, yielding a lower bound regarding all the odd terms in $(1+\beta)^N$. Since the odd terms in $(1+\beta)^N$ can be expressed by $\frac{(1+\beta)^N-(1-\beta)^N}{2}$, a lower bound can then be obtained for the N-undistillability case:

Theorem IV.2. Let β_0 be the zero point of $1 + (1+\beta)^N - (1-\beta)^N$ within $[-1, 0]$. When $\beta \geqslant \beta_0$, Werner state ρ_w is N-undistillable.

Proof of this is presented in Appendix B. By calculating the zero point, a lower bound is obtained where the corresponding Werner state is N-undistillable. Note that unlike in previous works, this bound β_0 is also independent of dimensionality d. By subsequently raising the dimensionality of Werner states within the set, thus raising $-\frac{1}{d}$, we can always obtain a set of Werner states that falls into $[\beta_0, -\frac{1}{d})$, which means that they are both NPT and N-undistillable for any finite N. However, as N increases, higher dimensionality is required for undistillability, and so the subset of N-undistillable NPT states shrinks to emptiness as N approaches infinity, which is similar to the circumstances encountered in [6,18,19]. Therefore, this method fails to find a state that is undistillable for arbitrarily many copies, while being NPT at the same time.

V. THE PROBLEM AS A PARTIAL TRACE INEQUALITY

The problem of Werner states' N-undistillability can be equivalently written as inequalities regarding the Frobenius norm of partial traces of a rank-2 matrix.

Take 2-undistillability as an example. $\langle\psi^{\mathrm{SR}\leqslant 2}|E(I\otimes G + G\otimes I)E^\dagger|\psi^{\mathrm{SR}\leqslant 2}\rangle$ can be written with regard to the Frobenius norms of two partial traces:

$$\langle\psi^{\mathrm{SR}\leqslant 2}|E(I\otimes G)E^\dagger|\psi^{\mathrm{SR}\leqslant 2}\rangle = ||\mathrm{Tr}_2(X_2(\psi))||_F^2, \tag{29}$$

$$\langle\psi^{\mathrm{SR}\leqslant 2}|E(G\otimes I)E^\dagger|\psi^{\mathrm{SR}\leqslant 2}\rangle = ||\mathrm{Tr}_1(X_2(\psi))||_F^2, \tag{30}$$

where $||\cdot||_F$ denotes Frobenius norm:

$$||X||_F = \sqrt{\sum_{i,j=0}^{d^2-1}|X_{ij}|^2} = \sqrt{\mathrm{Tr}(X^\dagger X)}. \tag{31}$$

$X_2(\psi)$ is a $d^2\times d^2$ matrix with rank $\leqslant 2$, obtained by state-operator isomorphism, from $|\psi^{\mathrm{SR}\leqslant 2}\rangle$, a pure bipartite $d^2\times d^2$ state with Schmidt rank $\leqslant 2$. For simplicity, we will be writing it as X_2 from now on.

The normalization of $|\psi^{\mathrm{SR}\leqslant 2}\rangle$ requires that $||X_2||_F^2 = \mathrm{Tr}(X_2^\dagger X_2) = 1$. Now the problem of Werner states' 2-undistillability is equivalent to the following: Find a range of β that makes the following inequality always hold for arbitrary X_2 with rank no larger than 2 (the requirement of $||X_2||_F^2 = 1$ can be lifted due to homogeneity):

$$||X_2||_F^2 + \beta^2|\mathrm{Tr}(X_2)|^2 + \beta\big[||\mathrm{Tr}_1(X_2)||_F^2 + ||\mathrm{Tr}_2(X_2)||_F^2\big] \geqslant 0. \tag{32}$$

N-undistillability has a similar form:

Theorem V.1. Werner state ρ_w is N-undistillable iff the following holds for all $d^N\times d^N$ X_2:

$$\sum_{S\subset\{1,\dots,N\}}\beta^{|S|}||\mathrm{Tr}_S(X_2)||_F^2 \geqslant 0, \tag{33}$$

where Tr_S takes partial traces of the subsystems in set S.

S is taken to be the subsets of $\{1,\dots,N\}$, including the case of $\emptyset$, where $|S|=0$, $||\mathrm{Tr}_S(X_2)||_F^2 = ||X_2||_F^2$, and the case of $\{1,\dots,N\}$, where $|S|=N$, $||\mathrm{Tr}_S(X_2)||_F^2 = ||\mathrm{Tr}(X_2)||_F^2$.

The proof of this is presented in Appendix C. A similar result is obtained by [28].

The partial trace inequalities are with regard to a matrix X_2 with rank 1 or 2. From now on we consider the case in which β is taken to be $-\frac{1}{2}$ according to a popular guess. For the 2-undistillability problem, the rank-1 case can be trivially proven by making use of the following lemma:

Lemma V.2. The inequalities

$$||\mathrm{Tr}_1(X_1)||_F^2 \leqslant ||X_1||_F^2,\ ||\mathrm{Tr}_2(X_1)||_F^2 \leqslant ||X_1||_F^2 \tag{34}$$

hold for any $d^2\times d^2$ square matrix X_1 with rank 1.

Proof of this lemma is presented in Appendix E. For X_2 with rank 2, the inequality of concern when $\beta = -\frac{1}{2}$ is

$$||\mathrm{Tr}_2(X_2)||_F^2 + ||\mathrm{Tr}_1(X_2)||_F^2 - \tfrac{1}{2}|\mathrm{Tr}(X_2)|^2 \leqslant 2||X_2||_F^2 = 2. \tag{35}$$

For any square matrix X_2 with rank 2, the singular decomposition can be applied, decomposing the matrix as the sum of two rank-1 matrices:

$$X_2 = \sigma_1 X_2^1 + \sigma_2 X_2^2 = \sigma_1\mathbf{u}^1\mathbf{v}^{1\dagger} + \sigma_2\mathbf{u}^2\mathbf{v}^{2\dagger}, \tag{36}$$

where $\sigma_1^2+\sigma_2^2=1$, and both σ_1 and σ_2 are positive. We introduce $d\times d$ matrices U_1, U_2, V_1, V_2 that are the result of state-operator isomorphisms, corresponding to $\mathbf{u}^1$, $\mathbf{u}^2$, $\mathbf{v}^1$, $\mathbf{v}^2$, respectively.

Equation (35) then becomes

$$\begin{aligned}&\sigma_1^2[\mathrm{Tr}(V_1U_1^\dagger U_1V_1^\dagger) + \mathrm{Tr}(U_1^\dagger V_1V_1^\dagger U_1)]\\&+\sigma_2^2[\mathrm{Tr}(V_2U_2^\dagger U_2V_2^\dagger) + \mathrm{Tr}(U_2^\dagger V_2V_2^\dagger U_2)]\\&+\sigma_1\sigma_2 2\,\mathrm{Re}[\mathrm{Tr}(V_1U_1^\dagger U_2V_2^\dagger) + \mathrm{Tr}(U_1^\dagger V_1V_2^\dagger U_2)]\\&-\frac{|\sigma_1\mathrm{Tr}(U_1V_1^\dagger)+\sigma_2\mathrm{Tr}(U_2V_2^\dagger)|^2}{2} \leqslant 2.\end{aligned} \tag{37}$$

For simplicity, the above is rewritten as

$$\sigma_1^2P + \sigma_2^2Q + \sigma_1\sigma_2R \leqslant 2, \tag{38}$$

where P, Q, R are

$$P = \mathrm{Tr}(U_1^\dagger V_1V_1^\dagger U_1) + \mathrm{Tr}(V_1U_1^\dagger U_1V_1^\dagger) - \frac{|\mathrm{Tr}(U_1V_1^\dagger)|^2}{2}, \tag{39}$$

$$Q = \mathrm{Tr}(U_2^\dagger V_2V_2^\dagger U_2) + \mathrm{Tr}(V_2U_2^\dagger U_2V_2^\dagger) - \frac{|\mathrm{Tr}(U_2V_2^\dagger)|^2}{2}, \tag{40}$$

$$R = 2\,\mathrm{Re}\bigg[\mathrm{Tr}(V_1U_1^\dagger U_2V_2^\dagger) + \mathrm{Tr}(U_1^\dagger V_1V_2^\dagger U_2) - \frac{\mathrm{Tr}^*(U_1V_1^\dagger)\mathrm{Tr}(U_2V_2^\dagger)}{2}\bigg]. \tag{41}$$

Maximization regarding variables σ_1, σ_2 reduces the question to proving

$$R^2 \leqslant 4(2-P)(2-Q), \tag{42}$$

with normalization and orthogonality conditions requiring

$$||U_1||_F^2 = ||V_1||_F^2 = ||U_2||_F^2 = ||V_2||_F^2 = 1 \tag{43}$$

and

$$\mathrm{tr}(V_2^\dagger V_1) = \mathrm{tr}(U_2^\dagger U_1) = 0. \tag{44}$$

The special case of $U_1 = V_1$, in other words X_2 being the sum of a normal matrix and a rank-1 matrix, has been proved in [28].

In fact, by a slight change of representation, we can also get an equivalent expression of Werner states' N-undistillability inequality, regarding only rank-1 matrices:

Theorem V.3. Werner state ρ_w is N-undistillable iff

$$\mathrm{Re}[f_N(X_1, X_1')]^2 \leqslant f_N(X_1', X_1')f_N(X_1, X_1), \tag{45}$$

where

$$f_N(X_1, X_1') = \sum_{S\subset\{1,\dots,N\}}\beta^{|S|}\mathrm{Tr}[\mathrm{Tr}_S^\dagger(X_1)\mathrm{Tr}_S(X_1')] \geqslant 0, \tag{46}$$

where $X_1 = \mathbf{w}^\dagger\mathbf{x}$, $X_1' = \mathbf{y}^\dagger\mathbf{z}$ are $d^N\times d^N$ rank-1 matrices, and their component vectors $\mathbf{w}, \mathbf{x}, \mathbf{y}, \mathbf{z}$ satisfy $\mathbf{w}\perp\mathbf{y}, \mathbf{x}\perp\mathbf{z}$.

Similar to the previous theorem, S is taken to be the subsets of $\{1,\dots,N\}$, including the case of $\emptyset$, where $|S|=0$, $\mathrm{Tr}_S(X_2) = X_2$, and the case of $\{1,\dots,N\}$, where $|S|=N$, $\mathrm{Tr}_S(X_2) = \mathrm{Tr}(X_2)$.

Proof of this equivalence is presented in Appendix D.

It is then established that the N-undistillability problem for arbitrary N can be written as inequalities concerning rank-1 matrices. Although the above form looks like a

Cauchy-Schwartz inequality, $f_N(X_1, X_1')$ cannot be regarded as an inner product and enable the direct application of the Cauchy-Schwartz inequality. $f_N(X_1, X_1')$ is obviously conjugate symmetric, and for rank-1 matrices X_1 and X_1', positivity of $f_N(X_1, X_1)$ and $f_N(X_1', X_1')$ can be ascertained. However, rank-1 matrices do not compose a vector space, since the sum of two rank-1 matrices can be a rank-2 matrix. Although arbitrary finite-rank matrices do compose a finite-dimensional vector space, proving positivity of $f_N(A, A)$ for arbitrary rank matrix A is both beyond our ability and our need, since proving positivity of $f_N(X_2, X_2)$ for arbitrary rank-2 matrix X_2 is, in fact, equivalent to Eq. (33), and is enough for proof of N-undistillability.

VI. CONVERSION TO A MULTIVARIABLE FUNCTION

We make another attempt at this problem by seeing it as a multivariable function. For simplicity, we consider only the real case of the 2-distillability problem, that is, X_1, X_1' are $d^2 \times d^2$ real matrices. For convenience of expression we use $f(C, D) = f_2(X_1, X_1')$ to denote the function concerned. Thus, the 2-undistillability problem is equivalent to proving the following inequality for all $d^2 \times d^2$-dimensional rank-1 matrices C, D:

$$f^2(C, D) \leqslant f(C, C)f(D, D), \tag{47}$$

where

$$\begin{aligned} f(C, D) = {} & \mathrm{Tr}(C^T D) + \beta\big[\mathrm{Tr}\big(C_1^T D_1\big) + \mathrm{Tr}\big(C_2^T D_2\big)\big] \\ & + \beta^2 \mathrm{Tr}(C^T)\mathrm{Tr}(D), \end{aligned} \tag{48}$$

where we have used $\mathrm{Tr}_1(C) = C_2, \mathrm{Tr}_2(C) = C_1, \mathrm{Tr}_1(D) = D_2, \mathrm{Tr}_2(D) = D_1$ for simplicity. A multivariable function $g(C)$ is defined if we see D as a constant D_0:

$$g(C)_{D_0} = f(C, C)f(D_0, D_0) - f^2(C, D_0), \tag{49}$$

where D_0 is an arbitrary $(d^2 \times d^2)$-dimensional real matrix with rank 1. Both C and D_0 can be written as outer products of d^2-dimensional real vectors $\mathbf{w}, \mathbf{x}, \mathbf{y}, \mathbf{z}$:

$$C = \mathbf{w}\mathbf{x}^T, D_0 = \mathbf{y}\mathbf{z}^T. \tag{50}$$

The multivariables of function $g(C)$ are taken to be the components of vector $\mathbf{w}, \mathbf{x}$, represented by w_{ij}, x_{ij}. Indices i and j take their values in $[0, 1, \dots, d-1]$, and are combined together to represent the $(i \times d + j)$th component of the vector. The problem is therefore transformed into proving that multivariable function $g(C)_{D_0}$ is always non-negative for all variables w_{ij}, x_{ij} and all possible parameters y_{ij}, z_{ij}. It is clear that when $C = D_0$, $g(D_0)_{D_0} = f^2(D_0, D_0) - f^2(D_0, D_0) = 0$, and we conjecture that these are global minimums.

We first prove that the gradients at these points are zero regardless of the parameters $\mathbf{y}, \mathbf{z}$ by calculating the Jacobian matrix, therefore showing that the $C = D_0$ points are indeed critical points. Then the Hessian matrix at this point is presented, in particular its three block parts, since the Hessian matrix is Hermitian. We conjecture that it is positive semidefinite. An additional proof of nonconvexity is also given in Appendix F, thus eliminating the easy case where any local minimum is also a global minimum.

A. The gradient at $C = D_0$ is zero

For simplicity, all $g(C)_{D_0}$ are written as $g(C)$ in the following text. Define

$$\begin{aligned} h_{1,ij}(w, x) = {} & 2w_{ij}\left(\sum_{p,q=0}^{d-1} x_{pq}^2\right) \\ & + 2\beta\left[\sum_{p,q=0}^{d-1} x_{pj}w_{iq}x_{pq} + \sum_{p,q=0}^{d-1} x_{iq}w_{pj}x_{pq}\right] \\ & + 2\beta^2 x_{ij}\left(\sum_{p,q=0}^{d-1} w_{pq}x_{pq}\right), \end{aligned} \tag{51}$$

$$\begin{aligned} h_{2,ij}(y, z, x) = {} & y_{ij}\left(\sum_{p,q=0}^{d-1} x_{pq}z_{pq}\right) \\ & + \beta\left[\sum_{p,q=0}^{d-1} x_{pj}y_{iq}z_{pq} + \sum_{p,q=0}^{d-1} x_{iq}y_{pj}z_{pq}\right] \\ & + \beta^2 x_{ij}\left(\sum_{p,q=0}^{d-1} y_{pq}z_{pq}\right). \end{aligned} \tag{52}$$

The partial derivatives of $f(C, C)$ and $f(C, D_0)$ are

$$\frac{\partial f(C, C)}{\partial w_{ij}} = h_{1,ij}(w, x), \ \frac{\partial f(C, C)}{\partial x_{ij}} = h_{1,ij}(x, w), \tag{53}$$

$$\frac{\partial f(C, D_0)}{\partial w_{ij}} = h_{2,ij}(y, z, x), \ \frac{\partial f(C, D_0)}{\partial x_{ij}} = h_{2,ij}(z, y, w). \tag{54}$$

Notice that $h_{1,ij}(w, x) = 2h_{2,ij}(w, x, x)$, $h_{1,ij}(x, w) = 2h_{2,ij}(x, w, w)$.

Therefore, at the critical points where $C = D_0$,

$$\left.\frac{\partial f(C, D_0)}{\partial w_{ij}}\right|_{C=D_0} = \frac{1}{2}\left.\frac{\partial f(C, C)}{\partial w_{ij}}\right|_{C=D_0}, \tag{55}$$

$$\left.\frac{\partial f(C, D_0)}{\partial x_{ij}}\right|_{C=D_0} = \frac{1}{2}\left.\frac{\partial f(C, C)}{\partial x_{ij}}\right|_{C=D_0}. \tag{56}$$

It then follows that the Jacobian at the $C = D_0$ point is zero:

$$\begin{aligned} \left.\frac{\partial g(C)}{\partial w_{ij}}\right|_{C=D_0} = {} & f(D_0, D_0)\left.\frac{\partial f(C, C)}{\partial w_{ij}}\right|_{C=D_0} \\ & - 2\left.\frac{\partial f(C, D_0)}{\partial w_{ij}}\right|_{C=D_0} f(D_0, D_0) = 0, \end{aligned} \tag{57}$$

$$\begin{aligned} \left.\frac{\partial g(C)}{\partial x_{ij}}\right|_{C=D_0} = {} & f(D_0, D_0)\left.\frac{\partial f(C, C)}{\partial x_{ij}}\right|_{C=D_0} \\ & - 2\left.\frac{\partial f(C, D_0)}{\partial x_{ij}}\right|_{C=D_0} f(D_0, D_0) = 0. \end{aligned} \tag{58}$$

It is then established that the gradients at the $C = D_0$ points are zero, and the points are indeed critical points.

B. Hessian matrix

Hessian matrices at the critical points are presented. Define

$$h_{3,ijkl}(x) = 2\delta_{ik}\delta_{jl}\left(\sum_{p,q=0}^{d-1} x_{pq}^2\right) + 2\beta\left[\delta_{ik}\sum_{p=0}^{d-1} x_{pj}x_{pl} + \delta_{lj}\sum_{q=0}^{d-1} x_{iq}x_{kq}\right] + 2\beta^2 x_{ij}x_{kl}, \tag{59}$$

$$h_{4,ijkl}(w,x) = 4w_{ij}x_{kl} + \beta\left[2\delta_{jl}\left(\sum_{q=0}^{d-1} w_{iq}x_{kq}\right) + x_{kj}w_{il} + 2\delta_{ik}\left(\sum_{p=0}^{d-1} w_{pj}x_{pl}\right) + x_{il}w_{kj}\right] + 2\beta^2\left[\delta_{ik}\delta_{jl}\left(\sum_{p,q=0}^{d-1} w_{pq}x_{pq}\right) + x_{ij}w_{kl}\right], \tag{60}$$

$$h_{5,ijkl}(y,z) = y_{ij}z_{kl} + \beta\left[\delta_{jl}\left(\sum_{q=0}^{d-1} y_{iq}z_{kq}\right) + \delta_{ik}\left(\sum_{p=0}^{d-1} y_{pj}z_{pl}\right)\right] + \beta^2\delta_{ik}\delta_{jl}\left(\sum_{p,q=0}^{d-1} y_{pq}z_{pq}\right). \tag{61}$$

The Hessian matrices at $C = D_0$ can be explicitly written as

$$\begin{pmatrix} \left(\frac{\partial^2 g(C)}{\partial w_{ij}\partial w_{kl}}\right)\Big|_{C=D_0} & \left(\frac{\partial^2 g(C)}{\partial w_{ij}\partial x_{kl}}\right)\Big|_{C=D_0} \\ \left(\frac{\partial^2 g(C)}{\partial x_{ij}\partial w_{kl}}\right)\Big|_{C=D_0} & \left(\frac{\partial^2 g(C)}{\partial x_{ij}\partial x_{kl}}\right)\Big|_{C=D_0} \end{pmatrix}, \tag{62}$$

where the three independent parts of the Hessian matrix are

$$\frac{\partial^2 g(C)}{\partial w_{ij}\partial w_{kl}}\Big|_{C=D_0} = f(D_0,D_0)h_{3,ijkl}(x) - 2h_{2,ij}(w,x,x)h_{2,kl}(w,x,x), \tag{63}$$

$$\frac{\partial^2 g(C)}{\partial x_{ij}\partial x_{kl}}\Big|_{C=D_0} = f(D_0,D_0)h_{3,ijkl}(w) - 2h_{2,ij}(x,w,w)h_{2,kl}(x,w,w), \tag{64}$$

$$\frac{\partial^2 g(C)}{\partial w_{ij}\partial x_{kl}}\Big|_{C=D_0} = f(D_0,D_0)h_{4,ijkl}(w,x) - 2h_{5,ijkl}(w,x)f(D_0,D_0) - 2h_{2,ij}(w,x,w)h_{2,kl}(x,w,w). \tag{65}$$

We conjecture that this Hessian matrix is positive semidefinite, thus making the critical points local minimums. In Appendix F we prove that the function is nonconvex, which means that further scrutiny is needed for characterization of this function.

VII. CONCLUSION AND DISCUSSION

We have broken down the process of verifying N-undistillability into iterative steps of 1-undistillability verifications by noticing that N-undistillability for arbitrary N is equivalent to 2^N-undistillability for arbitrary N, and then utilizing specific symmetric properties. In the Werner states case, new parameter intervals for N-undistillability of any finite N are presented, a result similar to that of [6,18,19], but different in the sense that our parameter intervals are unaffected by the dimensionality of the Hilbert space in which Werner states lie. Alternative expressions for inequalities applicable to both rank-2 and rank-1 matrices are given. Subsequently, the problem of 2-undistillability is converted into a matrix analysis problem. Both the finite and infinite versions of the above inequalities remain unsolved problems in mathematics. If we manage to find necessary and sufficient conditions for these inequalities, then the bound entanglement problem can be fully solved. The multivariable function treatment is also attempted, as well as proving critical points, nonconvexity, and conjecturing about Hessian positivity.

Recently, in [28], the N-undistillability of Werner states has been reformulated into a set of partial trace inequalities, which coincided with our Theorem V.1. In the regime of the 2-distillability of Werner states, a special case of the matrix being the sum of a rank-one matrix and a normal matrix is proved.

We believe the new perspectives presented here will assist further attempts at this famous open problem.

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APPENDIX A: PROOF OF LEMMA IV.1

Lemma A.1. Let $|\psi\rangle$ be an arbitrary pure quantum state, and s_j are the Schmidt coefficients of $|\psi\rangle$ arranged in descending order. Then

$$\sum_{j=1}^{k} s_j^2 = \max_{|\phi^{\mathrm{SR}\leqslant k}\rangle} |\langle\psi|\phi^{\mathrm{SR}\leqslant k}\rangle|^2, \tag{A1}$$

where $|\phi^{\mathrm{SR}\leqslant k}\rangle$ is an arbitrary quantum pure state with Schmidt rank being less than k, namely $\mathrm{SR}(|\phi^{\mathrm{SR}\leqslant k}\rangle) \leqslant k$.

Proof. State-operator isomorphism translates the problem to an equivalent form of proving

$$|\mathrm{Tr}(A^\dagger B)|^2 \leqslant \sum_{i=1}^{k} s_i^2(A), \tag{A2}$$

where both A and B are $d \times d$ matrices, and are the result of state-operator isomorphism from $|\psi\rangle$ and $|\phi^{SR\leqslant k}\rangle$. Specifically, for

$$|\psi\rangle = \sum_{i,j=0}^{d-1} \alpha_{ij}|ij\rangle, \tag{A3}$$

$$A = \begin{pmatrix} \alpha_{00} & \alpha_{01} & \cdots & \alpha_{0,d-1} \\ \alpha_{10} & \alpha_{11} & \cdots & \alpha_{1,d-1} \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_{d-1,0} & \alpha_{d-1,1} & \cdots & \alpha_{d-1,d-1} \end{pmatrix}. \tag{A4}$$

Similarly, for

$$|\phi^{SR\leqslant k}\rangle = \sum_{i,j=0}^{d-1} \beta_{ij}|ij\rangle, \tag{A5}$$

$$B = \begin{pmatrix} \beta_{00} & \beta_{01} & \cdots & \beta_{0,d-1} \\ \beta_{10} & \beta_{11} & \cdots & \beta_{1,d-1} \\ \vdots & \vdots & \ddots & \vdots \\ \beta_{d-1,0} & \beta_{d-1,1} & \cdots & \beta_{d-1,d-1} \end{pmatrix}. \tag{A6}$$

Therefore, A and B are both of Frobenius norm 1 due to normalization conditions, with B having the same rank as the Schmidt rank of $|\phi^{SR\leqslant k}\rangle$, namely $\leqslant k$. We use $s_i(A)$ and $|\lambda_i(A)|$ to denote the singular values and absolute values of eigenvalues of A arranged in descending order,

$$\begin{aligned} |\mathrm{Tr}(A^\dagger B)|^2 &\leqslant \left(\sum_{i=1}^{d} |\lambda_i(A^\dagger B)|\right)^2 \leqslant \left(\sum_{i=1}^{d} s_i(A^\dagger B)\right)^2 \\ &\leqslant \left(\sum_{i=1}^{k} s_i(A^\dagger) s_i(B)\right)^2 = \left(\sum_{i=1}^{k} s_i(A) s_i(B)\right)^2, \end{aligned} \tag{A7}$$

where the second and third inequality are from Theorem 3.3.13(a) and Theorem 3.3.14(a) in [29], and $d \to k$ change of index holds because the rest of B's singular values are all zeros after d. Then by Cauchy-Schwartz inequality,

$$\begin{aligned} |\mathrm{Tr}(A^\dagger B)|^2 &\leqslant \left(\sum_{i=1}^{k} s_i(A) s_i(B)\right)^2 \\ &\leqslant \left(\sum_{i=1}^{k} s_i^2(A)\right)\left(\sum_{j=1}^{k} s_j^2(B)\right) \\ &= \sum_{i=1}^{k} s_i^2(A), \end{aligned} \tag{A8}$$

where the last equality follows from the fact that B is of rank $\leqslant k$, and therefore only has k nonzero singular values. ■

APPENDIX B: PROOF OF THEOREM IV.2

Theorem B.1. Let β_0 be the zero point of $1 + (1+\beta)^N - (1-\beta)^N$ within $[-1, 0]$. When $\beta \geqslant \beta_0$, Werner state ρ_w is N-undistillable.

Proof. We can overlook the $\frac{1}{d^2+\beta d}$ factor since it does not affect positivity,

$$\left(\rho_w^{T_A}\right)^{\otimes N} = I^{\otimes N} + \sum_{m=1}^{N} \beta^m \sum_{\mathrm{seq}(m,N)} G^{i_1} \otimes G^{i_2} \otimes \cdots \otimes G^{i_N}, \tag{B1}$$

where $\mathrm{seq}(m, N)$ denotes all possible binary $i_1, \ldots, i_N$ sequences with m ones and $N-m$ zeros. For convenience, denote $Z_0 = \{n|i_n = 0\}$, $Z_1 = \{n|i_n = 1\}$,

$$\begin{aligned} &M_N G^{i_1} \otimes G^{i_2} \otimes \cdots \otimes G^{i_N} M_N^\dagger \\ &= M_N \sum_{j_1 \cdots j_{2N}} \big| \cdots j_{2n-1} j_{2n-i_n} \cdots \big\rangle \big\langle \cdots j_{2n-1+i_n} j_{2n} \cdots \big| M_N^\dagger \\ &= \sum_{j_1 \cdots j_{2N}} \big| \ldots j_{2n-1} \ldots, \ldots j_{2n-i_n} \ldots \big\rangle \\ &\quad \times \big\langle \ldots j_{2n-1+i_n} \ldots, \ldots j_{2n} \ldots \big| \\ &= d^m \sum_{j_{2n-1}, j_{2n}, n \in Z_0} |\psi_{j_{2n-1}, j_{2n}, n\in Z_0}\rangle\langle\psi_{j_{2n-1}, j_{2n}, n\in Z_0}|, \end{aligned} \tag{B2}$$

where the sum is taken over all indexes in the subscript within the range of $\{0, \ldots, d-1\}$ (the same goes for all similar sums below), and

$$\big|\psi_{j_{2n-1}, j_{2n}, n\in Z_0}\big\rangle = \frac{1}{\sqrt{d^m}} \sum_{j_{2n-1}, n\in Z_1} \big| \ldots j_{2n-1} \ldots, \ldots j_{2n-i_n} \ldots \big\rangle. \tag{B3}$$

Any pure quantum state $|\psi^{SR\leqslant 2}\rangle$ of Schmidt rank no larger than 2 can be decomposed into

$$|\psi^{SR\leqslant 2}\rangle = \sum_{j_{2n-1}, j_{2n}, n\in Z_0} p_{j_{2n-1}, j_{2n}, n\in Z_0} \big|\psi^{SR\leqslant 2}_{j_{2n-1}, j_{2n}, n\in Z_0}\big\rangle, \tag{B4}$$

where $|\psi^{SR\leqslant 2}_{j_{2n-1}, j_{2n}, n\in Z_0}\rangle$ is the normalized extraction of all $|\ldots j_{2n-1} \ldots, \ldots j_{2n} \ldots\rangle, n \in Z_0$ terms in $|\psi^{SR\leqslant 2}\rangle$, namely, if

$$|\psi^{SR\leqslant 2}\rangle = \sum_{k_1, \ldots, k_{2N}} c_{k_1, \ldots, k_{2N}} |k_1, \ldots, k_{2N}\rangle, \tag{B5}$$

then

$$\begin{aligned} \big|\psi^{SR\leqslant 2}_{j_{2n-1}, j_{2n}, n\in Z_0}\big\rangle = &\frac{1}{p_{j_{2n-1}, j_{2n}, n\in Z_0}} \sum_{j_{2n-1}, j_{2n}, n\in Z_1} c_{\ldots j_{2n-1} \ldots, \ldots j_{2n} \ldots} \\ &\times |\ldots j_{2n-1} \ldots, \ldots j_{2n} \ldots\rangle, \end{aligned} \tag{B6}$$

where

$$p_{j_{2n-1}, j_{2n}, n\in Z_0} = \sqrt{\sum_{j_{2n-1}, j_{2n}, n\in Z_1} |c_{\ldots j_{2n-1} \ldots, \ldots j_{2n} \ldots}|^2}. \tag{B7}$$

It can be proven that $|\psi^{SR\leqslant 2}_{j_{2n-1}, j_{2n}, n\in Z_0}\rangle$ also has Schmidt rank less than or equal to 2. According to state-operator isomorphism, the Schmidt rank of a state is equal to the rank of the corresponding operator. In fact, the operator corresponding to $|\psi^{SR\leqslant 2}_{j_{2n-1}, j_{2n}, n\in Z_0}\rangle$ is the extraction of d^m rows $\ldots j_{2n-1} \ldots, n \in Z_0$, and d^m columns $\ldots j_{2n} \ldots, n \in Z_0$. The row and column numbers $\ldots j_{2n-1} \ldots$ and $\ldots j_{2n} \ldots$ are written in base-d numeral systems. Therefore, the operator corresponding to

$|\psi^{\mathrm{SR}\leqslant 2}_{j_{2n-1},j_{2n},n\in Z_0}\rangle$ is a submatrix of the operator corresponding to $|\psi^{\mathrm{SR}\leqslant 2}\rangle$. The rank of a submatrix is no larger than the rank of the entire matrix, therefore $|\psi^{\mathrm{SR}\leqslant 2}_{j_{2n-1},j_{2n},n\in Z_0}\rangle$ must have Schmidt rank no larger than 2. Using Lem. IV.1, it is then clear that

$$\left|\left\langle\psi^{\mathrm{SR}\leqslant 2}_{j_{2n-1},j_{2n},n\in Z_0}\middle|\psi_{j_{2n-1},j_{2n},n\in Z_0}\right\rangle\right|^2 \leqslant \frac{2}{d^m}, \tag{B8}$$

and so

$$\begin{aligned}&\langle\psi^{\mathrm{SR}\leqslant 2}|M_N G^{i_1}\otimes G^{i_2}\otimes\cdots\otimes G^{i_N}M_N^\dagger|\psi^{\mathrm{SR}\leqslant 2}\rangle\\ &\leqslant d^m\frac{2}{d^m}\sum_{j_{2n-1},j_{2n},n\in Z_0}\left|p_{j_{2n-1},j_{2n},n\in Z_0}\right|^2 = 2.\end{aligned} \tag{B9}$$

Considering the fact that all even terms in $(\rho_w^{T_A})^{\otimes N}$ are nonnegative and using the above inequality on all odd terms, a lower bound is obtained:

$$\begin{aligned}&\langle\psi^{\mathrm{SR}\leqslant 2}|M_N(\rho_w^{T_A})^{\otimes N}M_N^\dagger|\psi^{\mathrm{SR}\leqslant 2}\rangle\\ &\geqslant 1+\sum_{k=1}^{\lceil\frac{N}{2}\rceil}2C_N^{2k-1}\beta^{2k-1} = 1+(1+\beta)^N-(1-\beta)^N.\end{aligned} \tag{B10}$$

For $\beta\in(-1,0)$, any β greater than the zero point β_0 would make $1+(1+\beta)^N-(1-\beta)^N$ greater than zero, thus ensuring the positivity of $\langle\psi^{\mathrm{SR}\leqslant 2}|M_N(\rho_w^{T_A})^{\otimes N}M_N^\dagger|\psi^{\mathrm{SR}\leqslant 2}\rangle$. ■

APPENDIX C: PROOF OF THEOREM V.1

Theorem C.1. Werner state ρ_w is N-undistillable iff the following holds for all $d^N\times d^N$ X_2:

$$\sum_{S\subset\{1,\dots,N\}}\beta^{|S|}||\mathrm{Tr}_S(X_2)||_F^2\geqslant 0, \tag{C1}$$

where Tr_S takes partial traces of the subsystems in set S.

Proof. We have already established that N-undistillability is equivalent to

$$\langle\psi^{\mathrm{SR}\leqslant 2}|M_N(\rho^{T_A})^{\otimes N}M_N^\dagger|\psi^{\mathrm{SR}\leqslant 2}\rangle\geqslant 0. \tag{C2}$$

In the Appendix B, it has been established that

$$(\rho_w^{T_A})^{\otimes N} = I^{\otimes N}+\sum_{m=1}^{N}\beta^m\sum_{\mathrm{seq}(m,N)}G^{i_1}\otimes G^{i_2}\otimes\cdots\otimes G^{i_N}, \tag{C3}$$

$$\begin{aligned}&M_N G^{i_1}\otimes G^{i_2}\otimes\cdots\otimes G^{i_N}M_N^\dagger\\ &= d^m\sum_{j_{2n-1},j_{2n},n\in Z_0}\left|\psi_{j_{2n-1},j_{2n},n\in Z_0}\right\rangle\left\langle\psi_{j_{2n-1},j_{2n},n\in Z_0}\right|,\end{aligned} \tag{C4}$$

where the sum is taken over all indexes in the subscript within the range of $\{0,\dots,d-1\}$ (the same goes for all similar sums below), and

$$\begin{aligned}&\left|\psi_{j_{2n-1},j_{2n},n\in Z_0}\right\rangle\\ &= \frac{1}{\sqrt{d^m}}\sum_{j_{2n-1},n\in Z_1}\left|\dots j_{2n-1}\dots,\dots j_{2n-i_n}\dots\right\rangle.\end{aligned} \tag{C5}$$

For a pure quantum state of the form

$$|\psi^{\mathrm{SR}\leqslant 2}\rangle = \sum_{j_1,\dots,j_N}c_{\dots j_{2n-1}\dots,\dots j_{2n}\dots}|\dots j_{2n-1}\dots,\dots j_{2n}\dots\rangle, \tag{C6}$$

$$\begin{aligned}&\langle\psi^{\mathrm{SR}\leqslant 2}|M_N G^{i_1}\otimes G^{i_2}\otimes\cdots\otimes G^{i_N}M_N^\dagger|\psi^{\mathrm{SR}\leqslant 2}\rangle\\ &= d^m\sum_{j_{2n-1},j_{2n},n\in Z_0}|\langle\psi_{j_{2n-1},j_{2n},n\in Z_0}|\psi^{\mathrm{SR}\leqslant 2}\rangle|^2\\ &= \sum_{j_{2n-1},j_{2n},n\in Z_0}\left|\sum_{j_{2n-1},n\in Z_1}c_{\dots j_{2n-1}\dots,\dots j_{2n-i_n}\dots}\right|^2\\ &= ||\mathrm{Tr}_{\{i_n|n\in Z_1\}}(X_2)||_F^2.\end{aligned} \tag{C7}$$

In the last equality, X_2 is the result of state-operator isomorphism from $|\psi^{\mathrm{SR}\leqslant 2}\rangle$. Noticing that

$$\langle\psi^{\mathrm{SR}\leqslant 2}|M_N I^{\otimes N}M_N^\dagger|\psi^{\mathrm{SR}\leqslant 2}\rangle = 1 = \beta^0||X_2||_F^2, \tag{C8}$$

it then follows that

$$\langle\psi^{\mathrm{SR}\leqslant 2}|M_N(\rho^{T_A})^{\otimes N}M_N^\dagger|\psi^{\mathrm{SR}\leqslant 2}\rangle\geqslant 0 \tag{C9}$$

is equivalent to

$$\sum_{S\subset\{1,\dots,N\}}\beta^{|S|}||\mathrm{Tr}_S(X_2)||_F^2\geqslant 0. \tag{C10}$$

■

APPENDIX D: PROOF OF THEOREM V.3

Theorem D.1. Werner state ρ_w is N-undistillable iff

$$\mathrm{Re}[f_N(X_1,X_1')]^2\leqslant f_N(X_1',X_1')f_N(X_1,X_1), \tag{D1}$$

where

$$f_N(X_1,X_1') = \sum_{S\subset\{1,\dots,N\}}\beta^{|S|}\mathrm{Tr}[\mathrm{Tr}_S^\dagger(X_1)\mathrm{Tr}_S(X_1')]\geqslant 0, \tag{D2}$$

where $X_1=\mathbf{w}^\dagger\mathbf{x}$, $X_1'=\mathbf{y}^\dagger\mathbf{z}$ are $d^N\times d^N$ rank-1 matrices, and their component vectors $\mathbf{w},\mathbf{x},\mathbf{y},\mathbf{z}$ satisfy $\mathbf{w}\perp\mathbf{y}$, $\mathbf{x}\perp\mathbf{z}$.

Proof. It has been proven that N-undistillability is equivalent to

$$\sum_{S\subset\{1,\dots,N\}}\beta^{|S|}||\mathrm{Tr}_S(X_2)||_F^2\geqslant 0. \tag{D3}$$

Since any rank-2 matrix can be decomposed via singular value decomposition:

$$X_2=\sigma_1X_1+\sigma_2X_1', \tag{D4}$$

Eq. (D3) can be written as

$$\begin{aligned}&\sum_{S\subset\{1,\dots,N\}}\beta^{|S|}||\mathrm{Tr}_S(X_2)||_F^2\\ &= \sum_{S\subset\{1,\dots,N\}}\beta^{|S|}\big[\sigma_1^2||\mathrm{Tr}_S(X_1)||_F^2+\sigma_2^2||\mathrm{Tr}_S(X_1')||_F^2\\ &\quad+2\sigma_1\sigma_2\mathrm{Re}(\mathrm{Tr}(\mathrm{Tr}_S(X_1)^\dagger\mathrm{Tr}_S(X_1')))\big]\\ &= \sigma_1^2f_N(X_1,X_1)+\sigma_2^2f_N(X_1',X_1')\\ &\quad+2\sigma_1\sigma_2\mathrm{Re}[f_N(X_1,X_1')]\\ &\geqslant 0.\end{aligned} \tag{D5}$$

The above should hold for all singular values σ_1, σ_2, which is then equivalent to

$$\mathrm{Re}[f_N(X_1, X_1')]^2 \leqslant f_N(X_1, X_1) f_N(X_1', X_1'), \tag{D6}$$

always holding when $X_1 = \mathbf{w}^\dagger \mathbf{x}$, $X_1' = \mathbf{y}^\dagger \mathbf{z}$ are $d^N \times d^N$ rank-1 matrices, and their component vectors $\mathbf{w}, \mathbf{x}, \mathbf{y}, \mathbf{z}$ satisfy $\mathbf{w} \perp \mathbf{y}, \mathbf{x} \perp \mathbf{z}$. ■

APPENDIX E: PROOF OF LEM. V.2

Lemma E.1. The inequalities

$$||\mathrm{Tr}_1(X_1)||_F^2 \leqslant ||X_1||_F^2, \; ||\mathrm{Tr}_2(X_1)||_F^2 \leqslant ||X_1||_F^2 \tag{E1}$$

hold for any $d^2 \times d^2$ square matrix X_1 with rank 1.

Proof. A rank-1 matrix X_1 can always be written as the outer product of two vectors (in this case, bipartite):

$$(X_1)_{ij,kl} = w_{ij} x_{kl}. \tag{E2}$$

Its partial traces can be computed accordingly:

$$[\mathrm{Tr}_2(X_1)]_{i,k} = \sum_{j=0}^{d-1} w_{ij} x_{kj}, \; [\mathrm{Tr}_1(X_1)]_{j,l} = \sum_{i=0}^{d-1} w_{ij} x_{il}. \tag{E3}$$

A direct calculation and application of Cauchy-Schwartz inequality yields the desired result:

$$||\mathrm{Tr}_2(X_1)||_F^2 = \sum_{i,k=0}^{d-1} \left| \sum_{j=0}^{d-1} w_{ij} x_{kj} \right|^2 \leqslant \sum_{i,k=0}^{d-1} \sum_{j=0}^{d-1} |w_{ij}|^2 \sum_{l=0}^{d-1} |x_{kl}|^2$$

$$= \sum_{i,j,k,l=0}^{d-1} |w_{ij}|^2 |x_{kl}|^2 = ||X_1||_F^2, \tag{E4}$$

$$||\mathrm{Tr}_1(X_1)||_F^2 = \sum_{j,l=0}^{d-1} \left| \sum_{i=0}^{d-1} w_{ij} x_{il} \right|^2 \leqslant \sum_{j,l=0}^{d-1} \sum_{i=0}^{d-1} |w_{ij}|^2 \sum_{k=0}^{d-1} |x_{kl}|^2$$

$$= \sum_{i,j,k,l=0}^{d-1} |w_{ij}|^2 |x_{kl}|^2 = ||X_1||_F^2. \tag{E5}$$

APPENDIX F: PROVING NONCONVEXITY

We now prove that the function of $g(C)_{D_0}$ is nonconvex by showing that its local minimum set is not a convex one. For

$$C = \mathbf{w}\mathbf{x}^T, \quad D_0 = \mathbf{y}\mathbf{z}^T, \tag{F1}$$

we set vectors $\mathbf{y}$ and $\mathbf{z}$ to identical forms of

$$y_{ij} = z_{ij} = \delta_{i0}\delta_{j1}. \tag{F2}$$

For simplicity, we first write the variables $\mathbf{w}, \mathbf{x}$ in a matrix form of

$$\begin{pmatrix} w_{00} & w_{01} & \cdots & w_{d-1,d-1} \\ x_{00} & x_{01} & \cdots & x_{d-1,d-1} \end{pmatrix},$$

where the two rows correspond to two vectors $\mathbf{w}$, $\mathbf{x}$, respectively. We take the middle point combination of the following two points:

$$\begin{pmatrix} 0 & 1 & \cdots 0 \\ 0 & 1 & \cdots 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 & \cdots 0 \\ 1 & 0 & \cdots 0 \end{pmatrix}.$$

Both of these points can be proven to have zero Jacobian matrix and positive-definite Hessian, effectively making them local minimums.

For a convex function, its local minimum set must be a convex set, so that a middle point combination of any two points should stay in the set. Their middle point combination is

$$\begin{pmatrix} 1 & 1 & 0 & \cdots 0 \\ 1 & 1 & 0 & \cdots 0 \end{pmatrix}.$$

The normalization factor does not change whether the Jacobian matrix is nonzero or not, and therefore is interchangeable and omitted here. At this particular point, the Jacobian matrix is nonzero and proportional to

$$[1, 1, 0, 0, 0, 0, 0, 0, 0, 1, 1, 0, 0, 0, 0, 0, 0, 0], \tag{F3}$$

which suggests that the middle point is not a local minimum, thus proving the nonconvexity of the set of local minimums. It then follows that the function of $g(C, D)$ is nonconvex.

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