Overcoming ambiguities in classical and quantum correlation measures

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Abstract – We identify ambiguities in the available frameworks for defining quantum, classical, and total correlations as measured by discord-like quantifiers. More specifically, we determine situations for which either classical or quantum correlations are not uniquely defined due to degeneracies arising from the optimization procedure over the state space. In order to remove such degeneracies, we introduce a general approach where correlations are independently defined, escaping therefore from a degenerate subspace. As an illustration, we analyze the trace-norm geometric quantum discord for two-qubit Bell-diagonal states.

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Introduction. – Quantum correlations are widely recognized as a resource for quantum information tasks [1]. In this scenario, entanglement plays a special role for applications in quantum computation and quantum communication [2]. On the other hand, it is now known that, even in the absence of entanglement, it is possible to achieve some quantum advantage, such as in protocols for work extraction via Maxwell’s demons [3], metrology [4,5], entanglement distribution [6–10], quantum state merging [11], among others. The source for the quantum power of such tasks can be attributed to more general quantum correlations, as measured by quantum discord [12]. Such correlations can be suitably applied to make quantum systems supersede their classical counterparts.

Quantum information science has then motivated the development of a general theory of quantum, classical, and total correlations in physical systems. In this context, quantum discord has been originally introduced by Ollivier and Zurek [12] as an entropic measure of quantum correlation in a bipartite system, which arises as a difference between the total correlation (as measured by the mutual information) before and after a local measurement is performed over one of the subsystems. In addition, a number of discord-like measures have also appeared through a geometric formulation, which are based, e.g., on the relative entropy [13,14], Hilbert-Schmidt norm [15,16], trace norm [17,18], and Bures norm [19,20]. All of these distinct versions can be generally described by a unified framework in terms of a distance function. Here, the term distance will be generically used as a measure of distinguishability between two density operators (not necessarily a proper distance). Then, a correlation measure (either classical, quantum, or total) can be obtained by computing the distance function associated with a state $\rho$ and a related classical or product state.

By focusing on the quantumness of $\rho$, we typically optimize the distance function via a pre-selected strategy over classical states, which leads to a unique value for the quantum correlation. We then compute the distance function between the optimal classical state and a product state (or a measured product state) to obtain the classical correlation. However, as we will explicitly show in this work, there may be more than a single optimal classical state. This set of optimal classical states, which are degenerate in the sense that they provide the same value for the quantum correlation, can lead to a nonunique (multivalued) classical correlation. Therefore, there is an ambiguity in the definition of the classical correlation. This result is independent of the distance function adopted, affecting all the discord-like measures (see, e.g., a brief discussion

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for the specific cases of the Bures distance [20] and the measurement-induced disturbance [21]). Moreover, by choosing first to optimize the distance function for the classical correlation, the nonuniqueness will be moved to the subsequent optimization of the quantum correlation. In order to remove those degeneracies for both classical and quantum correlations, we propose a general strategy based on an independent optimization procedure. As will be shown, this will lead to the uniqueness of the distance functions, providing a consistent theory of correlations.

**Distance functions.** – Discord-like measures of quantum correlation are typically devised to quantify the disturbance of quantum states under local measurements. In this sense, even separable states may exhibit quantumness. Quantum correlation is part of the total correlation exhibited by a quantum state, which is also composed by the classical correlation. Proposals of *bona fide* measures for quantum, classical, and total correlations are expected to obey a set of fundamental criteria [1,22]: i) product states have no correlations, ii) all correlations are invariant under local unitary operations, iii) all correlations are non-negative, iv) total correlations are nonincreasing under local operations, and v) classical states have no quantum correlations. Moreover, an extra assumption has been recently taken as necessary [17,23–25]: vi) quantum correlations are part of the total correlation in this sense, even separable states may exhibit quantumness. Quantum correlation is part of the total correlation under local measurements. In the general method proposed according to a pre-selected strategy. In eq. (2), $\rho$ would be shown, this will lead to the uniqueness of the distance functions, providing a consistent theory of correlations. It can be shown that a number of correlation quantities are compatible with the fundamental criteria of correlations listed above. Explicit examples in the class of entropic measures include the mutual information $K_I(\rho, \tau) = I(\rho) - I(\tau)$, the conditional entropy $K_P(\rho, \tau) = S(\rho_1 | a) - S(\tau_1 | a)$, and the von Neumann entropy $K_S(\rho, \tau) = S(\rho) - S(\tau)$. In the class of geometric measures, one has the Schatten 1-norm (trace norm) $K_G(\rho, \tau) = \| \rho - \tau \|_1$, with $\| X \|_1 = \text{Tr} [\sqrt{X^\dagger X}]$, among others. Concerning $M(\rho)$, it is usually defined as a positive operator-valued measure (POVM) over one or more of the subsystems such that: a) it minimizes the quantum correlation or b) it maximizes the classical correlation.

**Measurement-independent approach.** A measurement-independent approach has also been introduced for different discord-like measures [13,16,20,26]. In terms of the generalized function $K$, we can express the quantum, classical, and total correlations in this approach respectively by

\begin{align}
Q'(\rho) &= K [\rho, \chi_\rho], \quad (4) \\
C'(\rho) &= K [\chi_\rho, \pi_\chi], \quad (5) \\
T'(\rho) &= K [\rho, \pi_\rho]. \quad (6)
\end{align}

For the evaluation of the function $K$, $\chi_\rho$ denotes the classical state closest to $\rho$ among a pre-selected set of classical states $\{\chi\}$, whereas $\pi_\chi$ and $\pi_\rho$ represent the product states closest to $\chi_\rho$ and $\rho$, respectively. In comparison with the measurement-based formalism, the optimization of eqs. (4)–(6) may lead to $C' \neq C$ and $T' \neq T$ even in the case $Q' = Q$ (which occurs for $\chi_\rho = M(\rho)$ [26,27]). On the other hand, both approaches are equivalent in terms of obeying the fundamental criteria.

**Ambiguities.** – Both the measurement-based and the measurement-independent approaches yield well-defined frameworks as long as the optimized classical state involved (either $M(\rho)$ or $\chi_\rho$) is unique for any given $\rho$. However, this assumption is not true in general. Degenerate classical states, which lead to a single value of quantum correlation but nonunique values for the classical correlation (and vice versa in the case of the measurement-based framework), are often present in the optimization performed over state space. As an example, fig. 1 provides a sketch of such degeneracies in the measurement-independent formalism. As an explicit illustration of these ambiguities, let us consider a function $K$ based on the Schatten 1-norm and a classical state $M(\rho)$ emerging from a projective measurement over one qubit of a two-qubit system so that $M(\rho)$ minimizes the quantum correlation $Q$. Then, we have

\begin{align}
K [\rho, \tau] &= K_G [\rho, \tau] = \| \rho - \tau \|_1 = \sum_{i=1}^4 | \Gamma_i [\rho - \tau] |, \quad (7) \\
M(\rho) &= M_n(\rho) = \sum_{j=-+} \left( \Pi_j \otimes 1 \right) \rho \left( \Pi_j' \otimes 1 \right), \quad (8)
\end{align}
where \( Q, C, Q', \) and \( C' \) are obtained from eqs. (1), (2), (4), and (5), respectively, with the distance function \( K \) given in terms of the Schatten 1-norm. Now, let us prove that the optimized classical state in eq. (10) is nonunique, implying there are multiple values for the classical correlations. In order to provide a concrete example of ambiguity, let us consider a restricted class of Bell-diagonal states \( \rho_* \), which is given by

\[
\rho_* = \frac{1}{4} [\mathbb{I} \otimes \mathbb{I} + \vec{c}_* \cdot (\vec{\sigma} \otimes \vec{\sigma})],
\]

(16)

where the correlation vector is \( \vec{c}_* = (c, c, 0) \), with \( c > 0 \). In this case, the possible four eigenvalues of the operator \( \rho_* - M_\chi(\rho_*) \) are given by \( \{ \Gamma_i [\rho_* - M_\chi(\rho_*)] \} = \{-\alpha_-, \alpha_-, \alpha_+, \alpha_+\} \), where \( \alpha_\pm = c(1 \pm |n_z|)/4 \). So, taking into account these eigenvalues in eq. (7), we obtain that the quantum correlation reads

\[
Q_\chi(\rho_*) = \sum_{i=1}^{4} \left| \Gamma_i [\rho_* - M_\chi(\rho_*)] \right| = 2(\alpha_- + \alpha_+) = c,
\]

(17)

with \( \hat{n} \) an arbitrary unitary vector. This result is in agreement with eq. (13) applied to the state described in eq. (16). However, its independence of \( \hat{n} \) reveals the existence of an infinity number of optimized classical states associated with a unique value of \( Q_\chi(\rho_*) \). Such degeneracy implies into a continuum of inequivalent values for the classical correlation. Indeed, the eigenvalues of \( M_\chi(\rho_*) - M_\chi(\pi^m_\rho) \) are given by \( \{ \Gamma_i [M_\rho(\rho_*) - M_\chi(\pi^m_\rho)] \} = \{-\beta, -\beta, \beta, \beta\} \), where \( \beta = c\sqrt{1 - n_z^2}/4 \). This leads to

\[
C_\chi(\rho_*) = \sum_{i=1}^{4} \left| \Gamma_i [M_\rho(\rho_*) - M_\chi(\pi^m_\rho)] \right| = c\sqrt{1 - n_z^2},
\]

(18)

with \(-1 \leq n_z \leq 1\). Note that eq. (18) agrees with eq. (14) applied to the state \( \rho_* \) only in the case \( n_z = 0 \), i.e., when \( \hat{n} \) lies on the xy-plane. This includes the particular solutions \( \hat{n} = \pm \hat{x} \) or \( \pm \hat{y} \) associated with the classical state in eq. (10). The maximal discrepancy occurs for \( n_z = \pm 1 \) (\( \hat{n} = \pm \hat{z} \)), where the classical correlation in eq. (18) goes to zero. A schematic picture of this situation is shown in fig. 2. Concerning the measurement-independent framework, we find

\[
Q'_\chi(\rho_*) = Q_\chi(\rho_*) = c,
\]

(19)

\[
C'_\chi(\rho_*) \leq C_\chi(\rho_*) \leq C(n_\chi(\rho_*)).
\]

(20)

where we have used the relations \( M_\chi(\rho_*) = \chi_\rho_*, \)

\[
M_\chi(\pi^m_\rho) = \pi^m_\rho = (\mathbb{I} \otimes \mathbb{I})/4, \quad \| \chi_{\rho_*} - \chi_{\rho_*} \|_1 \leq \| \chi_{\rho_*} - \pi^m_{\rho_*} \|_1 \]

(21)

into the definitions of quantum and classical correlations. From eqs. (10) and (15), we can derive that

\[
C'_{\pm \mp}(\rho_*) = C'_{\pm \mp}(\rho_*) \neq 0,
\]

(22)

whereas from eqs. (20) and (18) we obtain

\[
C'_{\pm \mp}(\rho_*) = 0.
\]

This variation of \( C'_\chi(\rho_*) \) for distinct choices of \( \hat{n} \) is sufficient to show that the nonuniqueness also affects the measurement-independent approach.
New framework. – As long as the fundamental criteria of reasonable correlation measures are satisfied, it is plausible to add auxiliary strategies to the previous frameworks in order to overcome ambiguities originated from the degeneracies. As an example, we could adopt the following modified strategy (see subsect. “Measurement-based approach” for the original strategy): a’) maximize the classical correlation or $b’$) minimize the quantum correlation over the degenerate subspace. However, depending on the distance function $K$ and for general quantum states, it may not be a trivial task to find out the degenerate subspace as well as to optimize over the degenerate classical states. Here, we propose a new framework based on the measurement-based approach, which has the advantage of avoiding extra optimization over the degenerate subspace. In this new framework, the quantum, classical, and total correlations are independently obtained from

$$Q''(\rho) = K[\rho, M_-(\rho)],$$
$$C''(\rho) = K[M_+(\rho), M_+(\pi^m)],$$
$$T''(\rho) = K[\rho, \pi^m],$$

where $M_-(\rho)$ and $M_+(\rho)$ are classical states that minimizes $Q''$ and maximizes $C''$ within a pre-established set of measurements (e.g., orthogonal projective measurements), respectively. In this approach, degeneracies in $M_-(\rho)$ or $M_+(\rho)$ are irrelevant, being it sufficient to find out a unique solution for each optimal measurement. More specifically, $M_-(\rho)$ and $M_+(\rho)$ are independently optimized, with no direct connection between them. As an application, let us assume $K = K_G$, $\rho = \bar{\rho}$, and $M_+(\rho) = M_{\hat{n}_+}(\rho)$, i.e., orthogonal projective measurements, where $\hat{n}_- = (n_{x-}, n_{y-}, n_{z-})$ and $\hat{n}_+ = (n_{x+}, n_{y+}, n_{z+})$ denote the unitary vectors that minimize $Q''$ and maximize $C''$, respectively. From previous analysis, it follows that $\hat{n}_- = \hat{n}$ or $M_{\hat{n}_-}(\bar{\rho}) = M_\rho(\rho)$, with $c_m = \max\{c_k\}$, such that

$$Q''(\bar{\rho}) = Q(\rho) = 0.$$  

Concerning the evaluation of the classical correlation, we find $(\Gamma_i [M_{\hat{n}_+}(\bar{\rho}) - M_{\hat{n}_-}(\pi^m)]) = \{\gamma, -\gamma, \gamma, \gamma\}$, where we have defined $\gamma = \sqrt{\bar{v} \cdot \bar{u}/4}$ with $\bar{v} = (c_2^z, c_2^y, c_2^x)$ and $\bar{u} = (n_{x+}^z, n_{y+}^z, n_{z+}^z)$. These eigenvalues lead to

$$C''(\bar{\rho}) = \sum_{i=1}^{4} |\Gamma_i [M_{\hat{n}_+}(\bar{\rho}) - M_{\hat{n}_-}(\pi^m)]| = \sqrt{\bar{v} \cdot \bar{u}},$$

where $\bar{u}$ maximizes eq. (27) under the conditions $u_x + u_y + u_z = 1$ and $0 \leq u_k \leq 1$. By defining $v_+ = \max\{v_k\}$, $v_- = \min\{v_k\}$, $u_+ = \max\{u_k\}$, $u_0 = \min\{u_k\}$, and $u_- = \min\{u_k\}$, where max, int, and min, denote maximum, intermediate, and minimum, respectively, we can write

$$\bar{v} \cdot \bar{u} = v_x u_x + v_y u_y + v_z u_z = v_+ u_+ + v_0 u_0 + v_- u_-,$$

with

$$u_x + u_y + u_z = u_+ + u_0 + u_- = 1.$$  

Then, isolating $u_z$ in terms of $u_0$ and $u_-$ in eq. (29) and inserting the resulting expression in eq. (28), we obtain

$$\bar{v} \cdot \bar{u} = v_+ - (v_+ - v_0) u_0 - (v_+ - v_-) u_- \leq v_+,$$

where we have used the relations $v_+ \geq v_0$, $v_+ \geq v_-$, $0 \leq u_0 \leq 1$, and $0 \leq u_- \leq 1$. Evidently, the maximum value $v_+$ of the function $\bar{v} \cdot \bar{u}$ can be achieved for $u_- = 0$, $u_0 = 0$, and $u_+ = 1$, i.e., for $\hat{n}_+ = \hat{n}$, $\hat{n}_- = \hat{n}$. Consequently, $M_{\hat{n}_+}(\bar{\rho}) = M_{\hat{n}_-}(\bar{\rho}) = M_\rho(\rho)$. Thus, it follows that

$$C''(\bar{\rho}) = C(\rho) = c_+.$$  

Remarkably, the framework introduced here and the measurement-based approach with $M(\rho)$ given by eq. (10) (see ref. [27]) lead to the same expressions for the correlations in the particular case of the Bell-diagonal states, even though inequivalent results may appear for more general states. Furthermore, it is also important to emphasize that the alternative strategy of further optimization over the degenerate subspace (instead of independent optimization of $Q$ and $C$) also provides the same results. Indeed, since we have shown that there is at least one optimized classical state in common for $M_-(\rho)$ and $M_+(\rho)$, given by eq. (10), then eqs. (26) and (31) can also be obtained from the measurement-based formalism by assuming strategy a) in combination with a’) or b) followed by b’).

Conclusions. – In summary, we have identified ambiguities in the definition of either classical or quantum correlations, which potentially affect all the approaches used.
to define discord-like measures. Moreover, we have proposed a new framework to avoid such ambiguities by independent optimization of the correlation functions. These results are relevant for a consistent correlation theory and for practical applications of correlation measures, such as in quantum many-body systems [28,29], in the emergence of the pointer basis in open quantum systems [30,31], etc. As future challenges, it remains the application of the proposed framework for states more general than the Bell-diagonal qubit-qubit states, the investigation of its robustness against decoherence, and possible relevance in quantum information tasks.

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