Measuring Incompatibility and Clustering Quantum Observables with a Quantum Switch

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The existence of incompatible observables is a cornerstone of quantum mechanics and a valuable resource in quantum technologies. Here we introduce a measure of incompatibility, called the mutual eigenspace disturbance (MED), which quantifies the amount of disturbance induced by the measurement of a sharp observable on the eigenspaces of another. The MED provides a metric on the space of von Neumann measurements, and can be efficiently estimated by letting the measurement processes act in an indefinite order, using a setup known as the quantum switch, which also allows one to quantify the noncommutativity of arbitrary quantum processes. Thanks to these features, the MED can be used in quantum machine learning tasks. We demonstrate this application by providing an unsupervised algorithm that clusters unknown von Neumann measurements. Our algorithm is robust to noise and can be used to identify groups of observers that share approximately the same measurement context.

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Introduction.—One of the most striking features of quantum mechanics is the existence of incompatible observables. Incompatible observables are at the heart of Bohr's notion of complementarity [1] and of Heisenberg's uncertainty principle [2], and have nontrivial relations with Bell nonlocality [3,4] and other forms of nonclassicality [5–9]. In addition to their foundational relevance, they play center stage in quantum information technologies [4,10,11], where quantum incompatibility serves as a resource [12–14], in a similar way as quantum entanglement and coherence.

Several measures of incompatibility have been proposed in the past years, including robustness to noise (defined as the minimum amount of noise that has to be added to a set of incompatible observables in order to make them compatible) [15,16], sensitivity to eavesdropping (defined as the minimum amount of disturbance that an arbitrary entanglement-breaking channel would induce on a quantum system prepared in an unknown eigenstate of the given observables) [17], and disturbance on the measurement statistics (defined as the maximum distance between the probability distribution of observable A on a given input state and the probability distribution of A after a measurement of observable B has been performed on the same input state, with the maximum evaluated over all possible input states) [18]. Since all these measures are defined in terms of optimization problems, they are often hard to compute analytically, and numerical evaluation becomes unfeasible for systems of high dimension. In addition, there is generally no direct way to estimate these measures from experimental data: in most cases, the best known way to infer the incompatibility of two unknown observables is to perform a full tomography, which is unfeasible for quantum systems consisting of many particles.

In this Letter, we introduce a measure of incompatibility for sharp observables [19], called the mutual eigenspace disturbance (MED). The MED quantifies the noncommutativity of the spectral resolutions associated with the two observables, and can be naturally extended to a larger class of noncommutativity measures for unsharp measurements and general quantum processes. It has a simple closed-form analytical expression and, unlike other incompatibility measures, it constitutes a metric on the space of von Neumann measurements, a property that makes it suitable for machine learning applications. The MED and its generalizations to measures of noncommutativity can be directly estimated using the quantum switch [20,21], an operation that combines quantum processes in a coherently controlled order. Estimation of the MED via the quantum switch can be realized with existing technology [22–29]

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and its sample complexity is independent of the dimension of the system, meaning that the number of experiments needed to estimate the MED remains small even for multiparticle systems.

The experimental accessibility of the MED and its metric properties make it suitable for applications in quantum machine learning. To illustrate the idea, we provide a quantum algorithm that clusters noisy von Neumann measurements based on their mutual compatibility. This algorithm can be used to identify clusters of observers who share approximately the same measurement context [30–33], and thereby could share the same notion of an emergent classical reality [34–38]. Notably, the observers could be localized in distant laboratories, and the algorithm does not require access to their measurement outcomes, but only to the average evolution associated to their measurement devices.

MED.—For sharp observables, compatibility is equivalent to commutativity [39]. Let A and B be two sharp observables on a d-dimensional quantum system, and let $\mathbf{P} = (P_i)_{i=1}^{k_A}$ and $\mathbf{Q} = (Q_j)_{j=1}^{k_B}$ be the projectors on the eigenspaces of A and B, respectively. We now introduce a measure of noncommutativity between **P** and **Q**. Imagine that the system is initially in an eigenstate of A, say $|\alpha_i\rangle$, picked uniformly at random from the ith eigenspace, with i distributed according to the probability distribution $p_i := d_{A,i}/d$, where $d_{A,i}$ is the eigenspace's dimension. Then, the system undergoes the canonical (Lüders) measurement process associated with the observable B: with probability $p_B(j) = \langle\alpha_i|Q_j|\alpha_i\rangle$ the measurement yields outcome j, leaving the system in the postmeasurement state $Q_j|\alpha_i\rangle/\|Q_j|\alpha_i\rangle\|$. On average over all outcomes, the density matrix of the system is $\sum_j p_B(j)\, Q_j|\alpha_i\rangle\langle\alpha_i|Q_j/\|Q_j|\alpha_i\rangle\|^2 = \mathcal{B}(|\alpha_i\rangle\langle\alpha_i|)$, where $\mathcal{B}$ is the dephasing channel defined by the relation $\mathcal{B}(\rho) := \sum_j Q_j\rho Q_j$ for arbitrary density matrices ρ. Finally, a measurement of the observable A is performed. The probability to find the outcome i, associated with the original subspace, is $\mathrm{Tr}[P_i\mathcal{B}(|\alpha_i\rangle\langle\alpha_i|)]$. On average, the probability that the system is still found in the original eigenspace is

$$\mathsf{Prob}(A,\mathcal{B}) := \sum_i p_i \int \pi_i(d\alpha_i)\,\mathrm{Tr}[P_i\mathcal{B}(|\alpha_i\rangle\langle\alpha_i|)], \tag{1}$$

where $\pi_i(d\alpha_i)$ is the uniform probability distribution over the pure states in the ith subspace. Explicit calculation yields the expression

$$\mathsf{Prob}(A,\mathcal{B}) := \frac{1}{d}\sum_{ij}\mathrm{Tr}[P_iQ_jP_iQ_j], \tag{2}$$

which is related to an extension of the Kirkwood-Dirac quasiprobability distribution [40,41].

Note that the role of the projectors **P** and **Q** is completely symmetric. Operationally, this symmetry implies to the relation

$$\mathsf{Prob}(A,\mathcal{B}) = \mathsf{Prob}(B,\mathcal{A}), \tag{3}$$

where $\mathsf{Prob}(B,\mathcal{A})$ is the average probability that a randomly chosen state $|\beta_j\rangle$ from the jth eigenspace of B, drawn with probability $q_j := d_{B,j}/d$ (where $d_{B,j}$ is the eigenspace's dimension), is still found in the same eigenspace after the action of the dephasing channel $\mathcal{A}(\rho) := \sum_i P_i\rho P_i$.

Note also that the probabilities in Eq. (3) depend only on the dephasing channels $\mathcal{A}$ and $\mathcal{B}$. Accordingly, we will denote by $D(\mathcal{A},\mathcal{B}) := 1 - \mathsf{Prob}(A,\mathcal{B}) \equiv 1 - \mathsf{Prob}(B,\mathcal{A})$ the average probability of eigenstate disturbance. We then define the MED of the two observables A and B as

$$\mathrm{MED}(\mathcal{A},\mathcal{B}) := \sqrt{D(\mathcal{A},\mathcal{B})} = \sqrt{1 - \frac{1}{d}\sum_{i,j}\mathrm{Tr}[P_iQ_jP_iQ_j]}. \tag{4}$$

The MED exhibits several appealing properties for a measure of incompatibility: (1) it is *symmetric and nonnegative*, namely, $\mathrm{MED}(\mathcal{A},\mathcal{B}) = \mathrm{MED}(\mathcal{B},\mathcal{A}) \geq 0$ for every pair of dephasing channels $\mathcal{A}$ and $\mathcal{B}$, (2) it is *faithful*, namely, $\mathrm{MED}(\mathcal{A},\mathcal{B}) > 0$ if and only if A and B are incompatible, (3) it is *decreasing under coarse graining*, (4) it is a *a metric on von Neumann measurements*, corresponding to observables with a nondegenerate spectrum. (5) it is *robust to noise*: it remains faithful even if one of the channels $\mathcal{A}$ and $\mathcal{B}$ is replaced by the evolution resulting from a noisy measurement of the corresponding observable, (6) it is *maximal for maximally complementary observables* [42], that is, observables such that their eigenstates form mutually unbiased bases [43,44]. In general, one has the bound $\mathrm{MED}(\mathcal{A},\mathcal{B}) \leq \sqrt{1 - 1/\min\{k_A,k_B\}}$, and the maximum value $\mathrm{MED}(\mathcal{A},\mathcal{B}) = \sqrt{1-1/d}$ and is attained if and only if A and B are maximally complementary. The proof of the above properties is provided in the Supplemental Material [45]. There, we also extend the MED to a broader class of incompatibility measures, given by the expression

$$\mathrm{MED}_\rho(\mathcal{A},\mathcal{B}) := \sqrt{1 - \mathsf{Re}\sum_{i,j}\mathrm{Tr}[\rho P_iQ_jP_iQ_j]}, \tag{5}$$

where ρ is a density matrix. The original MED, defined above, corresponds to the case where ρ is the maximally mixed state I/d. Notably, the generalized MED (5) is also a metric on von Neumann measurements whenever the density matrix ρ is nonsingular, including, e.g., the case where ρ is a thermal state.

Experimental setup.—We now provide an experimental setup that can be used to estimate the MED of two observables and, more generally, the amount of noncommutativity between two arbitrary quantum processes.

The setup is based on the quantum switch [20,21], an operation that combines two unknown processes in a coherent superposition of two alternative orders. Previously, the quantum switch was shown to be able to distinguish between pairs of quantum channels with commuting or anticommuting Kraus operators [57,58], a task that can be practically achieved with photonic systems [22,59]. We now show that the quantum switch can be used to quantify the amount of noncommutativity of quantum measurements and, more generally, of arbitrary quantum processes.

Suppose that an experimenter is given access to two black boxes, acting on a d-dimensional quantum system. The two black boxes implement two quantum processes $\mathcal{C}$ and $\mathcal{D}$ with Kraus representations $\mathcal{C}(\rho) = \sum_i C_i \rho C_i^\dagger$ and $\mathcal{D}(\rho) = \sum_j D_j \rho D_j^\dagger$, respectively. The goal of the experimenter is to estimate the noncommutativity of the Kraus operators $(C_i)_i$ and $(D_j)_j$. To this purpose, one can combine the two boxes in the quantum switch [20,21], generating a new quantum process $\mathcal{S}_{\mathcal{C},\mathcal{D}}$ with Kraus operators

$$S_{ij} = C_i D_j \otimes |0\rangle\langle 0| + D_j C_i \otimes |1\rangle\langle 1|, \tag{6}$$

where $\{|0\rangle, |1\rangle\}$ are basis states of a control qubit. The action of the channel $\mathcal{S}_{\mathcal{C},\mathcal{D}}$ on a generic product state $\rho \otimes \omega$ is

$$\begin{aligned}\mathcal{S}_{\mathcal{C},\mathcal{D}}(\rho \otimes \omega) = \frac{1}{4}\sum_{ij}(&\{C_i, D_j\}\rho\{C_i, D_j\}^\dagger \otimes \omega \\ &+ \{C_i, D_j\}\rho[C_i, D_j]^\dagger \otimes \omega Z \\ &+ [C_i, D_j]\rho\{C_i, D_j\}^\dagger \otimes Z\omega \\ &+ [C_i, D_j]\rho[C_i, D_j]^\dagger \otimes Z\omega Z),\end{aligned} \tag{7}$$

where $[C_i, D_j] \coloneqq C_i D_j - D_j C_i$ denotes the commutator, $\{C_i, D_j\} \coloneqq C_i D_j + D_j C_i$ denotes the anticommutator, and $Z \coloneqq |0\rangle\langle 0| - |1\rangle\langle 1|$.

To estimate the noncommutativity of $\mathcal{C}$ and $\mathcal{D}$, the experimenter can initialize the control qubit in the maximally coherent state $\omega = |+\rangle\langle +|$, apply the quantum channel $\mathcal{S}(\mathcal{C}, \mathcal{D})$, and measure the control system in the Fourier basis $\{|+\rangle, |-\rangle\}$, with $|\pm\rangle \coloneqq (|0\rangle \pm |1\rangle)/\sqrt{2}$. Using Eq. (7), one can see that the probability of the outcome "−" is

$$p_- = \frac{1}{4}\sum_{ij}\mathrm{Tr}(\rho|[C_i, D_j]|^2), \tag{8}$$

where $|O|^2 \coloneqq O^\dagger O$ denotes the modulus square of an arbitrary operator O.

We define the *noncommutativity* of two generic quantum processes $\mathcal{C}$ and $\mathcal{D}$ relative to the state ρ as

$$\mathrm{NCOM}_\rho(\mathcal{C}, \mathcal{D}) \coloneqq \sqrt{2p_-} = \sqrt{\frac{\sum_{ij}\mathrm{Tr}(\rho|[C_i, D_j]|^2)}{2}} \tag{9}$$

(in the special case $\mathcal{C} = \mathcal{D}$ and $\rho = I/d$, a related definition was used in [60] to quantify the degree of noncommutativity of the Kraus operators of a given channel). It is evident from the definition that $\mathrm{NCOM}_\rho(\mathcal{C}, \mathcal{D})$ is symmetric and non-negative. When the matrix ρ is invertible, $\mathrm{NCOM}_\rho(\mathcal{C}, \mathcal{D})$ is a faithful measure of noncommutativity, i.e., $\mathrm{NCOM}_\rho(\mathcal{C}, \mathcal{D}) = 0$ if and only if every Kraus operator $\mathcal{C}$ commutes with every Kraus operator of $\mathcal{D}$. For composite systems, it is possible to show that the noncommutativity between a maximally entangled measurement and product measurement is at least $\sqrt{1 - 1/d_{\min}}$, $d_{\min}$ being the dimension of the smallest subsystem (see the Supplemental Material [45]).

In the special case where $\mathcal{C}$ and $\mathcal{D}$ are two dephasing channels $\mathcal{A}$ and $\mathcal{B}$, explicit calculation yields the relation

$$\mathrm{NCOM}_\rho(\mathcal{A}, \mathcal{B}) = \mathrm{MED}_\rho(\mathcal{A}, \mathcal{B}). \tag{10}$$

Hence, the MED of two unknown observables can be directly estimated from experimental data. Crucially, the sample complexity of the estimation procedure is independent of the dimension of the system: for a fixed error threshold ϵ and for every state ρ, the estimate of $\mathrm{MED}_\rho(\mathcal{A}, \mathcal{B})$ can be guaranteed to have error at most ϵ with probability at least $1 - \delta$ by repeating the experiment for $n = \log(2/\delta)/(2\epsilon^2)$ times (see the Supplemental Material [45]).

The experimental estimation of the MED is feasible with photonic systems, in particular in the case where the state ρ is maximally mixed, and its preparation can be achieved by generation two-photon Bell states. The preparation of the maximally mixed state is also standard in the DQC1 model of quantum computing [61] and can be well approximated in other models of quantum computing with highly mixed states [62]. In the Supplemental Material [45] we also discuss the advantages of the quantum switch set up with respect to other ways to estimating the MED.

Besides providing direct way to the experimental estimation of the MED, the relation with the noncommutativity also provides an alternative route to its analytical or numerical evaluation. In the Supplemental Material [45] we show that the noncommutativity can be equivalently rewritten as

$$\mathrm{NCOM}_\rho(\mathcal{C}, \mathcal{D}) = \sqrt{1 - \mathrm{Re}\,\mathrm{Tr}[D\check{C}(I \otimes \rho^T)]}, \tag{11}$$

where $\check{C}$ and D are two operators associated with the maps $\mathcal{C}$ and $\mathcal{D}$, respectively. When the operators $\check{C}$, D, and ρ have a suitable tensor network structure, Eq. (11) provides a way to efficiently evaluate the noncommutativity, avoiding the sums in Eqs. (5) and (9) which may contain an exponentially large number of terms when the system has exponentially large dimension. In the Supplemental Material [45] we also show another equivalent expression that reduces the noncommutativity to the overlap between two pure states, a task that can be carried out efficiently in a variety of physically relevant cases, including, e.g., matrix product [63–65] and MERA states [66].

Clustering algorithm for quantum observables.—We now provide a machine learning algorithm for identifying clusters of observables that are approximately compatible with one another. The algorithm is unsupervised: the learner does not need to be trained with labeled examples of observables belonging to different clusters.

The input of the algorithm is the access to m black boxes, implementing m unknown dephasing channels $\mathcal{A}_1, \ldots, \mathcal{A}_m$ associated to nondegenerate quantum observables $A_1, \ldots, A_m$. The quantum part of the algorithm is the estimation of the MED for every pair of observables. Then, the estimated values of the MED are fed into a classical clustering algorithm. Here we choose k medoids clustering with k-means++ style initial seeding [67,68]. Compared to the popular k-means method, k medoids works better (in terms of convergence) with arbitrary dissimilarity measures.

To illustrate the algorithm, we generate $m = 100$ random qubit observables, of the form $A_l = b_x^{(l)} X + b_y^{(l)} Y + b_z^{(l)} Z$, $l \in \{1, \ldots, m\}$, where X, Y, Z are the three Pauli matrices and $\mathbf{b}_l = (b_x^l, b_y^l, b_z^l) \in \mathbb{R}^3$ is a unit vector (the Bloch vector of the lth observable). The vectors are generated in the following way: for 50 observables, we start from the Bloch vector (1,0,0) and apply a rotation by a random angle θ with $|\theta| \leq 22.5°$ about a random rotation axis. For the remaining 50 observables, we start from the Bloch vector (0,0,1) and apply the same procedure. In this way, the 100 observables are naturally divided into two clusters, as in Fig. 1.

We performed a numerical experiment on the classical part of the algorithm, feeding the values of the MED into the k-medoids algorithm. For improved reliability, we repeated the experiment for 50 times, finding that in each repetition all the 100 observables are correctly clustered. Note that, while we fed the algorithm with the exact values of the MED, the robustness of the k-medoids [67,68] algorithm implies that the results are robust to errors in the estimation of the MED from actual experimental data.

Clustering with noisy observables.—Our clustering algorithm can also be extended to noisy measurements. Following [11], the noise is modeled by randomizing the measurement of each ideal observable with a trivial measurement, which produces the same outcome statistics for every possible input state. Mathematically, this means that the projective measurement $\mathbf{P}^{(l)}$, associated to the lth observable, is replaced by a nonprojective measurement $\mathbf{N}^{(l)} = (1 - \lambda_l)\mathbf{P}^{(l)} + \lambda_l \mathbf{T}^{(l)}$, where λ_l is the noise probability, and $\mathbf{T}^{(l)}$ is a trivial measurement, with POVM operators $T_i^{(l)} = p_i^{(l)} I$, for a fixed probability distribution $\mathbf{p}^{(l)} = (p_i^{(l)})$. For the measurement process associated to the noisy measurement $\mathbf{N}^{(l)}$, we take quantum instruments with Kraus operators of the form $N_{ij}^{(l)} = \sqrt{a_{ij}^{(l)} P_i^{(l)} + b_{ij}^{(l)} I}$, where $a_{ij}^{(l)}$ and $b_{ij}^{(l)}$ are arbitrary nonnegative coefficients subject to the constraints $\sum_j a_{ij}^{(l)} = 1 - \lambda_l$ and $\sum_j b_{ij}^{(l)} = \lambda_l p_i^{(l)}$ for every i and l. The k-medoids algorithm can then be applied, using the noncommutativity (9) of the noisy channels $\mathcal{N}_1, \ldots, \mathcal{N}_m$ defined by $\mathcal{N}_l(\rho) \coloneqq \sum_{ij} N_{ij}^{(l)} \rho N_{ij}^{(l)\dagger}$ for $l \in \{1, \ldots, m\}$.

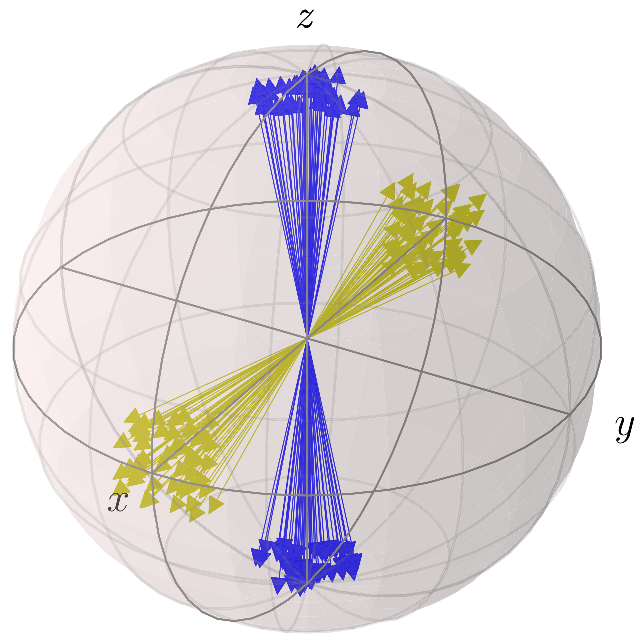

FIG. 1. Clustering of 100 qubit observables, using a k-medoids algorithm based on the values of the MED with k-means++ style initial seeding. The algorithm correctly identifies two clusters, one centered around the Pauli X observable (Bloch vectors in yellow), and one centered around the Pauli Z observable (Bloch vectors in blue).

To test the algorithm, we performed a numerical experiment on 100 randomly generated noisy qubit observables. For simplicity, we chose isotropic noise [69] and set the noise randomly following a uniform distribution, picking each probability $p_i^{(l)}$ uniformly at random in the interval (0,1), subject to the constraint $\sum_i p_i^{(l)} = 1,\ \forall\, l$. For the original observables, we generated the Bloch vectors as in the noiseless case. For the noise, we first defined a maximum noise level η and then we picked a random noise probability $\lambda_l = \eta R_l$ where each R_l is chosen independently, uniformly at random in the interval [0, 1]. The coefficients $a_{ij}^{(l)}$ and $b_{ij}^{(l)}$ are then chosen uniformly at random, subject to the constraints. The experiment has been performed for $\eta = 0.25$, 0.5, and 0.75, and for each setting

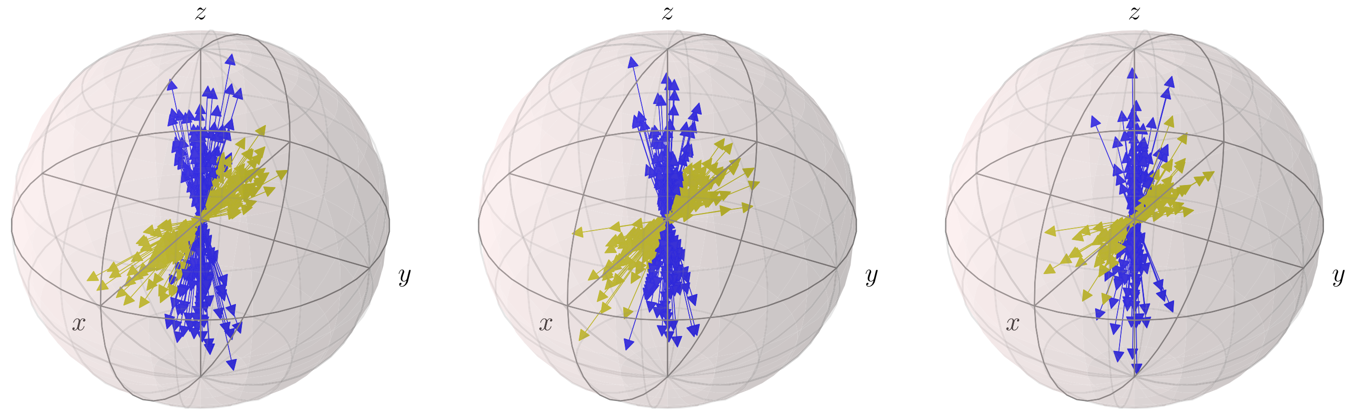

FIG. 2. Clustering of 100 noisy qubit measurements, using a k-medoids algorithm based on the values of the noncommutativity with k-means$++$ style initial seeding. The algorithm correctly identifies two clusters, centered around the Pauli X and Z observables, respectively. The three plots refer to numerical experiments with maximum noise level 0.25, 0.5, and 0.75, respectively.

the k-medoids algorithm has been run 50 times. The results of the experiment, plotted on Fig. 2, show that perfect clustering is still achieved in the presence of noise.

Conclusions and outlook.—In this Letter, we introduced the MED, an experimentally accessible measure of incompatibility for sharp observables. The MED quantifies the noncommutativity of the projectors associated to a pair of observables, and can be directly measured without access to the measurement outcomes, by letting the two measurement processes act in an indefinite order. Thanks to its properties, the MED can be used in quantum machine learning tasks, such as clustering unknown observables based on their degree of compatibility.

An interesting direction of future research is to extend the results of this Letter to infinite dimensional systems, unsharp observables, and general quantum channels. For sharp observables with discrete spectrum, our approach can be easily extended by taking a limit of finite dimensional subspaces. For observables with continuous spectrum, however, the situation is more complex, due to the fact that no repeatable measurement exists [70]. Regarding the extension to unsharp observables and general channels, one approach is to focus on the noncommutativity, which can be measured with the quantum switch. On the other hand, commutativity is not a necessary condition, and an open question is to determine whether there exists a measure of incompatibility that can be measured experimentally like the MED.

Another direction is the extension of the MED from pairs to arbitrary numbers of observables. One option would be to generalize our definition, examining the amount of disturbance on the eigenspace of one observable induced by measurements of the other observables. An appealing feature is that the resulting quantity could be estimated by placing the measurements in a superposition of orders, in a similar way as it was done in our Letter for the case of two observables.

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