Machine learning study of the relationship between the geometric and entropy discord

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Abstract – As an important resource to realize quantum information, quantum correlation displays different behaviors, freezing phenomenon and nonlocalization, which are dissimilar to the entanglement and classical correlation, respectively. In our setup, the ordering of the value of quantum correlation is represented for different quantization methods by considering an open quantum system scenario. The machine learning method (neural network method) is then adopted to train for the construction of a bridge between the Rényi discord ($\alpha = 2$) and the geometric discord (Bures distance) for $X$ form states. Our results clearly demonstrate that the machine learning method is useful for studying the differences and commonalities of different quantizing methods of quantum correlation.

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Introduction. – With the development of the quantum technology, many novel instruments and ideas arise to serve for people's life, such as quantum communication and quantum computer [1]. When we deal with the composite quantum systems in these applications, the superposition principle which is a basic theory of quantum mechanics and the tensorial structure of the Hilbert space have been widely applied to describe these composite quantum systems. The concept of entanglement [2] which is a kind of special superposition states is always naturally involved. The earliest researches show that entanglement is equivalent to quantum correlation and had been regarded as reasonable for many years. Simultaneously, many different quantification methods have been put forward in this period, including geometric [3] and entropy methods (the most famous is concurrence [4] for the entanglement of two partial systems), and many interesting properties of entanglement had been found for different quantum systems, such as sudden death and sudden spring [5–7].

About twenty years ago, Ollivier and Zurek [8] and Henderson and Vedral [9] introduced the concept of “quantum discord”. It told us that the entanglement does not account for all nonclassical correlations and that even the states with zero entanglement usually contain quantum correlations [8,10]. And there is a universal consensus that entanglement entirely captures quantum correlation only for a global pure state [11]. So, many related works have been presented for $X$ states [12,13] and some open quantum systems [7,14–23] in the past few years, and the unique freezing phenomenon is found, which reveals a robust feature of a family of two-qubit models subject to nondissipative decoherence [11,24–26].

In the experimental implementation perspective, the Rényi entropy is defined by

$$S_\alpha(\rho) = \frac{1}{1-\alpha} \log \text{Tr}[\rho^\alpha],$$

which has drawn much attention in the recent years, because the Rényi entropy shows quantitative bounds for different parameter $\alpha$ comparing the von Neumann entropy, and can be more easily implemented than the von Neumann entropy for measuring entanglement [27,28]. Here the parameter $\alpha \in (0, 1) \cup (1, \infty)$ and the logarithm is in base 2. Notably, the Rényi entropy will reduce to the von Neumann entropy when $\alpha \to 1$. As a natural extension of quantum discord, the Rényi entropy discord (RED) [29,30] is also put forward. Therefore, it is valuable to study the properties and the role of RED in the quantum information field.

From the geometric viewpoint, several other quantization methods are proposed, such as Hilbert-Schmidt [31]...
\(D_{HS}\), Bures distance \([3,11,32,33]\) \(D_{Br}\), trace-norm and Hellinger \([11,34]\) \(D_{HL}\). Unlike the quantum discord, the geometric discords quantify the quantum correlation by searching the minimum distance between the quantum states and zero quantum correlation states, and showed the classification of quantum states, such as classical states, quantum-classical states and quantum states. Based on these classification, it is better to understand the difference between the entanglement and the quantum correlation by geometric definition \([3,11]\). Simultaneously, the different quantization methods are ordered as

\[
D_{Br}(\rho) \geq \{D_{HL}(\rho), D_{HS}(\rho)\},
\]

which is discussed in refs. \([11,33]\). Here, \(E(\rho)\) denotes the geometric quantification of the entanglement. Unfortunately, the concurrence can be smaller or larger than quantum discord.

Although a series of works mentioned the above properties of geometric and entropy discords, respectively, no clearly relationship between the geometric and entropy style discords has been established because all the discords are defined by the complex nonlinear mathematical forms. The new idea to solve this problem is to find a method to obtain the relation only based on partial data (the value of quantum correlation of partial quantum states). As a part of both artificial intelligence and statistics, machine learning comes from the computer science field in which the goal is to learn the potential patterns from previously given data sets, and make a decision or prediction for future unknown situation based on this learned patterns. Recently, these learning tools have been used for dealing with some quantum problems, such as quantum state tomography \([35]\), and quantum many-body problem \([36]\). These results suggest that machine learning can be a new platform for solving some problems of quantum physics. In addition, establishing the relationship between geometric and entropy discords through the machine learning method will be beneficial to reveal some hidden physical character of the quantum state, for example, which quantum states can present the freezing phenomenon under the same condition for different discords \([37]\).

In this work, we calculate the value of entanglement and different discords for two qubits open system under the \(X\) form initial states, and show the order of these value. Notably, our result not only gives the powerful proof for refs. \([11]\) and \([33]\), but also firstly answers the question as to whether the RED of \(\alpha = 2\) can resolve the problem “quantum discord can be larger or smaller than the concurrence”. Furthermore, another highlight of this work is to construct the relationship between \(D_{Br}\) and the RED of \(\alpha = 2\) by the use of the machine learning method.

The ordering of the value of quantum correlation for different quantization methods. Stemming from the research works of Ollivier and Zurek \([8]\) and Henderson and Vedral \([9]\), many efforts have been devoted to study the quantum correlation for different systems by use of different methods. Reference \([3]\) shows that the geometric measures have a nice ordering feature (see eq. (2)). In contrast, the concurrence (entanglement) can be larger or smaller than the quantum discord \([22,38]\). Now, whether the Rényi discord is larger than the concurrence is still unknown, although it is monotone increasing with \(\alpha \) \([29,30]\) (for \(\alpha = 1\), the Rényi discord reduces to the quantum discord).

In what follows, we consider an open quantum system scenario and study the ordering of quantum correlation under different quantification methods.

Here, we consider the anisotropic coupling two-qubit system which is coupled to two correlated Fermi-spin environments, respectively. The Hamiltonian of the total system has the following form:

\[
H = H_s + \sum_{i=1,2} (H_{Ei} + H_{Es}) + qS_i^zS_j^z,
\]

\[
H_s = J_1(\sigma_i^1\sigma_j^2 + \sigma_i^2\sigma_j^1) + J_2\sigma_i^1\sigma_j^2 + \sum_{i=1,2} \omega_i\sigma_i^z,
\]

\[
H_{Ei} = \alpha_i S_i^2; H_{Es} = \gamma_i \sigma_i^z S_i^z;
\]

where, \(J_1\) and \(J_2\) are the anisotropic coupling parameters between two spin particles. \(\omega_i\) and \(\alpha_i\) are the frequencies of spin particle and environmental spin particle, respectively. \(q\) describes an Ising-type correlation between the environments. \(S_i^2 = \sum_{k=1}^{N_i} \sigma_k^{k,i}\) is the collective spin operators, \(\sigma_k^{k,i}\) are the Pauli matrices and each environment \(E_i\) consists of \(N_i\) particles with spin 1/2.

Here, the states \((j, m)\) denote the orthogonal bases in the environment Hilbert space \(H_B\) which satisfy \([22,39]\)

\[
S^2(j, m) = j(j + 1)(j, m), \quad S^2(j, m) = m(j, m), \quad S^2 = (S_x^2 + S_y^2 + S_z^2),\]

\[
j = 0, \ldots, N - \frac{1}{2}, \quad m = j, \ldots, -j.
\]

For the initial state \(\rho(0) = \rho_s(0) \otimes \rho_E(0)\) condition, the reduced density matrices \(\rho_s(t)\) of the system can be obtained,

\[
\rho_s(t) = \frac{1}{2} \sum_{j_1=0}^{N_1/2} \sum_{m_1} \sum_{j_2=0}^{N_2/2} \sum_{m_2} \frac{\nu(N_1, j_1)\nu(N_2, j_2)}{e^{i|m_1m_2|}e^{i|\alpha_1m_1|}e^{i|\alpha_2m_2|}} x V^\dagger U^\dagger(t)\rho_s(0)U(t)V,
\]

where \(V^\dagger = \left[\begin{array}{c|c|c|c|c|c|c}
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\hline
0 & e^{-iE_{1t}}Q_1 - e^{-iE_{2t}}Q_2 & 0 & 0 & 0 & 0 & 0 \\
\hline
0 & 2J_1(e^{-iE_{1t}} - e^{-iE_{2t}})Q_1 - Q_2 & 0 & 0 & 0 & 0 & 0 \\
\hline
0 & 2J_1(e^{-iE_{1t}} - e^{-iE_{2t}})Q_1 - Q_2 & 0 & 0 & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & 0 & 0 & 0 & e^{-iE_{2t}}
\end{array}\right]
\]

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where $|0\rangle$ and $|1\rangle$ denote the spin-up and -down states, respectively. So the two spin particles compose $\mathbb{C}^2 \otimes \mathbb{C}^2$ Hilbert space and the state space can be expanded by the basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$. $Q_{1,2} = Q + \sqrt{Q^2 + 4J_1^2} Q = \omega_1 + \gamma_1 m_1 - \omega_2 - \gamma_2 m_2, E_1 = \omega_1 + \gamma_1 m_1 + \omega_2 + \gamma_2 m_2 + J_2, E_2 = -J_2 + \sqrt{Q^2 + 4J_1^2}$ and $E_4 = -E_1 + 2J_2$. $\rho_s(t)$ is the matrix form of $\rho_s(t)$ under the basis $V$.

Notice, when the initial density matrix $\rho_s(0)$ has the X form [12,13],

$$\rho_s(0) = \begin{bmatrix} a & 0 & 0 & \delta \\ 0 & b & \beta & 0 \\ 0 & \beta^* & c & 0 \\ \delta^* & 0 & 0 & d \end{bmatrix}$$

which satisfies $a, b, c, d \geq 0$, $a + b + c + d = 1$, $||\delta||^2 \leq ad$ and $||\beta||^2 \leq bc$, it is easy to check that the matrix form of $\rho_s(t)$ is also the X form.

Figure 1 shows the difference between the different quantification methods of quantum correlation for X initial states (total 65880 states) generated by our considered open quantum system, including $D_{HS}$, $D_{HL}$, $D_{Br}$, RED and concurrence. The value of each dot denotes the value of the difference between the different quantification methods at different time. Note that this ordering is only between geometric methods ($D_{HS}$, $D_{HL}$, $D_{Br}$) or entropy style methods (RED, concurrence). The parameters are $\alpha_1 = 250 \text{ps}^{-1}$, $\alpha_2 = 200 \text{ps}^{-1}$, $\omega_1 = 5 \text{ps}^{-1}$, $\omega_2 = 6 \text{ps}^{-1}$, $q = 30 \text{ps}^{-1}$, $J_1 = 9 \text{ps}^{-1}$, $J_2 = 11 \text{ps}^{-1}$, $\beta = 1/77$, $N_1 = 14$, $N_2 = 12$, $\gamma_1 = 0.2 \text{ps}^{-1}$ and $\gamma_2 = 0.3 \text{ps}^{-1}$.

Figures 1(a), (b) further prove the reliability of the relationship $D_{Br}(\rho) \geq \{D_{HL}(\rho), D_{HS}(\rho)\}$. In contrast, fig. 1(c) shows that $D_{HL}$ can be larger or smaller than $D_{HS}$. Simultaneously, for entropy style quantization of quantum correlation, RED is still larger or smaller than the concurrence for the $\alpha = 2$ condition, as shown in fig. 1(d). The RED $= 2$ still cannot resolve the problem of whether quantum discord can be larger or smaller than the concurrence. Combined with the monotone increasing of RED with $\alpha$, we obtained that the RED shows a better value ordering of quantum correlation than quantum discord (RED reduces to quantum discord when $\alpha \to 1$) for $\alpha > 1$. As a conclusion, the value ordering of quantum correlation of different quantization methods in fig. 1 shows that $D_{Br}$ [3,11,32,33] and RED [29,30] quantization methods can be regarded as better than the others methods.

**The effect of the anisotropic coupling between qubits for freezing phenomenon.** As an interesting phenomenon in the process of quantum correlation evolution, the freezing discord shows a robust feature of a family of two-qubit models subject to nondissipative decoherence, that is, the quantum correlation does not change for a while, which was first found for classical correlations [40]. Later, Mazzola, Piilo, and Maniscalco [41] displayed a similar behavior for the quantum correlations, and Lang and Caves [42] provided a complete geometry picture explanation for Bell-diagonal states.

Later, some efforts have been devoted to discussing the condition for the frozen discord [11,24–26] of other special states, including X states and SCI states [25,26,37]. These results demonstrate that the freezing conditions may be different for various forms of discord, which is also related to the study in the third part of this work. Here, as a supplement of our previous work [22], the effect of the anisotropic coupling parameters $J_1$ and $J_2$ for quantum correlation are shown in fig. 2. It reveals that the isotropic coupling is beneficial to the preservation of the freezing phenomenon (see black line), with the amplitude of shock within the range from $10^{-2}$ to $10^{-3}$. This property can be explained by the information transfer between the system and the environment. The anisotropic coupling system can increase the different degrees of the information flow between system and the environment for different spin directions. Although there are some small differences (less than $10^{-2}$) in the evolution behavior of the freezing phenomenon, the same state also shows the freezing phenomenon under the same conditions, e.g., the
state \((a = \delta = 0, b = 0.4, c = 0.5, \beta = 0.4)\). This property promotes the study of constructing the relationship between \(D_{Br}\) and RED which paves the way to further study the freezing condition for different quantification methods. Simultaneously, considering the results of our previous works [7,21–23,26,37], we choose the coupling parameter \(q\) to generate the samples in the next item.

Machine learning study of the relationship between the \(D_{Br}\) and RED \((\alpha = 2)\). – From the point of view of invariant of physical laws, even for different methods, the same physical problem should have the same result. So there are some relations between the geometric and entropy style discords.

Cianciaruso et al. discussed the geometric measure of discord-type correlations based on the Bures distance \((d_{Bu})\) [11], which is defined as follows:

\[
D_{Br} \equiv \inf_{\chi'} d_{Bu}(\rho, \chi') = \inf_{\chi'} 2(1 - \text{Tr}([\sqrt{\rho} \sqrt{\chi'}]^2 / 2)),
\]

where the set of classical-quantum states \(\chi' = \sum_i p_i |i\rangle \otimes \omega_i^L\), \(p_i\) is a probability distribution, \(|i\rangle^A\) denotes an orthogonal basis for subsystem \(A\), \(\omega_i^L\) is an arbitrary ensemble of states for subsystem \(B\), and \(d_{Bu}(\rho, \chi')\) is the Bures distance.

Because it is difficult to obtain mathematically an analytic form of eq. (6) for general models, some numerical calculation methods were proposed in ref. [33] which are also adopted in this work to study \(D_{Br}\), based on the relation between quantum Fisher information and the Bures distance. The Bures distance can be rewritten as

\[
\mathcal{P}(\rho_{AB}) = \frac{1}{4} \min_{\Gamma} \mathcal{F}(\rho_{AB}; \Gamma),
\]

where \(F\) denotes the quantum Fisher information,

\[
\mathcal{F}(\rho_{AB}; \Gamma) = \frac{1}{4} \sum_{i,j,k,q_1,q_2} \sum_{\phi} \frac{1}{2} \left[|q_1 + q_2| \langle \psi_i | (\Gamma_A \otimes \Gamma_B) | \psi_j \rangle |^2, \right]
\]

with \(q_i, \phi\) denoting, respectively, the eigenvalues and eigenvectors of \(\rho_{AB}\), and the minimum is taken over the set of all local Hamiltonians \(\Gamma\).

The Rényi quantum discord of \(\rho_{AB}\) is an extension of quantum discord and is defined for \(\alpha \in (0, 1) \cup (1, 2)\) as follows [29,30]:

\[
D_\alpha(\rho_{AB}) = \inf \mathcal{I}_\alpha(E; B \mid X)_{\text{tau}, \text{EB}},
\]

where the Rényi conditional mutual information

\[
\mathcal{I}_\alpha(E; B \mid X)_{\text{tau}, \text{EB}} = \frac{\alpha}{\alpha - 1} \log \text{Tr}\left\{\left(\rho_X \text{Tr}_E \rho_{EBX} \frac{\rho_{EBX}}{\rho_X} \right)^\alpha \right\},
\]

where the the classical output \(X\) denotes the measurement acting on system \(A\) and \(E\) is an environment for the measurement map [30]. In this paper, we choose the von Neumann measurement \(\Pi_{lm} = |i\rangle \langle i| (i = 0, 1)\) with two angular parameters \(\theta\) and \(\phi\) : \(|0\rangle = \cos(\theta/2)|0\rangle + e^{i\phi} \sin(\theta/2)|1\rangle\) and \(|1\rangle = \sin(\theta/2)|0\rangle - e^{i\phi} \cos(\theta/2)|1\rangle\), \((0 \leq \theta \leq \pi/2; 0 \leq \phi \leq \pi)\).

Properties of the Rényi quantum discord are shown in table 2 of ref. [30].

Here, there are two points that caused our interest about studying the relationship between \(D_{Br}\) and RED for \(\alpha = 2\). One is some advantages of \(D_{Br}\) over other geometric discords, such as the ordering of quantum correlation [11,33], convex, monotonous [29,30] and the description of the freezing phenomenon [26]. The other is that there is a similar structure \(XEB(\cdot)\) which relates to the definition of fidelity for \(D_{Br}\) and RED for \(\alpha = 2\). Unfortunately, it is very difficult to get an analytical solution because of the nonlinear definitions of \(D_{Br}\) and RED and the structural dependence of the density matrix. So we apply a neural network to search for the relationship between \(D_{Br}\) and RED for \(\alpha = 2\).

Since the multi-layer neural network can simulate some complex relationship or function, we first consider the neural network model to construct the relationship between \(D_{Br}\) and RED based on the data of \(D_{Br}\) and RED and select tensorflow to implement. Artificial neural networks are constituted by a multi-layer perception that was inspired by the biological neural networks that constitute animal brains. It is a network of simple unit which was also named neuron. Each neuron is defined as a nonlinear mapping from the sum of its inputs to output. Through a training process, the weight parameters of units are adjusted so that the neural network extracts the potential patterns in data sets [43]. Figure 3 shows a structure graph of a general neural network. It has input data \(x_i\), hidden layer neural \(a_l^i\) and output data \(y\), satisfying

\[
z_l = W(l)A^{l-1} + b_l, \\
a_l^i = f(z_l^i),
\]

where the \(l\)-th layer neural cells denote \(A^l = [a_1^l, a_2^l \ldots a_n^l]\) and for \(l = 1\), \(A^1 = [x_1^1, x_2^1 \ldots x_n^1]\), \(z^l = [z_1^1, z_2^1 \ldots z_n^1]\).

In order to realize the nonlinear relation between input and output of each neural node, the activation function

\[
f(x) = \frac{1}{1 + e^{-x}}
\]

is used.

\[
\text{ReLU}(x) = \begin{cases} 
0, & x < 0 \\
x, & x \geq 0 
\end{cases}
\]

\[
\text{Softmax}(x) = \frac{e^x}{\sum_{i} e^{x_i}}
\]

\[
\text{Softplus}(x) = \ln(1 + e^x)
\]

and \(\text{LeakyReLU}(x) = \max(x, 0.1x)\). In this paper, we use \(\text{ReLU}(x)\) as the activation function.
$F(z)$ is required,

$$f(z) = \tanh(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}. \quad (11)$$

We adjust the parameters of the neural network to minimize the cost function by using back-propagation algorithm and gradient descent method,

$$\text{cost}(x) = \sum (y - y')^2,$$  \quad (12)

here, we have the summation for all the training data (training samples). $y'$ and $y$ denote the predicted value and real value of $D_{Br}$.

We constructed a 4-layer neural network for our problem. The number of neurons per layer is 7, 13, 1, 1. The learning process of a neural network is shown in Algorithm 1.

**Algorithm 1** Learning process of neural network

1: Input: matrix $n \times 7$ n data samples with 7 features
2: Output: matrix $n \times 1$, the predicted value $y'$ of $D_{Br}$ for each sample)
3: 1. Initial the parameters (W, b) in neural network.
4: 2. Split the data set into training data, validation data and test data randomly with proportion 60%, 20% and 20%.
5: for $t = 1:100000$ do
6: Minimize the difference between predicted value $y'$ and real value $y$ by updating the parameters using gradient descent on training data
7: End for
8: 3. use the validation data to choose the neural network with the minimal cost function

Samples: Because the matrix form of $\rho_s(t)$ is also the $X$ form for the $X$ initial state, the $X$ states samples are generated from the data of $\rho_s(t)$ for 60 samples per 6 seconds. Similarly, we change the parameter $q$ to generate another group of samples in the same process. The total number of samples are more than one hundred and twenty thousand with the repetition rate less than 1%. Based on eqs. (7) and (9), the values of $D_{Br}$ and RED ($\alpha = 2$) are obtained for these samples.

Feature: Based on eqs. (6), (7) and (9), we choose seven parameters, including the four eigenvalues of $\rho_s(t)$ and $\theta$ and $\phi$ which are introduced in the RED calculation process, and RED as the input features of the neural network. The data analysis reveals an important character of the data which is classified to $\theta = 0$ and $\theta = \frac{\pi}{4}$.

Neural network model: A bridge (relationship) has been built between RED ($\alpha = 2$) and $D_{Br}$ for the above two classifications. Here, we randomly choose 60% of the data as training data, 20% as validation data and 20% as test data. In fig. 4, the red line shows that at the end of training, the mean-square error (MSE) which is equal to the expectations of cost rapidly decreases at the first hundreds of epochs and eventually converges after a hundred thousand epochs. For $\theta = 0$ ($\theta = \pi/4$), the MSE is less than 0.004 (0.0027). This means that a good relationship is constructed based on our model.

Overfitting: For all machine learning applications, the training process should be carefully designed to avoid overfitting. Dropout is a regularization technique to prevent overfitting in neural networks by preventing complex co-adaptations on training data. This method is applied to prevent overfitting, which means that we temporarily remove some units from the network, along with all its incoming and outgoing connections. Moreover, we randomly choose units to drop at each epoch [44].

In fig. 4, the two lines are rapidly decreasing in the first few hundred iterations, and then gradually converge to zero. Moreover, comparing the blue and red lines, it is shown that the parameters that were applied to the training set data are also applicable to the test set as the distance between two lines is very small (magnitude 10^{-4}). That is to say, the parameters of the neural network can be generalized without overfitting. This also further demonstrates that the general relationship between RED ($\alpha = 2$) and $D_{Br}$ for $X$ states is correct. Although, our data and results stem from $X$ states which were generated by a quantum system, the results are also true for $X$ states generated by other quantum systems. This study method paves the way for the further study of the physical nature of quantum correlation.

Finally, from the physical perspective, the quantum correlation shows the different characteristics of the quantum states contrasting with the classical states or the changing degree of the quantum states when it suffers the local disturb. So, the system information presented by different discord-like definitions will be different. Searching for the link between these definitions, it will not only help us to understand the differences and commonalities of systematic information obtained by different definitions, but it will also help us to understand the total properties of quantum states, such as coherence, and the properties of entanglement.

**Conclusion.** – In this paper, two main results about quantum correlation are presented. One is that the
ordering of the value of quantum correlation is obtained with different quantization methods for an open quantum system scenario. It also hints that $D_{BR}$ and RED quantization methods may be better than the others methods. In addition, the anisotropic coupling between qubits can affect the freezing phenomenon. The other is that the machine learning method is firstly applied to study quantum correlation and successfully construct the relationship between geometric ($D_{BR}$) and entropy (RED) style discord for $X$ form states. This bridge will help to study the difference of quantum correlation between different quantization methods.

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