Operationally Invariant Measure of the Distance between Quantum States by Complementary Measurements

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We propose an operational measure of distance of two quantum states, which conversely tells us their closeness. This is defined as a sum of differences in partial knowledge over a complete set of mutually complementary measurements for the two states. It is shown that the measure is operationally invariant and it is equivalent to the Hilbert-Schmidt distance. The operational measure of distance provides a remarkable interpretation of the information distance between quantum states.

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Introduction.—Mathematical formulations of all the fundamental physical theories are based on the concept of an abstract space. The structure of the space and the theories is defined by its metric. For example, the Minkowski metric defines the mathematical structure of the special theory of relativity and the Rieman metric defines the structure of the general theory of relativity. In quantum mechanics, the Hilbert-Schmidt distance may be the natural metric of the Hilbert space. What are the fundamental laws which dictate the metrics in physical theories? This question is investigated in this paper for the case of quantum theory and the Hilbert-Schmidt distance.

When two quantum states are given, what do we do to measure how close they are? This is an important issue in various investigations of quantum mechanics. For example, we need to measure how close the teleported state is to the original state in order to check the credibility of the quantum teleportation protocol. Other examples appear in quantum cloning, quantum state reconstruction, and practical quantum gate operation [1]. We need a measure of closeness, depending on the kind of information process involved. In particular, two measures have been applied to the wide realm of quantum information processing: fidelity [2] and Hilbert-Schmidt distance [3]. These measures are equivalent to each other if the systems are in pure states.

The fidelity, $F = |\langle \psi | \phi \rangle|^2$, is the transition probability between two pure states, $|\psi\rangle$ and $|\phi\rangle$. When the fidelity is extended to incorporate mixed states [2], its interpretation becomes vague in an operational perspective. Instead, the fidelity may be indirectly interpreted in terms of statistical distance or "statistical distinguishability" in the measurement that optimally resolves neighboring density operators [4]. On the other hand, the Hilbert-Schmidt distance is a metric defined on the space of operators. It is unclear how to impose an operational interpretation on the Hilbert-Schmidt distance.

Another possible measure of closeness is quantum relative entropy which has also been proposed as a candidate for a measure of entanglement [5,6].

A quantum state is a representation of our knowledge on individual outcomes in future experiments [7]. We can, then intuitively, say that the difference between this knowledge for two quantum states measures how much the two states are "close to each other" with respect to the future predictions. Bohr [8] remarked that "... phenomena under different experimental conditions, must be termed complementary in the sense that each is well defined and that together they exhaust all definable knowledge about the object concerned." This suggests that the closeness of two quantum states should be defined with regard to a complete set of mutually complementary measurements. We require that such a measure of closeness between two states is invariant under the specific choice of a complete set of mutually complementary measurements.

In this Letter, we introduce a measure of distance between two quantum states, which conversely tells us the closeness. The measure of distance is operationally defined as a sum of the differences in partial knowledge over a complete set of mutually complementary "unbiased" measurements. The measure has several remarkable properties. (i) The measure is operationally invariant: It is uniquely defined, being independent of the specific choice of a complete set of complementary measurements. (ii) The measure is equivalent to the Hilbert-Schmidt distance. (iii) The operational measure of distance can be interpreted as an information distance between two quantum states. In addition, the fact that the operational measure is equivalent to the Hilbert-Schmidt distance suggests that the intrinsic structure of Hilbert space reflects information-theoretical foundations of quantum theory.

Mutually complementary measurement.—Two measurements are mutually complementary if precise

knowledge in one of them implies that all possible outcomes in the other are equally probable [9]. Consider a nondegenerate and orthogonal measurement A represented by a set of eigen projectors $\{\hat{A}_i\}$. Suppose a quantum system in d-dimensional Hilbert space is prepared in such a state that the outcome in the measurement A can be predicted with certainty; for instance, the system's density operator is given by $\hat{\rho} = \hat{A}_i$. Let B be another nondegenerate and orthogonal measurement represented by a set of eigen projectors $\{\hat{B}_i\}$. For a given state (density operator) \hat{A}_i , the probability of an outcome j in the measurement B is given by $p_{j|i} = \text{Tr}\hat{B}_j\hat{A}_i$. The measurement B is mutually complementary to A if outcomes of measurement B are equally probable:

$$p_{j|i} = \frac{1}{d}, \quad \forall i, j = 1, 2, ..., d.$$
 (1)

A set of complementary measurements is a complete set if the measurement operators can expand any density operators on the Hilbert space [see Eq. (13)]. For a spin-1/2 system, such a complete set of complementary measurements is associated with three Pauli spin operators $\{\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z\}$.

Definition of operational distance.—Consider two quantum systems of the d-dimensional Hilbert space. In order to indicate how close their density operators ρ_1 and ρ_2 are to each other, we consider a complete set of mutually complementary measurements $M = \{m_{\alpha}\}$ which are nondegenerate and orthogonal. Consider a measuring device set up with the observable for measurement m_{α} and let $\{\hat{m}_{\alpha,i}\}$ be the set of the eigen operators and $\{p_{\alpha,i} = \text{Tr}(\hat{m}_{\alpha,i}\hat{\rho})\}$ be the set of probabilities corresponding to the outcomes for a given density operator $\hat{\rho}$. The measurement is performed independently and equivalently for each quantum system and its probability vector is denoted as $\vec{p}_{\alpha}(S)$ for system S. The distance of the two probability vectors, $\vec{p}_{\alpha}(1)$ and $\vec{p}_{\alpha}(2)$, is defined as

$$D_{\alpha}(\hat{\rho}_1, \hat{\rho}_2) = |\vec{p}_{\alpha}(1) - \vec{p}_{\alpha}(2)|^2.$$
 (2)

The distance D_{α} is called a single operational distance for measurement m_{α} among a complete set of mutually complementary measurements. The total operational distance may be defined by summing single operational distances over the complete set of complementary measurements:

$$D_{\text{total}}(\hat{\boldsymbol{\rho}}_1, \hat{\boldsymbol{\rho}}_2) = \sum_{\alpha} D_{\alpha}(\hat{\boldsymbol{\rho}}_1, \hat{\boldsymbol{\rho}}_2). \tag{3}$$

Number of complementary measurements.—Consider a Hilbert-Schmidt space \mathcal{B} of bound operators for a system S in d-dimensional Hilbert space \mathcal{H}_d , in which the inner product of $\hat{A}, \hat{B} \in \mathcal{B}$ is defined as [10]

$$(\hat{A}|\hat{B}) = \operatorname{Tr}\hat{A}^{\dagger}\hat{B}. \tag{4}$$

The space \mathcal{B} forms a d^2 -dimensional vector space where each element is an operator. A Hilbert-Schmidt norm of \hat{A} is given by $\|\hat{A}\|^2 \equiv (\hat{A}|\hat{A})$. For operator space \mathcal{B} , one may choose a complete orthogonal basis set in terms of

Hermitian operators, $B_o = \{\hat{\lambda}_{\alpha}, \text{ for } \alpha = 0, 1, ..., d^2 - 1\}$, such that $\hat{\lambda}_0 = 1$ and $(\hat{\lambda}_{\alpha} | \hat{\lambda}_{\beta}) = d\delta_{\alpha\beta}$. The orthogonality implies that each $\hat{\lambda}_{\alpha}$ for $\alpha \neq 0$ is traceless: $\text{Tr}\hat{\lambda}_{\alpha} = 0$.

A Hermitian operator \hat{H} and a density operator $\hat{\rho}$ of S are represented by the observable basis set B_{ρ} as

$$\hat{H} = \frac{h_0}{d} \mathbb{1} + \frac{1}{d} \sum_{\alpha=1}^{d^2 - 1} h_\alpha \hat{\lambda}_\alpha, \tag{5}$$

$$\hat{\boldsymbol{\rho}} = \frac{1}{d} \mathbb{1} + \frac{1}{d} \sum_{\alpha=1}^{d^2 - 1} \rho_{\alpha} \hat{\boldsymbol{\lambda}}_{\alpha}, \tag{6}$$

where $h_0 = \operatorname{Tr} \hat{H}$, $h_\alpha = \operatorname{Tr} \hat{\lambda}_\alpha \hat{H}$, and $\rho_\alpha = \operatorname{Tr} \hat{\lambda}_\alpha \hat{\rho}$. Here $\rho_0 = 1$ due to the unit trace of a density operator. In particular, we call $\vec{\rho} = (\rho_1, \rho_2, \ldots, \rho_{d^2-1})$ a generalized Bloch vector. Because $\operatorname{Tr} \hat{\rho}^2 \leq 1$, the norm of $\vec{\rho}$ is upper bounded: $|\vec{\rho}|^2 \leq d-1$. If $\hat{\rho}$ is pure, $|\vec{\rho}|^2 = d-1$. The generalized Bloch vectors stay within a Bloch sphere S_B of radius $\sqrt{d-1}$. However, not all generalized Bloch vectors within S_B correspond to density operators, implying there is no one-to-one correspondence between density operators and generalized Bloch vectors within the Bloch sphere S_B . In fact, the set of Bloch vectors specifying density operators is restricted by the positivity of density operators such that a given density operator $\hat{\rho}$ should hold

$$(\hat{\boldsymbol{\rho}}|\hat{\boldsymbol{\sigma}}) \ge 0 \Leftrightarrow \vec{\boldsymbol{\rho}} \cdot \vec{\boldsymbol{\sigma}} \ge -1,\tag{7}$$

for any pure density operator $\hat{\sigma}$ with $|\vec{\sigma}|^2 = d - 1$.

We shall derive a condition of mutual complementarity with respect to generalized Bloch vectors. Consider two measurements A and B of $\{\hat{A}_i\}$ and $\{\hat{B}_i\}$, respectively. The orthogonality and the completeness relation of $\{\hat{A}_i\}$ raise relations among their generalized Bloch vectors $\{\hat{a}_i\}$ as, noting that \hat{A}_i has unit trace,

$$\operatorname{Tr} \hat{A}_i \hat{A}_j = \delta_{ij} \to \vec{a}_i \cdot \vec{a}_j = d\delta_{ij} - 1, \tag{8}$$

$$\sum_{i=1}^{d} \hat{A}_i = 1 \to \sum_{i=1}^{d} \vec{a}_i = \vec{0}, \tag{9}$$

where $\vec{0}$ is a null vector. Similar relations hold for the generalized Bloch vectors $\{\vec{b}_i\}$ of the measurement B. The condition (1) of mutual complementarity between A and B is now written as

$$\vec{a}_i \cdot \vec{b}_j = 0, \quad \forall i, j = 1, 2, ..., d.$$
 (10)

This condition implies that the subspace spanned by $\{\vec{a}_i\}$ is orthogonal to that by $\{\vec{b}_i\}$ within S_B when A and B are mutually complementary.

The subspace spanned by $\{\vec{a}_i\}$ is (d-1) dimensional due to the constraints in Eqs. (8) and (9). Further, the set satisfies an overcompleteness relation in the subspace as

$$\frac{1}{d} \sum_{i=1}^{d} \vec{a}_i \vec{a}_i = \mathbb{1}_{d-1}, \tag{11}$$

where $\vec{a}_i \vec{a}_j$ is a tensor product of two vectors \vec{a}_i and \vec{a}_j

and $\mathbb{1}_{d-1}$ is an identity matrix in the subspace. Noting that the Bloch space is $(d^2 - 1)$ dimensional, it can be divided into (d + 1) subspaces in (d - 1) dimension. For the d-dimensional Hilbert space \mathcal{H}_d , there are thus (d+1) measurements that are mutually complementary and they form a complete set of complementary measurements. We note here that, even though a pair of mutually complementary measurements always exists, the existence of a complete set needs to be investigated in the virtue of the condition (7) and was constructed explicitly for d being a prime or a power of a prime number [11]. This finding does not, however, exclude a possibility to find a complete set of mutually complementary measurements for other dimensions. To avoid any confusion, we are concerned with quantum systems in dimensions of prime numbers and their powers.

We present a nontrivial example of d being a prime number for a complete set of mutually complementary measurements [11]. Consider a measurement which is represented by a basis set $\{|\phi_j^0\rangle = |j\rangle\}$ and further d measurements, among which the α th measurement is represented by the basis vectors

$$|\phi_j^{\alpha}\rangle = \frac{1}{\sqrt{d}} \sum_{k=1}^d \exp[(2\pi i/d)(\alpha k^2 + jk)]|k\rangle, \qquad (12)$$

for j = 1, 2, ..., d. One can verify that each of these (d + 1) basis sets is orthonormal and that all the basis sets are mutually complementary.

Equivalence to Hilbert-Schmidt distance.—We shall derive one of the main results that the total operational distance is equivalent to the Hilbert-Schmidt distance. Let M be a complete set of (d+1) complementary measurements. For $m_{\alpha} \in M$ with eigen projectors $\{\hat{m}_{\alpha,i}\}$, let $\vec{m}_{\alpha,i}$ be the generalized Bloch vector of $\hat{m}_{\alpha,i}$. Because the set $\{\vec{m}_{\alpha,i}\}$ is overcompleted in the Bloch space due to Eq. (11),

$$\frac{1}{d} \sum_{\alpha=1}^{d+1} \sum_{i=1}^{d} \vec{m}_{\alpha,i} \vec{m}_{\alpha,i} = \sum_{\alpha=1}^{d+1} \mathbb{1}_{d-1}^{\alpha} = \mathbb{1}^{d^2 - 1}, \quad (13)$$

where $\mathbb{1}_{d-1}^{\alpha}$ is a projection matrix onto the α th subspace and $\mathbb{1}_{d^2-1}$ is an identity matrix in the Bloch space.

We obtain a single operational distance explicitly by complementary measurement $m_{\alpha} \in M$ and the total operational distance for given two density operators $\hat{\rho}_1$ and $\hat{\rho}_2$. For a measurement $m_{\alpha} \in M$, the single operational distance is given by Eq. (2) as

$$D_{\alpha}(\hat{\rho}_{1}, \hat{\rho}_{2}) = \frac{1}{d^{2}} \sum_{i=1}^{d} |\vec{m}_{\alpha, i} \cdot [\vec{\rho}(1) - \vec{\rho}(2)]|^{2}, \quad (14)$$

where $\vec{\rho}(S)$ is a generalized Bloch vector for the system S. Summing up the single operational distances over the complete set of complementary measurements, the total distance is obtained by Eq. (3) as

$$D_{\text{total}}(\hat{\rho}_1, \hat{\rho}_2) = \|\hat{\rho}_1 - \hat{\rho}_2\|^2, \tag{15}$$

where we have used the completeness relation (13).

We remark some properties of the total distance D_{total} . First, the total distance is invariant to the specific choice of a complete set of complementary measurements. In fact, in deriving Eq. (15), no particular set of complementary measurements has been chosen. Second, the total distance is equal to the Hilbert-Schmidt distance of the two operators $\hat{\rho}_1$ and $\hat{\rho}_2$ in the Hilbert-Schmidt space \mathcal{B} . Third, the total distance is bounded:

$$0 \le D_{\text{total}} \le 2. \tag{16}$$

where the bound values 0 and 2 are obvious as shown later in Eq. (21).

Relation between operational distance and information content.—Brukner and Zeilinger [12] introduced the total information content of a quantum system in the density operator $\hat{\rho}$ and it was successfully applied for entanglement teleportation [13], state estimation [14], and a criterion for the violation of Bell's inequalities [15]. Their measure can be written as

$$I(\hat{\boldsymbol{\rho}}) = N \|\hat{\boldsymbol{\rho}} - \hat{\boldsymbol{\rho}}_r\|^2, \tag{17}$$

where N is a normalization factor and $\hat{\rho}_r = \frac{1}{d}\mathbb{1}$ is a completely random state. Comparing Eq. (17) with Eq. (15), the total information content $I(\hat{\rho})$ can be described in terms of the total operational distance $D_{\text{total}}(\hat{\rho}, \hat{\rho}_r)$ such that $I(\hat{\rho})$ indicates the distance of the quantum state $\hat{\rho}$ from the completely random state $\hat{\rho}_r$. The more information a density operator $\hat{\rho}$ contains, the further it is away from $\hat{\rho}_r$. Reciprocally, the total operational distance between two density operators $\hat{\rho}_1$ and $\hat{\rho}_2$, $D_{\text{total}}(\hat{\rho}_1, \hat{\rho}_2)$, describes a difference in their information contents. These results imply that the total operational distance can be interpreted as an *information distance* between two quantum states.

Comparison with fidelity.—In the following discussion, we compare the total operational distance with the fidelity. The fidelity has been commonly employed for a measure of closeness in quantum information processing. The fidelity F is defined by [2]

$$F(\hat{\boldsymbol{\rho}}_1, \hat{\boldsymbol{\rho}}_2) = (\text{Tr}\sqrt{\sqrt{\hat{\boldsymbol{\rho}}_1}\hat{\boldsymbol{\rho}}_2\sqrt{\hat{\boldsymbol{\rho}}_1}})^2, \tag{18}$$

for two density operators $\hat{\rho}_1$ and $\hat{\rho}_2$. The fidelity is bounded by its definition: $0 \le F \le 1$. The two density operators are exactly the same if F = 1, and they are completely different if F = 0. Note for the total operational distance that two operators are equal if D = 0 and they are completely different if D = 2.

One may compare a set of test density operators $\{\hat{\rho}\}$ to a reference density operator $\hat{\sigma}$ so as to find out which density operator is the closest to $\hat{\sigma}$. For that purpose, let us denote the fidelity as $F_{\hat{\sigma}}(\hat{\rho}) \equiv F(\hat{\sigma}, \hat{\rho})$ for a reference density operator $\hat{\sigma}$. Similarly, $D_{\hat{\sigma}}(\hat{\rho}) \equiv D_{\text{total}}(\hat{\sigma}, \hat{\rho})$.

Consider a measure $M(\vec{q})$ of physical quantities $\{\vec{q}\}$. The measure M establishes the ordering of physical quantities such that $M(\vec{q}_1) \leq M(\vec{q}_2) \leq \cdots$. Another measure $N(\vec{q})$ of physical quantities is *equivalent* to $M(\vec{q})$ if N

is a monotonic function of M, in other words, if the ordering is either preserved $[N(\vec{q}_1) \leq N(\vec{q}_2) \leq \cdots]$ or completely reversed $[N(\vec{q}_1) \geq N(\vec{q}_2) \geq \cdots]$. The fidelity $F_{\hat{\sigma}}$ is equivalent to the total operational distance $D_{\hat{\sigma}}$ over a set of test density operators T for a reference $\hat{\sigma}$ if, for each pair of two test density operators $\hat{\rho}_1$, $\hat{\rho}_2 \in T$,

$$F_{\hat{\sigma}}(\hat{\rho}_1) \le F_{\hat{\sigma}}(\hat{\rho}_2) \Leftrightarrow D_{\hat{\sigma}}(\hat{\rho}_1) \ge D_{\hat{\sigma}}(\hat{\rho}_2).$$
 (19)

Further, the fidelity F is equivalent to the total distance D over a set of test density operators T for a set of reference density operators S if $F_{\hat{\sigma}}$ is equivalent to $D_{\hat{\sigma}}$ for any reference $\hat{\sigma} \in S$.

If the set of test and reference density operators is confined to pure states, the fidelity is equivalent to the total operational distance. Note that for a set of pure states the fidelity is given by the Hilbert-Schmidt inner product of two density operators $\hat{\sigma} = |\sigma\rangle\langle\sigma|$ and $\hat{\rho} = |\rho\rangle\langle\rho|$ in Eq. (4):

$$F_{\hat{\boldsymbol{\sigma}}}(\hat{\boldsymbol{\rho}}) = \operatorname{Tr}\hat{\boldsymbol{\sigma}}\,\hat{\boldsymbol{\rho}} = (\hat{\boldsymbol{\sigma}}|\hat{\boldsymbol{\rho}}).$$
 (20)

Further,

$$D_{\hat{\boldsymbol{\sigma}}}(\hat{\boldsymbol{\rho}}) = P(\hat{\boldsymbol{\sigma}}) + P(\hat{\boldsymbol{\rho}}) - 2F_{\hat{\boldsymbol{\sigma}}}(\hat{\boldsymbol{\rho}}), \tag{21}$$

where $P(\hat{\rho}) = ||\hat{\rho}||^2$ is the purity of $\hat{\rho}$. As $P(\hat{\sigma}) = P(\hat{\rho}) = 1$, it is clear in Eq. (21) that the total operational distance is a monotonic function of the fidelity.

The total operational distance is, however, inequivalent to the fidelity as general mixed states are concerned. For simplicity, let a reference be a pure state, $\hat{\sigma} = |\sigma\rangle\langle\sigma|$, and let $P(\hat{\rho})$ be the purity of a test state $\hat{\rho}$. In this case, the fidelity $F_{\sigma}(\rho)$ is written as in Eq. (20) and the total distance is given as in Eq. (21) with $P(\hat{\sigma}) = 1$. Now the total distance is not just a function of $F_{\hat{\sigma}}(\hat{\rho})$ but also a function of $P(\hat{\rho})$. As F and P are independent quantities over a set of test states $\{\hat{\rho}\}$, the equivalence (19) no longer holds.

Quantum tomography and operational distance for a qubit.—As an example to obtain the operational distance in an experiment, we consider quantum tomography on light fields which are an ensemble of polarization degrees of freedom [16]. The tomographic experiment obtains Stokes parameters by four intensity measurements [17] (i) with a filter that transmits 50% of the incident radiation regardless of its polarization, (ii) with a polarizer that transmits only horizontally polarized light, (iii) with a polarizer that transmits only light polarized at 45° to the horizontal axis, and (iv) with a polarizer that transmits only right-circularly polarized light. The latter three cases are propositions for a complete set of mutually complementary measurements for a polarization qubit. Thus, the operational distance of two ensembles of light fields may be estimated using the tomography setup.

In summary, we proposed a measure to find how close two quantum states are. This is operationally defined with respect to a complete set of mutually complementary measurements. It was shown that the operational measure is equivalent to the Hilbert-Schmidt distance, which implies that our result can also be understood as an operational determination of the Hilbert-Schmidt distance. The measure provides a remarkable interpretation as an information distance between quantum states. The comparison with the fidelity shows that the measure is not necessarily equivalent to the fidelity.

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