Bell nonlocality measure of density matrix based on trace distance

Yuxuan Fu and Liting Li [*]

School of Computer Science and Technology, University of Science and Technology of China, Hefei, Anhui, 230027, China

[*] Corresponding author's e-mail: ltli@mail.ustc.edu.cn

Abstract: Quantum information technology exhibits advantages in terms of algorithm efficiency, communication security, and other aspects compared to classical information technology, partially due to quantum nonlocality, which is a characteristic that distinguishes quantum mechanics from classical mechanics. Compared to quantum entanglement and quantum steering, Bell nonlocality exhibits stronger quantum properties in a certain sense. However, research on efficient estimation of Bell nonlocality of general quantum states remains rare. This work proposes a generalized Bell nonlocality measure of density matrices. Our method generalizes the fundamental matrix for classical correlation and applies it to experimental scenarios of various dimensions. We prove that this measure of Bell nonlocality is well-defined. We also propose a relaxation algorithm for numerically estimating this measure. Applying the see-saw method, the algorithm obtains an upper bound on this measure. Numerical experiments show the effectiveness of our method in low dimensions and suggest that it could be used in high dimensions.

1. Introduction

The emergence of quantum information science offers a novel approach to overcoming the predictions of Moore's Law [1]. From the initial proposition of the "EPR paradox" [2] to the concept of local hidden variable models (LHVM) [3], there has been increasing exploration into quantum entanglement and Bell nonlocality. These properties, absent in classical mechanics, serve as crucial physical resources widely employed in the design of quantum algorithms [4-5] and information processing protocols [6-9]. These quantum characteristics are also the fundamental reason why quantum information technology exhibits advantages compared to classical methods.

For a considerable period, researchers believed Bell nonlocality and quantum entanglement were fundamentally the same until Werner and WOLF [10] demonstrated that entanglement and Bell nonlocality are two distinct properties of quantum states. Furthermore, Wiseman et al. [11] provided a rigorous mathematical explanation for LHVM, indicating that steerability is stronger than nonseparability and weaker than Bell nonlocality, forming a strict hierarchy, as depicted in Figure 1. This indicates that any quantum state possessing Bell nonlocality must entangled and steerable.

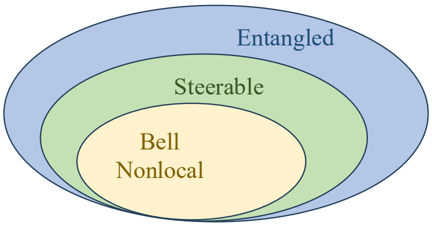

Figure 1. Hierarchy between quantum entanglement, quantum steering, and Bell nonlocality.

In 2014, De [12] proposed a quantum resource theory for nonlocality, which introduced requirements for a well-defined measure of Bell nonlocality and demonstrated previous measures [13-16]. Subsequently, there have been several researchers proposing measures of Bell nonlocality. However, these measures are either solely of correlations instead of density matrices [17], or are based on Bell's inequality which is hard to solve [18], or solved in low dimensions [19-20]. Quantifying Bell nonlocality of density matrices is challenging due to the high dimensionality, involvement of numerous unknown variables, and complex constraint conditions, and the problem is a high-order non-convex optimization, making it difficult to have a general solution method.

In this paper, we propose a Bell nonlocality measure of the density matrix based on trace distance, extending the results of Brito [16]. In Section 2, we introduce the fundamental matrix for classical correlations. In Section 3, we present our Bell nonlocality measure of the density matrix and provide proofs in Section 4. Section 5 and Section 6 derive numerical methods for computing upper bounds on this Bell nonlocality measure and conduct experimental validation. Finally, Section 7 summarizes our work.

2. Classical correlation fundamental matrix

An LHVM refers to the joint conditional probability distribution of outcomes a and b given measurement choices x and y for a physical system, satisfying the following equation [3]:

$$p(a,b \mid x,y) = \sum_{\lambda} p_{\lambda} p(a \mid x,\lambda) p(b \mid y,\lambda), \sum_{\lambda} p_{\lambda} = 1 \tag{1}$$

A system for which all generated correlations can be described by LHVM is considered Bell-local; otherwise, it is Bell-nonlocal. However, determining Bell's nonlocality based on LHVM is challenging. In the unified framework of Bell's theorem mentioned by Chaves et al. [21], the method of constructing the fundamental matrix using deterministic functions aids in reformulating Bell's theorem. We refer to this matrix as the classical correlation fundamental matrix.

Each experimental scenario corresponds to a unique coefficient matrix T. We set two subsystems, A and B, to be quantum systems with d levels each. On Subsystem A, Alice can choose d_x measurements, denoted by x, where each measurement may yield d_a outcomes, denoted by a. The same applies to Subsystem B. We provide matrix T according to the following steps.

Step 1: For $p(a,b \mid x,y)$, we arrange it sequentially to get an $n = d_x \times d_a \times d_y \times d_b$ dimensional vector, denoted as q.

Step 2: We define functions $f(\times,\lambda_a)$ and $g(\times,\lambda_b)$, where $f(\times,\lambda_a)$ represents all functions from X to A, totaling $\mathrm{d}_a^{\mathrm{d}_x}$ functions. $\lambda_a = (a_0, a_1, \ldots, a_{d_x-1})$ denotes that the function $f(\times,\lambda = i)$ maps $x = 0, x = 1, \ldots, x = d_x - 1$ to $a_0, a_1, \ldots, a_{d_x-1}$. The definition of function $g(\times,\lambda = i)$ is similar.

Step 3: The classical correlation fundamental matrix T is an $n \times m$ dimensional binary matrix, where $n = d_x \times d_a \times d_y \times d_b$, and $m = d_a^{d_x} \times d_b^{d_y}$. The element in the j-th row and i-th column of matrix T is defined as:

$$T_{j,i} = \delta_{a,f(x,\lambda_a = i(0:d_a^{d_x}-1))} \delta_{b,g(y,\lambda_b = i(d_a^{d_x}:m))} \tag{2}$$

where $j = (x,a,y,b), i = (a_0, a_1, \ldots, a_{d_x-1}, b_0, b_1, \ldots, b_{d_y-1})$.

Step 4: The LHVM equation can be equivalently expressed by using the classical correlation fundamental matrix as:

$$q = T \cdot \lambda \text{ or } q(j) = \sum_i T_{j,i}\lambda_i, \text{ where } \sum_i \lambda_i = 1. \tag{3}$$

3. Bell nonlocality measure for density matrix

3.1 Bell nonlocality measure for correlations

The set formed by classical correlations p is a convex set, called the classical correlation set, denoted as C_c, where any vector within the set can be represented as a convex combination of column vectors of the classical correlation fundamental matrix T.

$$C_c = \{p \mid p = T \cdot \lambda, \sum_i \lambda_i = 1\} \tag{4}$$

Brito et al. [16] proposed using the trace distance from the correlation vector to C_c to quantify the Bell nonlocality of correlations. Because the trace distance satisfies the triangle inequality and has low complexity, it is algorithm-friendly. It is additionally agreed upon that different measurement choices are equiprobable, i.e., $P(x,y) = \frac{1}{d_x \times d_y}$. Therefore, the Bell nonlocality measure of the correlation $q(a,b \mid x,y)$, as shown in Figure 2, can be represented as its distance to the classical correlation set:

$$NL(q) = \frac{1}{d_x \times d_y} \min_{p \in C_c} D(p(a,b \mid x,y), q(a,b \mid x,y)) = \frac{1}{2 \times d_x \times d_y} \min_{p \in C_c} \|p - q\|_{l1} \tag{5}$$

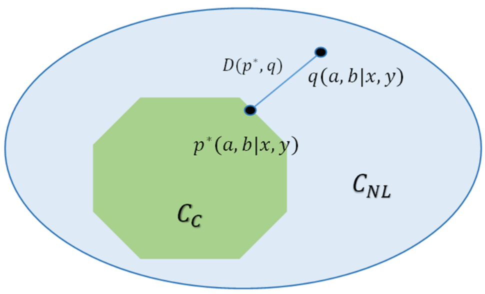

Figure 2. Bell nonlocality measure based on trace distance.

The most crucial part of the measure, $\min_{p \in C_c} \|p - q\|_{l1}$, can be rewritten as a linear programming problem:

$$\begin{gathered} \min_{t \in R^n, \lambda \in R^m} \langle 1_n, t \rangle \\ \text{subject to } -t \leq q - T \cdot \lambda \leq t, \\ \sum_i \lambda_i = 1, \quad \lambda \geq 0. \end{gathered} \tag{6}$$

3.2 Bell nonlocality measure for the density matrix

Density matrices, under different measurement choices, can generate various correlations q. To quantify the Bell nonlocality of density matrices, we use the maximum value of Bell nonlocality among all correlations as the measure of the density matrix's Bell nonlocality.

Additionally, some technical details need to be defined. Firstly, the setup of experimental scenarios should be consistent with the definition of the classical correlation fundamental matrix. Secondly, since we are only concerned with the probability distribution of the system after measurement and do not care about the change in the system's state, we adopt POVM measurements. The POVM operators

$\{A_a^x\}$ and $\{B_b^y\}$ should satisfy the positive semi-definiteness condition and the completeness condition. With the definition of $NL(q)$, we obtain the Bell nonlocality measure for the density matrix as follows.

$$\begin{aligned} NL(\rho) &= \max_{\{A_a^x\}\{B_b^y\}\text{ are POVMs}} NL(q), \quad \text{with } q(a,b\mid x,y) = \mathrm{Tr}\left(A_a^x \otimes B_b^y \rho\right) \\ &= \max_{\{A_a^x\}\{B_b^y\}\text{ are POVMs}} \min_{p\in C_c} D(p,q) \\ &= \max_{\{A_a^x\}\{B_b^y\}\text{ are POVMs}} \min_{t\in\mathbb{R}^n,\lambda\in\mathbb{R}^m} \langle 1_n, t\rangle \\ \text{subject to } & -t \le q - T\cdot\lambda \le t, \\ & \sum_i \lambda_i = 1, \quad \lambda \ge 0. \end{aligned} \tag{7}$$

The inner layer of this nested optimization problem involves minimizing, while the outer layer involves maximizing. To unify the two, we calculate the dual problem for the inner optimization problem:

$$\begin{aligned} &\max_{v\in R^n,\alpha\in R} \langle 2v - 1_n, q\rangle - \alpha \\ &\text{subject to } T^T\left(1_n - 2v\right) + \alpha 1_n \ge 0, \\ &\qquad 0 \le v \le 1. \end{aligned} \tag{8}$$

By utilizing the dual problem, we ultimately provide the complete definition:

$$\begin{aligned} NL(\rho) &= \max_{\{A_a^x\}\{B_b^y\}\subset\mathbb{C}^{d^2\times d^2}} \min_{t\in\mathbb{R}^n,\lambda\in\mathbb{R}^m} \langle 1_n, t\rangle, \quad \text{with } q(a,b\mid x,y) = \mathrm{Tr}\left(A_a^x \otimes B_b^y \rho\right) \\ &= \max_{\{A_a^x\}\{B_b^y\}\subset\mathbb{C}^{d^2\times d^2}} \max_{v\in\mathbb{R}^n,\alpha\in\mathbb{R}} \langle 2v - 1_n, q\rangle - \alpha \\ &= \max_{\{A_a^x\}\{B_b^y\}\subset\mathbb{C}^{d^2\times d^2}, v\in\mathbb{R}^n,\alpha\in\mathbb{R}} \langle 2v - 1_n, q\rangle - \alpha \\ \text{subject to } & T^T\left(1_n - 2v\right) + \alpha \times 1_n \ge 0, \\ & 0 \le v \le 1, \\ & \sum_a A_a^x = I_d, \text{ for any } x, \quad \sum_b B_b^y = I_d, \text{ for any } y, \\ & A_a^x, B_b^y \ge 0, \text{for any } a,b,x,y. \end{aligned} \tag{9}$$

4. The effectiveness of the measure

The fundamental requirements for a well-defined Bell nonlocality measure for density matrices can be derived from that for correlations, just as defined by De [12]:

(N1) $NL(\rho) = 0$, if ρ is Bell-local.

(N2) $NL(\rho 1) \ge NL(\rho 2)$, if $\rho_2 = p_0 l + \sum_{i=1} p_i \mathcal{O}_i(\rho_1)$, where $\{p_i\}$ forms a convex combination, l is a local quantum state, and $\mathcal{O}$ denotes relabeling R, output coarse graining G, and input substitution K.

Proof of (N1): For a Bell-nonlocal density matrix ρ, all correlations generated by ρ are classical correlations, that is $q \in C_c$, any q with ρ. In this case, property (N1) is satisfied.

Proof of (N2): We demonstrate that the measure is convex. For the density matrix $\lambda\rho_1 + (1-\lambda)\rho_2$, there exists an optimal set of POVM operators, $\{A_a^{x^\star}\}$ and $\{B_b^{y^\star}\}$, such that the maximum value is attained with this set of POVM operators. So:

$$NL(\lambda\rho_1 + (1-\lambda)\rho_2) = NL(q^\star)$$

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$$q^{\star}(x,a,b,y)=\mathrm{Tr}(A_a^{x^\star}\otimes B_b^{y^\star}(\lambda\rho_1+(1-\lambda)\rho_2))=\lambda\mathrm{Tr}(A_a^{x^\star}\otimes B_b^{y^\star}\rho_1)+(1-\lambda)\mathrm{Tr}(A_a^{x^\star}\otimes B_b^{y^\star}\rho_2)$$
$$=\lambda q_1+(1-\lambda)q_2$$

We set $p^\star$ as the optimal solution of $\min_{p\in C_c} D(p,q^\star)$, and $p_1^\star$ and $p_2^\star$ as the optimal solutions of $\min_{p\in C_c} D(p,q_1)$ and $\min_{p\in C_c} D(p,q_2)$, respectively.

$$\begin{aligned} NL(q^\star)&=\min_{p\in C_c} D(p,q^\star)=D(p^\star,q^\star)\\ &\le D(\lambda p_1^\star+(1-\lambda)p_2^\star,\lambda q_1+(1-\lambda)q_2)\\ &\le \lambda D(p_1^\star,q_1)+(1-\lambda)D(p_2^\star,q_2)\\ &\le \lambda NL(\rho_1)+(1-\lambda)NL(\rho_2)\end{aligned}$$

Next, we provide proofs for R, G, and K. Relabeling R essentially change the order of labeling in the experimental scenarios. For any correlation q, relabeling its indices without altering its content does not affect the nonlocality of the density matrix. Output coarse graining operation G merges some of the outputs. By utilizing the triangle inequality of the trace norm, we can show that $NL(G(\rho))$ does not increase. Input substitution K preserves the locality of correlation relations and does not increase under unchanged dimensions.

5. Relaxation and numerical solving

5.1 Modeling and relaxation

The original problem is a maximization optimization problem, with a non-convex cubic objective function and semi-definite constraints. Additionally, the constraints of (ν,α) and the POVM operators can be separated. Therefore, the entire problem is a non-convex optimization problem with separable semi-definite constraints. This type of problem is usually difficult to solve directly.

To solve it effectively, we introduce relaxation variables, replacing the quadratic outer product terms with relaxation variable matrices K, and transforming the cubic objective function into a quadratic bilinear function, thereby reducing dimensionality. Meanwhile, we retain the remaining bilinear terms and utilize separable constraint conditions to reduce relaxation errors. The solution provides an upper bound.

We denote $K_{x,a,y,b}=A_a^x\otimes B_b^y$ and then have $A_a^x=\mathrm{Tr}_B(K_{x,a,y,b}), B_b^y=\mathrm{Tr}_A(K_{x,a,y,b})$.

Replacing the outer product terms of the POVM operators with K, and reorganizing the original problem yields:

$$NL(\rho)=\max_{\{K_{a,b,x,y}\}\text{ are }4\times4\text{ matrices}} NL(q),\ \text{with } q_i=\mathrm{Tr}\left[K_i\rho\right]$$
$$=\max_{\{K_{a,b,x,y}\}\text{ are }4\times4\text{ matrices}}\left(\frac{1}{2\times d_x\times d_y}\min_{\lambda\in R^m}\left\|q-T\cdot\lambda\right\|_{l1}\right)$$

$$= \frac{1}{2 \times d_x \times d_y} \max_{\{K_{a,b,x,y}\} \text{ are } 4\times 4 \text{ matrices}} \max_{\alpha \in R, v \in R^n} \left(\langle 2v - 1_n, q \rangle - \alpha \right)$$

$$= \frac{1}{2 \times d_x \times d_y} \max_{\{K_{a,b,x,y}\} \text{ are } 4\times 4 \text{ matrices}, \alpha \in R, v \in R^n} \left(\langle 2v - 1_n, q \rangle - \alpha \right)$$

Subject to

$$\begin{aligned} &\mathrm{Tr}_B\left(K_{a,b,x,y}\right) = \mathrm{Tr}_B\left(K_{a,b',x,y'}\right) =: A_a^x, \quad \forall a, x, \\ &\mathrm{Tr}_A\left(K_{a,b,x,y}\right) = \mathrm{Tr}_A\left(K_{a',b,x',y}\right) =: B_b^y, \quad \forall b, y, \\ &A_a^x, B_b^y \geq 0 \quad \forall a, b, x, y, \\ &\sum_a A_a^x = I \quad \forall x, \quad \sum_b B_b^y = I \quad \forall y, \\ &T^T\left(1_n - 2v\right) + 1_m \cdot \alpha \geq 0, \\ &0_n \leq v \leq 1_n. \end{aligned} \tag{10}$$

After relaxation, the new problem becomes a continuous separable constraint bilinear problem. Introducing the relaxation variable K will magnify the solution, and the solution to the relaxation problem provides an upper bound.

Using $n = d_x \times d_a \times d_y \times d_b$ matrices K to represent $n' = d_x \times d_a + d_y \times d_b$ POVM elements is redundant. We derive equality constraints for the matrix group variables $\{K_{x,a,y,b}\}$ based on the properties of the POVM operators, thus improving experimental efficiency.

By summing over indices a and b simultaneously on both sides of the equation $K_{x,a,y,b} = A_a^x \otimes B_b^y$, we obtain the following constraints:

$$\sum_a \sum_b K_{x,a,y,b} = I_d \otimes I_d = I_{d^2} \tag{11}$$

Furthermore, since each POVM operator can be derived from $d_y \times d_b$ K matrices, we have the following constraints.

$$\sum_b K_{x,a,y=0,b} = \sum_b K_{x,a,y=1,b} = \ldots = \sum_b K_{x,a,y=d_y-1,b} \tag{12}$$

$$\sum_a K_{x=0,a,y,b} = \sum_a K_{x=1,a,y,b} = \ldots = \sum_a K_{x=d_x-1,a,y,b} \tag{13}$$

5.2 Solution of the see-saw method

We utilize the see-saw iterative algorithm [10] for solving the optimization problem. Its main idea is to alternately optimize the two parts of variables with separable constraints until the objective function value converges to an acceptable accuracy. The two optimization subproblems in this relaxation problem are linear optimization and semi-definite optimization.

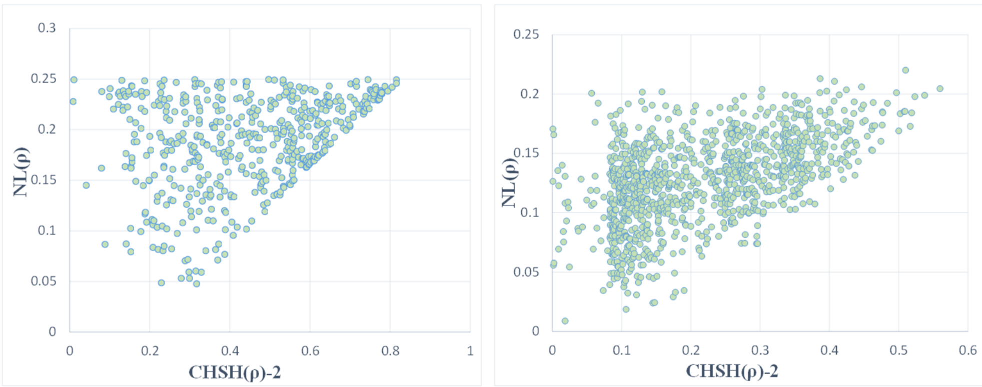
We should acknowledge that the see-saw method has some drawbacks. Like most numerical optimization methods for non-convex problems, the see-saw method cannot guarantee convergence to the global optimum. Secondly, the see-saw method depends on the initial value selection, and the algorithm may converge to a local optimum. However, we still consider the see-saw method as a good tool for finding the upper bound of the density matrix Bell nonlocality. As seen from subsequent experiments, the see-saw method can quickly converge to some extremum after several iterations, and it can also avoid falling into local optima by random initial values multiple times.

6. Numerical evaluation

This section conducts numerical evaluations on the relaxation problem. We use MATLAB R2023a and the CVX package for optimization modeling. The SDPT3 solver is used to address the semi-definite programming (SDP) portion of the overall optimization problem.

6.1 The numerical results for the scenario $(2, 2, 2, 2)$

Figure 3 illustrates the relationship between the maximum violation of the CHSH inequality and $NL(\rho)$ when optimization is successful on entangled pure states and mixed states, and $NL(\rho)$ provides an upper bound. Figure 3 (a): When there is weaker Bell nonlocality, the upper bound is relaxed, whereas when there is stronger Bell nonlocality, $NL(\rho)$ are more accurate. Figure 3 (b): $NL(\rho)$ provides an upper bound also, with the bound being more relaxed when the nonlocality is weak and becoming more accurate as the nonlocality increases.



(a) entangled pure states (b) mixed states

Figure 3. Maximum violation of the CHSH inequality and $NL(\rho)$ on entangled pure states and mixed states.

Table 1 presents the success probability under current settings on entangled pure states and mixed states. For local mixed states, the see-saw method yields a result of 0 with a success probability of 0.989. For both entangled pure states and nonlocal mixed states, the success probability increases with the increase in the violation of the CHSH inequality. When the violation of the CHSH inequality approaches its maximum value, the success probability tends to be close to 1.

Table 1. Probability of success on entangled pure states and mixed states.

CHSH(ρ)-2	Probability of success on entangled pure states	Probability of success on mixed states
<0	/	0.989247312
0-0.15	0.173611111	0.789655172
0.15-0.5	0.614349776	0.930706522
0.5-0.828	0.985915493	1

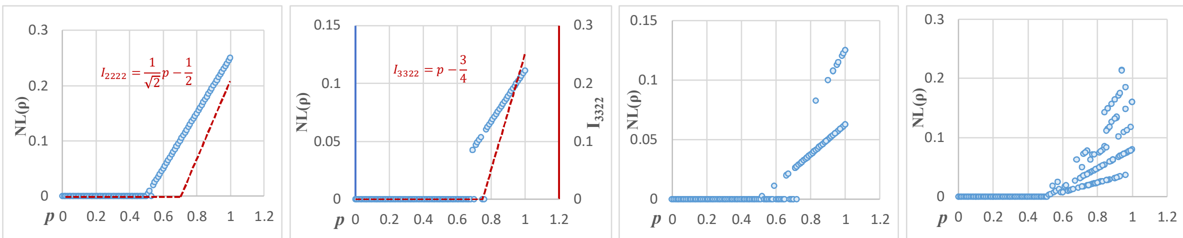
On product pure states, the CHSH inequality is always satisfied and never violated. $NL(\rho)$ also yields a value of 0 with a probability exceeding 99%.

6.2 The numerical results for the scenario $(n, n, 2, 2)$

This scenario corresponds to Alice and Bob being able to perform n measurements, each yielding one of two possible outcomes. It corresponds to the well-known I_{nn22} inequality. Since there is currently no analytical solution for the maximum violation of the I_{nn22} inequality for general quantum states, this study selects the Werner state for experimentation: $\rho(p) = p\ |\beta_{00}\rangle\langle\beta_{00}| + (1-p)\frac{I}{4}$.

When $p=1$, the Werner state is one of the Bell states and maximizes the I_{nn22} inequality, with its violation decreasing linearly with p. This serves as a reference for our Bell nonlocality. It is worth noting that the metrics for these two Bell nonlocality measures are different, so direct numerical comparisons are meaningless. Only the trends are considered for reference. The maximum violation of the I_{nn22} inequality in quantum mechanics occurs at $p=1$, with values of 0.2071 for $n=2$ and 0.25 for $n=3$.

Figure 4 illustrates the Bell nonlocality $NL(\rho)$ of the Werner state computed for different values of p at $n=2,3,4,5$. Figure 4 (a): For $n=2$, $NL(\rho)$ is 0 for $p<0.5$, consistent with analytical results. For $p>0.5$, $NL(\rho)$ linearly increases with p, reaching a maximum value of 0.25 at $p=1$. Bell nonlocality $NL(\rho)$ with p for Figure 4 (b): for $n=3$, $NL(\rho)$ is 0 for $p<0.71$, consistent with analytical results. For $p>0.71$, $NL(\rho)$ linearly increases with p, reaching a maximum value of 0.11 at $p=1$. Figure 4 (a-b) demonstrate that over the entire range $0 \le p \le 1$, the numerical results exhibit a trend similar to the maximum violations of the I_{2222} and I_{3322} inequalities. Figure 4 (c-d): for $n=4$ and $n=5$, $NL(\rho)$ shows a trend of initially being 0 and then linearly increasing with p, similar to $n=2$ and $n=3$. However, as n increases, the dimension of the problem rapidly increases, leading to multiple linear trends in the optimal solutions due to the presence of local optima.

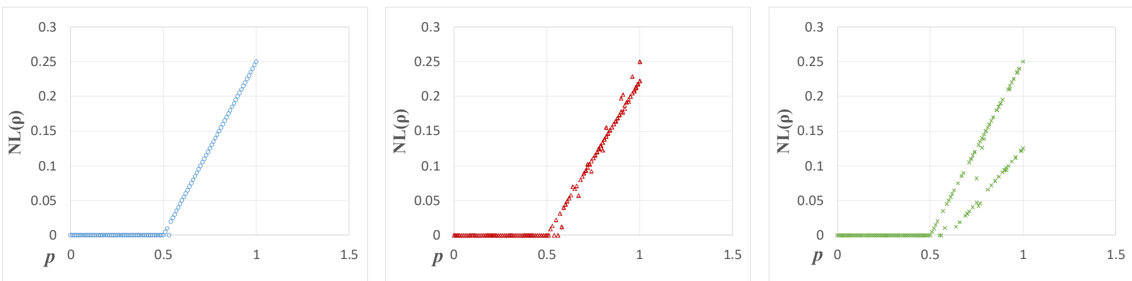


(a) n=2 (b) n=3 (c) n=4 (d) n=5

Figure 4. Bell nonlocality $NL(\rho)$ with p for $(n,n,2,2), n=2,3,4,5$.

6.3 The numerical results for the scenario $(2,2,n,n)$

The scenario is a multi-output extension of the CHSH scenario, corresponding to the CGLMP inequality. Both parties are able to choose from two measurements, each capable of producing n outcomes. Since the CGLMP inequality lacks a general analytical solution, we use the Werner state for analysis again.



(a) n=2,I_{2222} (b) n=3,I_{2233} (c) n=4,I_{2244}

Figure 5. Bell nonlocality $NL(\rho)$ with p for $(2,2,n,n), n=2,3,4$.

Figure 5 illustrates the Bell nonlocality $NL(\rho)$ of the Werner state for different values of the parameter p at different n. It can be observed that $NL(\rho)$ exhibits a linear relationship with p, with a certain degree of amplification in the numerical solutions. Additionally, as n increases, the number of local optimal solutions in the numerical optimization program increases, leading to decreased program stability.

7. Conclusion

Nonlocality is a significant physical resource and it constitutes an essential characteristic of quantum mechanics' foundational principles. Quantifying the nonlocality of density matrices can aid in identifying quantum states with stronger Bell nonlocality. The paper has two main contributions. Firstly, we propose a widely applicable measure of Bell nonlocality for density matrices in quantum systems. Building upon the classical correlation fundamental matrix, we extend the Bell nonlocality measure based on trace distance from correlation relations to density matrices. We also demonstrate that this measure is well-defined. Secondly, we introduce a relaxation algorithm which can efficiently estimate this measure. By introducing relaxation variables to reduce the complexity of the original problem, and employing the see-saw method, this algorithm demonstrates promising effectiveness in solving the problem.

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