Measuring incompatibility and clustering quantum observables with a quantum switch

Ning Gao,\textsuperscript{1} Dantong Li,\textsuperscript{1} Anchit Mishra,\textsuperscript{1} Junchen Yan,\textsuperscript{1} Kyrylo Simonov,\textsuperscript{2} and Giulio Chiribella\textsuperscript{1,3,4}

\textsuperscript{1}QICI Quantum Information and Computation Initiative, Department of Computer Science, The University of Hong Kong, Pokfulam Road, Hong Kong
\textsuperscript{2}Fakultät für Mathematik, Universität Wien, Oskar-Morgenstern-Platz 1, 1090 Vienna, Austria
\textsuperscript{3}Quantum Group, Department of Computer Science, University of Oxford, Wolfson Building, Parks Road, Oxford, OX1 3QD, United Kingdom
\textsuperscript{4}Perimeter Institute for Theoretical Physics, 31 Caroline Street North, Waterloo, Ontario, Canada

(Dated: May 10, 2023)

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 can be used to identify groups of observers that share approximately the same measurement context.

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 non-trivial relations with Bell nonlocality [3, 4] and other forms of nonclassicality [5–9]. In addition to their foundational relevance, they play central 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 paper 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 to 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] 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 $P = (P_i)_{i=1}^k$ and $Q = (Q_j)_{j=1}^b$ 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 $i$-th 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 to 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 post-measurement state $Q_j | \alpha_i \rangle / \| Q_j | \alpha_i \rangle \|. \quad \text{[1]}

On average over all outcomes, the density matrix of the system is $\sum_j p_B(j) Q_j | \alpha_i \rangle \langle \alpha_i | Q_j \| = \mathcal{B} | \alpha_i \rangle \langle \alpha_i |$, 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 $\rho$. Finally, a measurement of the observable $A$ is performed. The probability to find the outcome $i$, associated to the original subspace, is $\text{Tr}[P_i \mathcal{B} | \alpha_i \rangle \langle \alpha_i |]$. On average, the probability that the system is still found in the original eigenspace is

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

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

$$\text{Prob}(A, \mathcal{B}) := \frac{1}{d} \sum_{ij} \text{Tr}[P_i Q_j P_j], \quad \text{[1]}

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

$$\text{Prob}(A, \mathcal{B}) = \text{Prob}(B, \mathcal{A}), \quad \text{[1]}

where $\text{Prob}(B, \mathcal{A})$ is the average probability that a randomly chosen state $| \beta_i \rangle$ from the $j$-th eigenspace of $B$, drawn with probability $q_j := d_{R,j}/d$ (where $d_{R,j}$ 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 $D(\mathcal{A}, \mathcal{B}) := 1 - \text{Prob}(A, \mathcal{B}) \equiv 1 - \text{Prob}(B, \mathcal{A})$ the average probability of eigenstate disturbance. We then define the MED of the two observables $A$ and $B$ as

$$\text{MED}(\mathcal{A}, \mathcal{B}) := \sqrt{D(\mathcal{A}, \mathcal{B})} = \sqrt{1 - \frac{1}{d} \sum_{ij} \text{Tr}[P_i Q_j P_j]}. \quad \text{[1]}

The MED exhibits several appealing properties for a measure of incompleteness:

1. it is symmetric and nonnegative, namely $\text{MED}(\mathcal{A}, \mathcal{B}) = \text{MED}(\mathcal{B}, \mathcal{A}) \geq 0$ for every pair of dephasing channels $\mathcal{A}$ and $\mathcal{B}$,

2. it is faithful, namely $\text{MED}(\mathcal{A}, \mathcal{B}) > 0$ if and only if $A$ and $B$ are incompatible,

3. it is decreasing under coarse-graining,

4. it is a metric on von Neumann measurements, corresponding to observables with non-degenerate 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 $\text{MED}(\mathcal{A}, \mathcal{B}) \leq \sqrt{1 - \min(k_A, k_B)}$, and the maximum value $\text{MED}(\mathcal{A}, \mathcal{B}) = \sqrt{1 - 1/d}$ is attained if and only if $A$ and $B$ are maximally complementary.

The proof of the above properties is provided in Appendix A. There, we also extend the MED to a broader class of incompatibility measures, given by the expression

$$\text{MED}_\rho(\mathcal{A}, \mathcal{B}) := \sqrt{1 - \text{Re} \sum_{ij} \text{Tr}[\rho P_i Q_j P_j]}, \quad \text{[1]}

where $\rho$ is a density matrix. The original MED, defined above, corresponds to the case where $\rho$ is the maximally mixed state $1/d$. Notably, the generalized MED (5) is also a metric on von Neumann measurements whenever the density matrix $\rho$ is non-singular, including e.g. the case where $\rho$ 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 anti-commuting Kraus operators [45, 46], a task that can be practically achieved with photonic systems [22, 47]. 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 $\mathcal{E}$ and $\mathcal{D}$ with Kraus representations $\mathcal{E}(\rho) = \sum_i C_i \rho C_i^\dagger$ 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 $(C_i)_j$ and $(D_j)_j$. To this purpose, one can combine the two boxes in the quantum switch [20, 21], generating a new quantum process $\mathcal{S}_{\mathcal{E}, \mathcal{D}}$ with Kraus operators

$$S_{ij} = C_i D_j \otimes \langle 0 | 0 \rangle + D_j C_i \otimes \langle 1 | 1 \rangle \quad \text{[1]}

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

$$\mathcal{E} \otimes \omega(\rho \otimes \omega) = \frac{1}{4} \sum_{ij} \left( \{C_i, D_j\} \rho \{C_i, D_j\}^\dagger \otimes \omega + \{C_i, D_j\} \rho \{C_i, D_j\}^\dagger \otimes \omega Z \right) + \{C_i, D_j\} \rho \{C_i, D_j\}^\dagger \otimes Z \omega + \{C_i, D_j\} \rho \{C_i, D_j\}^\dagger \otimes Z \omega Z \right),$$

(7)

where $\{C_i, D_j\} := C_i D_j - D_j C_i$ denotes the commutator, $\{C_i, D_j\} := C_i D_j + D_j C_i$ denotes the anti-commutator, and $Z := |0\rangle \langle 0| - |1\rangle \langle 1|$. To estimate the noncommutativity of $\mathcal{E}$ and $\mathcal{D}$, the experimenter can initialize the control qubit in the maximally coherent state $\omega = |+\rangle \langle +|$, apply the quantum channel $\mathcal{E}(\mathcal{D}, \omega)$, and measure the control system in the Fourier basis $\{|+\rangle, |-\rangle\}$, with $|\pm\rangle := (|0\rangle \pm |1\rangle) / \sqrt{2}$. Using Eq. (7), one can see that the probability of the outcome “−” is

$$p_- = \frac{1}{4} \sum_{ij} \text{Tr} \left( \rho \{C_i, D_j\}^2 \right),$$

(8)

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

We define the non-commutativity of two generic quantum processes $\mathcal{E}$ and $\mathcal{D}$ relative to the state $\rho$ as

$$\text{NCOM}_\rho(\mathcal{E}, \mathcal{D}) := \sqrt{2p_-} = \sqrt{\frac{\sum_{ij} \text{Tr} \left( \rho \{C_i, D_j\}^2 \right)}{2}}$$

(9)

(in the special case $\mathcal{E} = \mathcal{D}$ and $\rho = I/d$, a related definition was used in [48] to quantify the degree of non-commutativity of the Kraus operators of a given channel). It is evident from the definition that $\text{NCOM}_\rho(\mathcal{E}, \mathcal{D})$ is symmetric and non-negative. When the matrix $\rho$ is invertible, $\text{NCOM}_\rho(\mathcal{E}, \mathcal{D})$ is a faithful measure of non-commutativity, i.e. $\text{NCOM}_\rho(\mathcal{E}, \mathcal{D}) = 0$ if and only if every Kraus operator $\mathcal{E}$ 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 $\sqrt{1 - 1/d_{\text{min}}}$, $d_{\text{min}}$ being the dimension of the smallest subsystem (see Appendix B).

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

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

(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 $\epsilon$ and for every state $\rho$, the estimate of $\text{MED}_\rho(\mathcal{A}, \mathcal{B})$ can be guaranteed to have error at most $\epsilon$ with probability at least $1 - \delta$ by repeating the experiment for $n = \log \frac{2}{\delta} / (2\epsilon^2)$ times (see Appendix C).

The experimental estimation of the MED is feasible with photonic systems, in particular in the case where the state $\rho$ 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 [49] and can be well approximated in other models of quantum computing with highly mixed states [50]. In Appendix D 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/numerical evaluation. In Appendix E we show that the noncommutativity can be equivalently rewritten as

$$\text{NCOM}_\rho(\mathcal{E}, \mathcal{D}) = \sqrt{1 - \text{Re} \text{Tr}[D \hat{C} (I \otimes \rho T)]},$$

(11)

where $\hat{C}$ and $D$ are two operators associated to the maps $\mathcal{E}$ and $\mathcal{D}$, respectively. When the operators $\hat{C}$, $D$ and $\rho$ 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 Appendix F 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 [51–53] and MERA states [54].

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

The input of the algorithm is the access to \( m \) black boxes, implementing \( m \) unknown dephasing channels \( A_1, \ldots, A_m \) associated to non-degenerate 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 \([55, 56]\). 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 \( A_l = a_x^{(l)} X + a_y^{(l)} Y + a_z^{(l)} Z \), \( l \in \{1, \ldots, m\} \), where \( X, Y, Z \) are the three Pauli matrices and \( b_l = (b_x^{(l)}, b_y^{(l)}, b_z^{(l)}) \in \mathbb{R}^3 \) is a unit vector (the Bloch vector of the \( l \)-th 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 \( \theta \) with \( |\theta| \leq 22.5^\circ \) 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 Figure 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 \([55, 56]\) 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 modelled 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 \( P^{(l)} \), associated to the \( l \)-th observable, is replaced by a non-projective measurement \( N^{(l)} = (1 - \lambda_l) P^{(l)} + \lambda_l T^{(l)} \), where \( \lambda_l \) is the noise probability, and \( T^{(l)} \) is a trivial measurement, with POVM operators \( T^{(l)} = p_l^{(l)} I \), for a fixed probability distribution \( p^{(l)} = \{ p_i^{(l)} \} \) for every \( l \) and \( i \). The \( k \)-medoid algorithm can then be applied, using the non-commutativity (9) of the noisy channels \( N_1, \ldots, N_m \) defined by

\[
N_{ij}^{(l)} := \sum_{ij} N_{ij}^{(l)} N_{ij}^{(l)\dagger} \quad \text{for} \ l \in \{1, \ldots, m\}.
\]

To test the algorithm, we performed a numerical experiment on 100 randomly generated noisy qubit observables. For simplicity, we chose isotropic noise \([57]\) 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 \( \eta \) 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 \( a_i^{(l)} \) and \( b_i^{(l)} \) 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 the results show that 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 paper we introduced the MED, an experimentally accessible measure of incompati-
bility 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 paper 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 [58]. 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 to how the MED was done in our paper for the case of two observables.

ACKNOWLEDGMENTS

We thank N. Yunger Halpern, S. De Bièvre, and D. R. M. Arvidsson-Shukur for comments on an earlier version of this manuscript, and to L. A. Rozema and M. Antesberger for a discussion on the experimental realization of the proposals in this work. This research is supported by the Hong Kong Research Grant Council through Grants No. 17300918 and No. 17307520, and through the Senior Research Fellowship Scheme SRFS2021-7S02. This publication was made possible through the support of the ID# 62312 grant from the John Templeton Foundation, as part of the 'The Quantum Information Structure of Spacetime' Project (QISS). The opinions expressed in this project are those of the authors and do not necessarily reflect the views of the John Templeton Foundation. Research at the Perimeter Institute is supported by the Government of Canada through the Department of Innovation, Science and Economic Development Canada and by the Province of Ontario through the Ministry of Research, Innovation and Science.

Appendix A: Properties of the MED and its generalization

Here we establish the main properties of the MED, including symmetry, nonnegativity, faithfullness, robustness to noise, being a metric for von Neumann measurements, and reaching its maximum value for mutually unbiased bases. Some of the properties will be established for a generalized version of the MED, which can also be experimentally accessed using the quantum switch.

In the following, we will often consider the generalized MED

$$\text{MED}_\rho(\mathcal{A}, \mathcal{B}) := \sqrt{1 - \sum_{i,j} \text{Re}\text{Tr}[\rho P_i Q_j P_i Q_j]}.$$ (A1)

Note that, by definition, one has

$$\text{MED}_\rho(\mathcal{A}, \mathcal{B}) = \text{MED}(\mathcal{A}, \mathcal{B}),$$ (A2)

for every pair of observables $A$ and $B$. In the following we establish a number of properties of $\text{MED}_\rho$ and MED. As it turns out, some of the properties of $\text{MED}_\rho$ require the density matrix $\rho$ to have some properties, such as being invertible, or commuting with the projectors onto the eigenspaces of $A$ and $B$. All these properties are automatically satisfied by the choice $\rho = I/d$.

Symmetry. By definition, one has

$$\text{MED}_\rho(\mathcal{A}, \mathcal{B}) = \sqrt{1 - \sum_{i,j} \text{Re}\text{Tr}[\rho P_i Q_j P_i Q_j]}$$

$$= \sqrt{1 - \sum_{i,j} \text{Re}\text{Tr}[\rho P_j Q_i P_j Q_i]}$$

$$= \sqrt{1 - \sum_{i,j} \text{Re}\text{Tr}[(\rho P_j Q_i P_j Q_i)^\dagger]}$$

$$= \sqrt{1 - \sum_{i,j} \text{Re}\text{Tr}[Q_j P_i Q_j P_i]}$$

$$= \text{MED}_\rho(\mathcal{B}, \mathcal{A}).$$ (A3)

Here the fourth equality follows from the property $(XY)^\dagger = Y^\dagger X^\dagger$, valid for arbitrary operators $X$ and $Y$, along with the fact that the operators $P_i$, $P_i$, and $Q_j$ are self-adjoint. The fifth equality follows from the cyclic property of the trace.

Nonnegativity. The generalized MED can be equivalently expressed as

$$\text{MED}_\rho(\mathcal{A}, \mathcal{B}) = \sqrt{\sum_{i,j} \text{Tr}[[P_i Q_j] \rho [P_i Q_j]^\dagger]}.$$ (A4)

The right-hand side is non-negative, because each of the operators $[P_i Q_j] \rho [P_i Q_j]^\dagger$ is non-negative, and therefore has a non-negative trace.
Faithfulness. We now show that the generalized MED is faithful for every invertible state \( \rho \) for two arbitrary dephasing channels \( A \) and \( B \), \( \Med_{\rho}(A, B) > 0 \) if and only if the observables \( A \) and \( B \) are incompatible.

The proof is based on Eq. (A4), which shows that \( \Med_{\rho}(A, B) \) is non-negative and equals to zero if and only if \( \text{Tr} \{ [P_i, Q_j] \rho [P_i, Q_j]^\dagger \} = 0 \) for every \( i \) and every \( j \). By the cyclicality of the trace, this condition holds if and only if \( \text{Tr} \{ \sqrt{\rho} [P_i, Q_j] [P_i, Q_j]^\dagger \sqrt{\rho} \} = 0 \) for every \( i \) and every \( j \). Moreover, since each operator \( \sqrt{\rho} [P_i, Q_j] [P_i, Q_j]^\dagger \sqrt{\rho} \) is positive, its trace is zero if and only if the operator itself is zero. Finally, since \( \rho \) is invertible, the condition \( \sqrt{\rho} [P_i, Q_j] [P_i, Q_j]^\dagger \sqrt{\rho} = 0 \) holds if and only if \( [P_i, Q_j] [P_i, Q_j]^\dagger = 0 \), or equivalently, if and only if \( [P_i, Q_j] = 0 \). Summarizing, the condition \( \Med_{\rho}(A, B) = 0 \) is equivalent to the condition \( [P_i, Q_j] = 0, \forall i, j \), which is equivalent to the compatibility of the observables \( A \) and \( B \).

Monotonicity under coarse-graining. Here we show that \( \Med_{\rho}(A, B) \) is non-increasing under coarse-graining, provided that the density matrix \( \rho \) commutes with the measurement that is being coarse-grained:

**Proposition 1** If the state \( \rho \) commutes with the observable \( A \), then one has \( \Med_{\rho}(A, B) \geq \Med_{\rho}(A', B) \) whenever \( A' \) is the dephasing channel associated to a coarse-grained measurement of \( A \).

**Proof.** Let \( P' := (P_i')_{i=1}^o \) be a coarse-graining of the measurement \( P = (P_i)_{i=1}^o \), meaning that there is a surjective function \( f : \{1, \ldots, o\} \to \{1, \ldots, o'\} \) such that

\[
P'_i = \sum_{j: f(j) = i} P_j.
\]

(A5)

Note that, by definition, one has the operator inequality

\[
P_i \leq P'_f(i).
\]

(A6)

Now, suppose that the density matrix \( \rho \) commutes with the projectors \( (P_i')_{i=1}^{o'} \). In this case, one has the relation

\[
\text{Tr}[\rho P_i P_j P_i' P_j'] = \text{Tr}[\sqrt{\rho} P_i P_j \sqrt{\rho} (Q_j P_i' Q_j')]
\]

\[
\geq 0,
\]

valid for every pair of indices \( i \) and \( i' \). Here, the last inequality follows from the fact that the operators \( \sqrt{\rho} P_i \sqrt{\rho} \) and \( Q_j P_i' Q_j' \) are positive semidefinite, and therefore the trace of their product is non-negative.

In particular, Eq. (A7) implies that \( \text{Tr}[\rho P_i P_j P_i' P_j'] \) is a real number. Hence, the real part in the definition of the generalized MED can be dropped, and one has

\[
\Med_{\rho}(A, B) = 1 - \sum_{i,j} \text{Tr}[\rho P_i P_j P_i' P_j'].
\]

(A8)

Since \( \rho \) commutes also with the projectors \( (P'_k)_{k=1}^{o'} \), we also have the relation

\[
\Med_{\rho}(A', B) = 1 - \sum_{k,j} \text{Tr}[\rho P_k' P_j' P_k' P_j'],
\]

(A9)

where \( A' \) is the dephasing channel associated to the coarse-grained measurement \( (P'_k)_{k=1}^{o'} \).

At this point, it is easy to see that \( \Med_{\rho}(A', B) \leq \Med_{\rho}(A, B) \). Indeed, one has the bound

\[
\sum_{k,j} \text{Tr}[\rho P_k' P_j' P_k' P_j'] = \sum_{k,j} \sum_{i,j} \text{Tr}[\rho P_i P_j P_i' P_j']
\]

\[
= \sum_{i,j} \text{Tr}[\rho P_i P_j P_i' P_j']
\]

\[
+ \sum_{k,j} \sum_{i,j} \text{Tr}[\rho P_i P_j P_i' P_j']
\]

\[
\geq \sum_{i,j} \text{Tr}[\rho P_i P_j P_i' P_j'],
\]

(A10)

where the last inequality follows from Eq. (A7). The inequality \( \Med_{\rho}(A', B) \leq \Med_{\rho}(A, B) \) then follows by combining Eq. (A10) with Eqs. (A8) and (A9).

**Metric on von Neumann measurements.** We now show that the generalized MED based on an invertible state is a metric on the set of rank-one projective measurements.

**Lemma 1** For every pair of dephasing channels \( A \) and \( B \) associated to rank-one measurements, one has the expression

\[
\Med_{\rho}(A, B) = \frac{1}{\sqrt{2}} \| (\tau_{AB} - \tau_{AB}) (\sqrt{\rho} \otimes I) \|_2,
\]

(A11)

where \( \| X \|_2 = \sqrt{\text{Tr}[X^* X]} \) is the Hilbert-Schmidt norm, and \( \tau_{AB} \) and \( \tau_{AB} \) are the Choi operators of \( A \) and \( B \), given by

\[
\tau_{AB} := \sum_{m,n} A(m) \langle n | \otimes | m \rangle \langle n | = \sum_i P_i \otimes \bar{F}_i,
\]

(A12)

\[
\tau_{AB} := \sum_{m,n} B(m) \langle n | \otimes | m \rangle \langle n | = \sum_j Q_j \otimes \bar{Q}_j,
\]

(A13)

with \( \bar{X} \) denoting the complex conjugate of a matrix \( X \).

**Proof.** Let us define the product

\[
\langle X, Y \rangle_{\rho} := \text{Tr}[(\rho \otimes I) X^* Y].
\]

(A14)

For every self-adjoint operator \( \tau \), we have the relation

\[
\| \tau (\sqrt{\rho} \otimes I) \|_2^2 = \text{Tr}[(\sqrt{\rho} \otimes I) \tau^2 (\sqrt{\rho} \otimes I)]
\]

\[
= \text{Tr}[\rho \otimes I \tau^2]
\]

\[
= \langle \tau, \tau \rangle_{\rho}.
\]

(A15)

Using the two equations above, we obtain

\[
\| (\tau_{AB} - \tau_{AB}) (\sqrt{\rho} \otimes I) \|_2^2 = \langle (\tau_{AB} - \tau_{AB}, (\tau_{AB} - \tau_{AB}) \rangle_{\rho}
\]

\[
= \langle \tau_{AB} - \tau_{AB} \rangle_{\rho} + \langle \tau_{AB} - \tau_{AB} \rangle_{\rho}
\]

\[
= \langle \tau_{AB}, \tau_{AB} \rangle_{\rho} - \langle \tau_{AB}, \tau_{AB} \rangle_{\rho}.
\]

(A16)
Note that one has

\begin{align}
\langle \tau_{\mathcal{A}}, \tau_{\mathcal{B}} \rangle_p &= \text{Tr}[(\rho \otimes I) \tau_{\mathcal{A}}^2] \\
&= \text{Tr}[(\rho \otimes I) \tau_{\mathcal{B}}] \\
&= \sum_i \text{Tr}[\rho P_i] \times \text{Tr}[\overline{P}_i] \\
&= \sum_{i,j} \text{Tr}[\rho Q_j] \\
&= 1,
\end{align}

where the second equality follows from the fact that \( \tau_{\mathcal{B}} \) is a projector, the third equality follows from Eq. \((A12)\), the fourth equality follows from the fact that the measurement is rank-one (and therefore \( \text{Tr}[\overline{P}_i] = 1 \) for every \( i \)), and the fifth equality follows from the normalization condition \( \sum_i P_i = I \).

Similarly, we have

\begin{align}
\langle \tau_{\mathcal{B}}, \tau_{\mathcal{A}} \rangle_p &= \text{Tr}[(\rho \otimes I) \tau_{\mathcal{B}}^2] \\
&= \sum_j \text{Tr}[\rho Q_j] \times \text{Tr}[\overline{Q}_j] \\
&= \sum_{i,j} \text{Tr}[\rho P_i Q_j] \\
&= \sum_{i,j} \text{Tr}[\rho P_i Q_j P_i Q_j],
\end{align}

where the last equality follows from the fact that the operators \( P_i \) and \( Q_j \) are rank-one.

Similarly, we have

\begin{align}
\langle \tau_{\mathcal{A}}, \tau_{\mathcal{B}} \rangle_p &= \text{Tr}[(\rho \otimes I) \tau_{\mathcal{A}}^2 \tau_{\mathcal{B}}] \\
&= \sum_{i,j} \text{Tr}[\rho P_i Q_j P_i] \times \text{Tr}[\overline{P}_i \overline{Q}_j] \\
&= \sum_{i,j} \text{Tr}[\rho P_i Q_j P_i] \\
&= \sum_{i,j} \text{Tr}[\rho P_i Q_j P_i Q_j],
\end{align}

where the last equality follows from the fact that the operators \( P_i \) and \( Q_j \) are rank-one.

Eq. \((A21)\) shows that \( \text{MED}_p(\mathcal{A}, \mathcal{B}) \) coincides with the Hilbert-Schmidt norm \( ||(\tau_{\mathcal{A}} - \tau_{\mathcal{B}})(\sqrt{\rho} \otimes I)||_2 \) up to a constant factor. \(\blacksquare\)

**Lemma 2** For every invertible density matrix \( \rho \), \( \text{MED}_p \) is a metric on the space of von Neumann measurements.

**Proof.** To prove that \( \text{MED}_p \) is a metric, we need to show that

1. \( \text{MED}_p(\mathcal{A}, \mathcal{B}) = \text{MED}_p(\mathcal{B}, \mathcal{A}) \) for every \( \mathcal{A} \) and \( \mathcal{B} \) (symmetry)
2. \( \text{MED}_p(\mathcal{A}, \mathcal{B}) \geq 0 \) for every \( \mathcal{A} \) and \( \mathcal{B} \), with the equality if and only if \( \mathcal{A} = \mathcal{B} \) (nonnegativity and identity of indiscernibles)
3. \( \text{MED}_p(\mathcal{A}, \mathcal{C}) \leq \text{MED}_p(\mathcal{A}, \mathcal{B}) + \text{MED}_p(\mathcal{B}, \mathcal{C}) \) (triangle inequality).

Symmetry was established at the beginning of this Supplemental Material, in Eq. \((A3)\).

Nonegativity of the generalized MED was also established earlier in this Supplemental Material in the demonstration of faithfulness of \( \text{MED}_p \). When \( \rho \) is invertible, we also showed that \( \text{MED}(\mathcal{A}, \mathcal{B}) = 0 \) implies \( [P_i, Q_j] = 0 \) for every \( i \) and \( j \). For von Neumann measurements, \( (P_i)_i \) and \( (Q_j)_j \) are two maximal sets of rank-one projectors, and the commutation condition means that there exists a permutation \( \pi : \{1, \ldots, d\} \rightarrow \{1, \ldots, d\} \) such that \( P_i = Q_{\pi(i)} \). In this case, one has \( \mathcal{A}(X) = \sum_i P_i X P_i = \sum_i Q_{\pi(i)} X Q_{\pi(i)} = \sum_j Q_j X Q_j = \mathcal{B}(X) \) for every \( d \times d \) matrix \( X \).

Finally, the triangle inequality can be deduced from Eq. \((A11)\) of Lemma 1 and from the triangle inequality of the Hilbert-Schmidt norm. \(\blacksquare\)

**Robustness to noise.** We have seen that the generalized MED based on an invertible state \( \rho \) is a faithful measure of noncommutativity. We now show that this faithfulness property is preserved even when the ideal projective measurements of \( A \) and \( B \) are replaced by noisy measurements. Precisely, we consider the noisy scenario where the canonical channels \( \mathcal{A} \) and \( \mathcal{B} \) are replaced by quantum channels \( \mathcal{A}' \) and \( \mathcal{B}' \) of the form \( \mathcal{A}' = \sum_{i,k} A^i_{k,l} \rho A^i_{k,l} \) and \( \mathcal{B}'(\rho) = \sum_{j,l} B_{j,l} \rho B_{j,l}^\dagger \), with

\begin{equation}
\sum_k A^i_{k,l} A^i_{k,l} = (1 - \lambda) P_i + \lambda p_i I \tag{A22}
\end{equation}

and

\begin{equation}
\sum_l B^\dagger_{j,l} B_{j,l} = (1 - \mu) Q_j + \mu q_j I \tag{A23}
\end{equation}

with suitable probabilities \( \lambda, \mu \in [0,1] \) and suitable probability distributions \( p \) and \( q \). In the following, we show robustness under the assumption that at least one of the two channels \( \mathcal{A}' \) and \( \mathcal{B}' \) is self-adjoint (recall that a linear map...
$\mathcal{M}$ is self-adjoint if, for every pair of $d \times d$ matrices $X$ and $Y$, one has $\text{Tr}[X, \mathcal{M}(Y)] = \text{Tr}[\mathcal{M}(X)Y]$. In the noisy case, we consider the noncommutativity

$$\text{NCOM}_p(\mathcal{A}', \mathcal{B}') = \sqrt{\frac{\sum_{i,j,k,l} \text{Tr} \left( p \left[ A_{i,k}, B_{j,l} \right] \right)^2}{2}}. \quad (A24)$$

If this quantity is zero, then each of the commutators $[A_{i,k}, B_{j,l}]$ must vanish, i.e. one must have the relations

$$[A_{i,k}, B_{j,l}] = 0 \quad \forall i, j, k, l \quad (A25)$$

and

$$[A_{i,k}^\dagger, B_{j,l}^\dagger] = 0 \quad \forall i, j, k, l, \quad (A26)$$

where the second relation is obtained from the first by taking the adjoint on both sides of the equality sign.

Note that the above relations must hold for every possible Kraus decomposition of the channels $\mathcal{A}'$ and $\mathcal{B}'$. If channel $\mathcal{A}'$ is self-adjoint, the operators $(A_{i,k})_{i,k}$ also form a Kraus representation, and therefore one must have the relation

$$[A_{i,k}^\dagger, B_{j,l}^\dagger] = 0 \quad \forall i, j, k, l. \quad (A27)$$

and, taking the adjoint on both sides of the equality

$$[A_{i,k}, B_{j,l}] = 0 \quad \forall i, j, k, l. \quad (A28)$$

Similarly, if channel $\mathcal{B}'$ is self-adjoint, the above relations must hold. Using Eqs. (A22), (A23), (A25), (A26), (A27), and (A28), we then obtain

$$(1-\lambda)(1-\mu) [P_i, Q_j] = \sum_{k,l} [A_{i,k}^\dagger A_{i,k}, B_{j,l}^\dagger B_{j,l}] = 0 \quad \forall i, j. \quad (A29)$$

Hence, if the noncommutativity of the channels $\mathcal{A}'$ and $\mathcal{B}'$ is zero, then the ideal measurements $(P_i)$ and $(Q_j)$ must be compatible, for every value of the noise parameters $\lambda$ and $\mu$ except in the trivial case $\lambda = 1$ or $\mu = 1$, in which the original measurements are replaced by white noise.

Maximality for maximally complementary observables. We now show the inequality $\text{MED}(\mathcal{A}, \mathcal{B}) \leq \sqrt{1-1/(k_A k_B)}$, where $k_A$ ($k_B$) is the number of projectors in the spectral decomposition of the observable $A$ ($B$). The maximum value is given by $\text{MED}(\mathcal{A}, \mathcal{B}) = \sqrt{1-1/d}$ and attained if and only if $A$ and $B$ are maximally complementary [42] or in other words, their POVM operators are rank-one projectors onto the basis vectors of two mutually unbiased bases.

The proof uses a series of lemmas.

Lemma 3 Let $A, B$ be $n \times n$ Hermitian matrices: If $A$ and $B$ are positive semi-definite, then $AB$ is diagonalizable and has non-negative eigenvalues.

Proof. The proof can be found in Corollary 7.6.2(b) of Ref. [59]. ■

Lemma 4 For every pair of observables $A$ and $B$, one has the bound $\text{MED}(\mathcal{A}, \mathcal{B}) \leq \sqrt{1-1/k_B}$ where $k_B$ is the number of distinct eigenvalues of $B$. The equality holds only if $\text{Tr}[P_i Q_j]$ is independent of $j$.

Proof. Using the definitions (A1) and (A2), we focus on a term $\sum_j \text{Tr}[P_i Q_j P_i Q_j]$, fixing thereby the index $i$. If $P_i$ is a projector of rank $r_i$, then

$$\text{rank}(P_i Q_j) \leq r_i. \quad (A30)$$

Both $P_i$ and $Q_j$ are orthogonal projectors, they are Hermitian and positive semi-definite operators. Using Lemma 3, we can diagonalize the operator $P_i Q_j$ as

$$P_i Q_j = X_{ij} \Lambda_{ij} X^{-1}_{ij},$$

where $\Delta_{ij}$ is a diagonal matrix with non-negative entries. Let $r_{ij}$ be the rank of $\Lambda_{ij}$ and assume that the first $r_{ij}$ diagonal entries of $\Lambda_{ij}$, denoted by $\lambda_{ij,1}, \cdots, \lambda_{ij,r_i}$, are non-zero. Then, we can write

$$\text{Tr}[P_i Q_j] = \sum_{s=1}^{r_{ij}} \lambda_{ij,s}. \quad (A31)$$

Taking into account the relation $\sum_{k=1}^{k_B} \text{Tr}[P_i Q_j] = \text{Tr}[P_i] =: r_i$, we find

$$\sum_{j=1}^{k_B} \sum_{s=1}^{r_{ij}} \lambda_{ij,s} = r_i. \quad (A32)$$

On the other hand,

$$\sum_{j=1}^{k_B} \text{Tr}[P_i Q_j P_i Q_j] = \sum_{j=1}^{k_B} \sum_{s=1}^{r_{ij}} (\lambda_{ij,s})^2. \quad (A33)$$

The minimum of (A33) under the constraint (A32) can be computed with the method of Lagrange multipliers. The coefficients that minimize (A33) are given by

$$\lambda^\text{min}_{ij,s} = \frac{r_i}{\sum_{l=1}^{k_B} r_{il}}, \quad \forall j \in \{1, \ldots, k_B\}, \forall s \in \{1, \ldots, r_{ij}\}. \quad (A34)$$

Plugging the optimal coefficients into the right hand side of Eq. (A33) we then obtain

$$\sum_{j=1}^{k_B} \text{Tr}[P_i Q_j P_i Q_j] \geq \frac{r_i^2}{\sum_{l=1}^{k_B} r_{il}}. \quad (A35)$$

Now, recall that $r_{il} = \text{rank}(P_i Q_j) \leq \text{rank}(P_i) = r_i$. Plugging this relation into the previous inequality, we obtain

$$\sum_{j=1}^{k_B} \text{Tr}[P_i Q_j P_i Q_j] \geq \frac{r_i}{k_B}. \quad (A36)$$
Finally, summing over $i$ yields the lower bound
\begin{equation}
\sum_{i=1}^{k_A} \sum_{j=1}^{k_B} \text{Tr}[P_i Q_j P_i Q_j] \geq \frac{d}{k_B}.
\end{equation}
(A37)

Hence, we obtained
\begin{equation}
\text{MED}(\mathcal{A}, \mathcal{B}) = \sqrt{1 - \frac{1}{k_B}},
\end{equation}
(A38)

A necessary condition for achieving the equality is that the eigenvalues $\lambda_{ij,s}$ depend only on $i$ (and not on $j$ and $s$), cf. Eq. (A34). This condition implies in particular that the sum $\sum_s \lambda_{ij,s} = \text{Tr}[P_i Q_j]$ is independent of $j$. ■

**Lemma 5** For every two observables $A$ and $B$, one has the bound $\text{MED}(\mathcal{A}, \mathcal{B}) \leq \sqrt{1 - \frac{1}{\min\{k_A, k_B\}}}$. The equality is achieved only if
\begin{equation}
\text{Tr}[P_i Q_j] = \frac{d}{k_A k_B} \quad \forall i \in \{1, \ldots, k_A\}, \forall j \in \{1, \ldots, k_B\}.
\end{equation}
(A39)

**Proof.** Lemma 4 implies the upper bound $\text{MED}(\mathcal{A}, \mathcal{B}) \leq \sqrt{1 - \frac{1}{k_A}}$. Moreover, the symmetry of the MED yields the condition $\text{MED}(\mathcal{A}, \mathcal{B}) = \text{MED}(\mathcal{B}, \mathcal{A}) \leq \sqrt{1 - \frac{1}{k_A}}$ (the inequality following again from Lemma 4). Hence, one has the bound $\text{MED}(\mathcal{A}, \mathcal{B}) \leq \sqrt{1 - \frac{1}{\min\{k_A, k_B\}}}$. By Lemma 4, the equality holds only if $\text{Tr}[P_i Q_j]$ is independent of $j$, and only $\text{Tr}[Q_j P_i] = \text{Tr}[P_i Q_j]$ is independent of $i$. In summary, it is necessary that $\text{Tr}[P_i Q_j]$ is constant, say $\text{Tr}[P_i Q_j] = c$ for some constant $c$ and for every $i$ and $j$. The value of the constant can be obtained from the condition
\begin{equation}
d = \text{Tr}[I] = \sum_{i=1}^{k_A} \sum_{j=1}^{k_B} \text{Tr}[P_i Q_j] = k_A k_B c,
\end{equation}
(A40)

which implies $c = d/(k_A k_B)$. ■

**Lemma 6** For every two observables $A$ and $B$, one has the bound $\text{MED}(\mathcal{A}, \mathcal{B}) \leq \sqrt{1 - \frac{1}{d}}$ and the equality holds if and only if $A$ and $B$ are non-degenerate and their eigenvectors form two mutually unbiased bases.

**Appendix B: Noncommutativity between entangled and product measurements**

The mathematical description of a measurement process, including both the measurement statistics and the post-measurement states, is provided by a quantum instrument, that is, a collection of completely positive, trace non-increasing maps $(\mathcal{E}_i)_{i=1}^k$, such that the sum $\sum_{i=1}^k \mathcal{E}_i$ is trace-preserving. Here the index $i$ labels the possible measurement outcomes, which occur on an input state $\rho$ with probability $p(i|\rho) = \text{Tr}[\mathcal{E}_i(\rho)]$, leaving the system in the post-measurement state $\rho_i = \mathcal{E}_i(\rho)/\text{Tr}[\mathcal{E}_i(\rho)]$. The average evolution due to the measurement is then given by the quantum channel $\mathcal{C} := \sum_{i=1}^k \mathcal{E}_i$.

We define the noncommutativity between two instruments as the noncommutativity of the corresponding average evolutions:
\begin{equation}
\text{NCOM}_\rho \left( (\mathcal{E}_i)_{i=1}^k, (\mathcal{D}_j)_{j=1}^d \right) := \text{NCOM}_\rho(\mathcal{E}, \mathcal{D}),
\end{equation}
(B1)

with $\mathcal{E} := \sum_{i=1}^k \mathcal{E}_i$ and $\mathcal{D} := \sum_{j=1}^d \mathcal{D}_j$.

We now provide a lower bound on the noncommutativity between a maximally entangled measurement and a product measurement. Consider the case of a bipartite system, consisting of two subsystems $S_1$ and $S_2$, of dimensions $2 \leq d_1 \leq d_2$. By "maximally entangled measurement" we mean a quantum instrument $(\mathcal{E}_i)_{i=1}^{k_A}$ of the form $\mathcal{E}_i(\rho) = C_i \rho C_i^\dagger$, with $C_i = A_i |\Psi_i\rangle \langle \Phi_i|$ where $|\Phi_i\rangle$ and $|\Psi_i\rangle$ are maximally entangled.
states, and $0 \leq \lambda_i \leq 1$ is a suitable coefficient. By a "product measurement", we mean an instrument $(\mathcal{D}_j)_{j=1}^{k_B}$ of the form $\mathcal{D}_j(\rho) = D_j \rho D_j^†$ with $D_j = \mu_j |\gamma_j\rangle \langle \alpha_j| \otimes |\delta_j\rangle \langle \beta_j|$, where $|\alpha_j\rangle$ and $|\beta_j\rangle$ ($|\gamma_j\rangle$ and $|\delta_j\rangle$) are pure states of system $S_1$ ($S_2$), and $0 \leq \mu_j \leq 1$ is a suitable coefficient. (Note that we are not assuming that the instrument $(\mathcal{D}_j)_{j=1}^{k_B}$ can be realized by local operations and classical communication.) In other words, our notion of product measurement corresponds to fine-grained separable instruments [60], which are not necessarily realizable through local operations and classical communication.

The noncommutativity of the instruments $(\mathcal{E}_i)_{i=1}^{k_A}$ and $(\mathcal{D}_j)_{j=1}^{k_B}$ is given by

\[
\text{NCOM}_\rho\left((\mathcal{E}_i)_{i=1}^{k_A}, (\mathcal{D}_j)_{j=1}^{k_B}\right) = \sqrt{\frac{1}{2} \sum_{i,j} \text{Tr}\left[\rho \left|\langle C_i | D_j \rangle \right|^2\right]} = \sqrt{1 - \frac{1}{d_1}} \sum_{i,j} \text{Tr}[C_i^† D_j^† C_i D_j \rho].
\]  

(B2)

Here we consider the case where the state $\rho$ is maximally mixed, namely $\rho = I_1/d_1 \otimes I_2/d_2$. In this case, one has the bound

\[
\text{Re} \left[ \sum_{i,j} \text{Tr}[C_i^† D_j^† C_i D_j] \right] \leq \sum_{i,j} \left| \text{Tr}[C_i^† D_j^† C_i D_j] \right| \leq \sum_{i,j} \lambda_i^2 \left| \langle \Phi_i | D_j | \Phi_i \rangle \right|^2 \leq \frac{1}{d_1} \sum_{i,j} \lambda_i^2 \mu_j \left| \langle \Phi_i | D_j | \Phi_i \rangle \right|^2.
\]  

(B3)

the last bound following form the expression $D_j = \mu_j |\gamma_j\rangle \langle \alpha_j| \otimes |\delta_j\rangle \langle \beta_j|$ and from the fact that the state $|\Psi_i\rangle$ is maximally entangled.

Using the polar decomposition $D_j = U|D_j|$, we then have the bound

\[
\sum_i \lambda_i^2 \left| \langle \Phi_i | D_j | \Phi_i \rangle \right|^2 = \sum_i \lambda_i^2 \left| \langle \Phi_i | U|D_j| U^† | \Phi_i \rangle \right|^2 \leq \sum_i \lambda_i^2 \left| \langle \Phi_i | |D_j| \right| \left| \Phi_i \rangle \right| \left| \Phi_i \rangle \right|^2 \times \sum_i \lambda_i^2 \left| \langle \Phi_i | U|D_j| U^† | \Phi_i \rangle \right|^2 = \text{Tr}[|D_j|^2] = \mu_j.
\]  

(B4)

Summarizing, we obtained the bound

\[
\text{Re} \left[ \sum_{i,j} \text{Tr}[C_i^† D_j^† C_i D_j] \right] \leq \frac{1}{d_1} \sum_j \mu_j^2 = \frac{1}{d_1} \left( d_1 d_2 \right).
\]  

(B5)

where the last equality follows by taking the trace on both sides of the completeness relation $\sum_{j=1}^{k_B} \mu_j^2 |\alpha_j\rangle \otimes |\beta_j\rangle \langle \beta_j| = I_1 \otimes I_2$, implied by the normalization of the instrument $(\mathcal{D}_j)_{j=1}^{k_B}$.

Hence, the noncommutativity is lower bounded as

\[
\text{NCOM}_{\rho} \left((\mathcal{E}_i)_{i=1}^{k_A}, (\mathcal{D}_j)_{j=1}^{k_B}\right) \geq \sqrt{1 - \frac{1}{d_1}}.
\]  

(B6)

The above bound can be immediately extended to the multipartite case, by considering a bipartition of the system into the lowest dimensional subsystem and all the remaining ones.

**Appendix C: Sample complexity of (generalized) MED estimation**

Our protocol provides a direct estimate of the MED in terms of the probability that a Fourier basis measurement on the control system yields outcome "-". The probability can be estimated from the frequency of the outcome "-" in a number of repetitions of the experiment. We now show that the number of repetitions is independent of the system’s dimension and scales inverse polynomially with the desired level of accuracy.

The proof is standard, and is provided here just for completeness. The result of the Fourier basis measurement defines a Bernoulli variable with outcomes $k \in \{0, 1\}$. Here, outcome 1 corresponds to the outcome corresponding to the basis vector $|+\rangle$, while outcome 0 corresponds to the basis vector $|-\rangle$. The probability mass function of this Bernoulli variable is $f(k; p_-)$ defined by

\[
f(-; p_-) = p_- \quad \text{and} \quad f(+; p_-) = 1 - p_-.
\]  

(C1)

If the experiment is repeated for $n$ times, the outcomes are a sequence of independent Bernoulli variables $X_1, X_2, ..., X_n$, with each variable distributed according to the probability mass function $f(k; p_-)$. The sum of these variables, denoted by $S = \sum_i X_i$, is distributed according to the binomial distribution $B(n; S; n, p_-) := p_-^S (1 - p_-)^{n-S} \binom{n}{S}$. Then, Hoeffding’s inequality [61] implies that the empirical frequency $S/n$ is close to $p_-$ with high probability, namely

\[
\forall \epsilon > 0, P \left( \left| \frac{S}{n} - p_- \right| < \epsilon \right) \geq 1 - 2e^{-2\epsilon^2 n}.
\]
Hence, the minimum number of repetitions of the experiment needed to guarantee that the empirical frequency has probability at most $\delta$ to deviate from the frequency by at most $\epsilon$ is

$$n(\epsilon, \delta) = \left\lceil \frac{1}{2\epsilon^2} \log \frac{\delta}{2} \right\rceil. \quad (C2)$$

This expression shows that the sample complexity is independent of the dimension of the system under consideration. In particular, the sample complexity does not increase when the MED is measured on multiparticle systems, in contrast with the sample complexity of process tomography which increases exponentially with the number of particles.

### Appendix D: Comparison with other experimental schemes

A naïve way to estimate the MED is to characterize the channels $\mathcal{A}$ and $\mathcal{B}$ via process tomography [62–67], or the projective measurements $\mathcal{P}$ and $\mathcal{Q}$ via measurement tomography [68], and then use Eq. (4). However, process and measurement tomography requires access to the outcomes of two measurements of the observable $A$. The estimation of the MED would then proceed by performing a measurement of the observable $A$, and finally, another measurement of the observable $A$. The total probability that the two measurements of $A$ give equal outcomes is equal to $\text{Prob}(A, \mathcal{B}) = 1 - \text{MED}(\mathcal{A}, \mathcal{B})^2$. In this case, the complexity of estimating the MED does not grow exponentially with the system’s size.

The main difference between the above scheme and the scheme using the quantum switch is that the above scheme requires access to the outcomes of two measurements of the observable $A$. The ability to estimate the incompatibility without access to the outcomes offers an advantage in situations where the experimenter wants to discover the incompatibility of two observables measured by two parties in their local laboratories. In this case, the quantum switch scheme allows the experimenter to estimate the incompatibility/noncommutativity in a black box fashion, by sending input states to the two laboratories and observing their outputs states, without any access to the outcomes generated inside the laboratories.

### Appendix E: Proof of Eq. (11) in the main text

From Eq. (9) in the main text, we have

$$\text{NCOM}_p(\mathcal{E}, \mathcal{D}) = \sqrt{\frac{\sum_{i,j} \text{Tr} \left( \rho \left| C_i D_j \right|^2 \right)}{2}}$$

$$= 1 - \text{Re} \left( \sum_{i,j} \text{Tr} \left( C_i D_j \rho C_i^\dagger D_j^\dagger \right) \right)$$

$$= 1 - \text{Re} \left( \sum_{j} \text{Tr} \left( \mathcal{E}(D_j \rho) \ D_j^\dagger \right) \right)$$

$$= 1 - \text{Re} \left( \sum_{j} \langle D_j | \mathcal{E}(D_j \rho) \rangle \right), \quad (E1)$$

where we used the double-ket notation $|X\rangle := \sum_{m,n} (m|X|n) \otimes |n\rangle$ for an arbitrary operator $X$, and the property $\langle X | Y \rangle = \text{Tr}[X^\dagger Y] = \text{Tr}[YX^\dagger]$, valid for arbitrary $X$ and $Y$ (in our case, $X = D_j$ and $Y = \mathcal{E}(D_j \rho)$).

Now, consider the operator $\hat{C}$ defined through the relation [69]

$$\hat{C}|X\rangle := \mathcal{E}(X), \quad \forall X. \quad (E2)$$

Using this definition, the noncommutativity can be expressed as

$$\text{NCOM}_p(\mathcal{E}, \mathcal{D}) = \sqrt{1 - \text{Re} \left( \sum_{j} \langle D_j | \hat{C} (I \otimes \rho^T) | D_j \rangle \right)}$$

$$= 1 - \text{Re} \left[ \sum_{j} \langle D_j | \hat{C} (I \otimes \rho^T) | D_j \rangle \right]$$

$$= 1 - \text{Re} \left[ \text{Tr} \left( \sum_{j} \left| D_j \right| \langle D_j | \hat{C} (I \otimes \rho^T) \right) \right]$$

$$= 1 - \text{Re} \left[ \text{Tr} \left[ D \hat{C} (I \otimes \rho^T) \right] \right]. \quad (E3)$$

where $D := \sum_j |D_j\rangle \langle D_j | = (\mathcal{D} \otimes \mathcal{I})(|I\rangle \langle I|)$ is the Choi operator of $\mathcal{D}$, with $\mathcal{I}$ being identity channel.

In particular, when the state $\rho$ is maximally mixed, the noncommutativity takes the simple expression

$$\text{NCOM}_p(\mathcal{E}, \mathcal{D}) = \sqrt{1 - \frac{\text{Re} \left[ \langle D \hat{C} \rangle \right]}{d}}. \quad (E4)$$

The operator $\hat{C}$ is in one-to-one correspondence with the map $\mathcal{E}$. Explicitly, Eq. (E2) implies the explicit expression

$$\hat{C} = \sum_i C_i \otimes \overline{C}_i, \quad (E5)$$

where $\overline{C}_i$ is the complex conjugate of the matrix $C_i$. The operator $\hat{C}$ can be equivalently expressed in terms of its Choi...
were in and out” and “out” label the input and output systems of channel $\mathcal{C}$, respectively, and $\text{SWAP}_{\text{in},\text{out}}$ is the swap operator, defined by the relation

$$\text{SWAP}_{\text{in},\text{out}}(\rho) = |\psi\rangle\langle\psi| \otimes |\phi\rangle\langle\phi|,$$

where $|\psi\rangle$ and $|\phi\rangle$ are pure states of the input and output systems, respectively. Eq. (E6) can be verified explicitly using the expressions

$$\tilde{C} = \sum_i C_i \otimes C_i$$

and $C = \sum_i |C_i\rangle\langle C_i|.$

### Appendix F: Expression of the noncommutativity of two channels in terms of their unitary realizations

Here we provide an alternative expression of the noncommutativity (and therefore of the MED) in terms of the unitary realizations of the two channels $\mathcal{C}$ and $\mathcal{D}.$ Consider two unitary realizations, of the form

$$\mathcal{C}(\rho) = \text{Tr}_F \left[ U_{\text{SE}} (\rho \otimes |\eta\rangle\langle\eta|_E) U_{\text{SE}}^\dagger \right],$$

$$\mathcal{D}(\rho) = \text{Tr}_F \left[ V_{\text{SF}} (\rho \otimes |\phi\rangle\langle\phi|_F) V_{\text{SF}}^\dagger \right],$$

where $E$ and $F$ are two suitable quantum systems, serving as the environments, $|\eta\rangle$ and $|\phi\rangle$ are pure states of $E$ and $F$, respectively, and $U_{\text{SE}}$ and $V_{\text{SF}}$ are two unitary evolutions between the target system (denoted by $S$) and the environments $E$ and $F$, respectively.

To compute the action of the channel $\mathcal{D}(\mathcal{C}, \mathcal{D})$, we consider the quantum switch of the unitary gates $U_{\text{SE}} \otimes I_F$ and $V_{\text{SF}} \otimes I_E$, and then take the partial trace over the environments. The quantum switch of the unitary gates $U_{\text{SE}} \otimes I_F$ and $V_{\text{SF}} \otimes I_E$ yields the controlled unitary gate

$$W = (U_{\text{SE}} \otimes I_F)(V_{\text{SF}} \otimes I_E) \otimes |0\rangle\langle 0|_C + (V_{\text{SF}} \otimes I_E)(U_{\text{SE}} \otimes I_F) \otimes |1\rangle\langle 1|_C,$$

where the subscript $C$ denotes the control system, and it is implicitly understood that the Hilbert spaces in the tensor product are suitably arranged according to the subscripts of the corresponding systems.

Hence, the action of the channel $\mathcal{D}(\mathcal{C}, \mathcal{D})$ on the state $\rho \otimes |+\rangle\langle +|$ is given by

$$\Delta_{\mathcal{D}, \mathcal{C}}(\rho \otimes |+\rangle\langle +|) = \text{Tr}_F \left[ W (\rho \otimes |\eta\rangle\langle\eta|_E \otimes |\phi\rangle\langle\phi|_F \otimes |+\rangle\langle +|_C) W^\dagger \right].$$

To reduce the above expression to the case where the input state is pure, we take a purification of $\rho,$ given by a pure state $|\Psi\rangle \in \mathcal{H}_S \otimes \mathcal{H}_R,$ where $R$ is a suitable purifying system. Let us define the state

$$|\Gamma\rangle_{SREF} := (W \otimes I_R) |\Psi\rangle_{SR} \otimes |\eta\rangle_E \otimes |\phi\rangle_F \otimes |+\rangle_C,$$

and $|\Lambda_0\rangle_{SREF} := (U_{\text{SE}} \otimes I_F)(V_{\text{SF}} \otimes I_E) \otimes |0\rangle \otimes |\eta\rangle \otimes |\phi\rangle,$

$$|\Lambda_1\rangle_{SREF} := (V_{\text{SF}} \otimes I_E)(U_{\text{SE}} \otimes I_F) \otimes |1\rangle \otimes |\eta\rangle \otimes |\phi\rangle.$$

The probability of the outcome - when the output state is measured on the Fourier basis is then given by

$$p_- = \langle - | \text{Tr}_S [\Delta_{\mathcal{D}, \mathcal{C}}(\rho \otimes |+\rangle\langle +|_C)] | - \rangle$$

$$= \langle - | \text{Tr}_{SREF} [\langle \Gamma | \Gamma \rangle_\mathcal{C}] | - \rangle$$

$$= ||\langle \Gamma_{SREF} = (\langle - | U_{\text{SE}} \otimes I_F) |\Psi\rangle_{SR} \otimes |\eta\rangle_E \otimes |\phi\rangle_F \otimes |+\rangle_C ||^2$$

$$= \frac{1}{4} |||\Lambda_0\rangle - |\Lambda_1\rangle ||^2$$

$$= 1 - \text{Re} \langle \Lambda_0 | \Lambda_1 \rangle \frac{2}{2}.$$
