Quantum speedup in the identification of cause-effect relations

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The ability to identify cause-effect relations is an essential component of the scientific method. The identification of causal relations is generally accomplished through statistical trials where alternative hypotheses are tested against each other. Traditionally, such trials have been based on classical statistics. However, classical statistics becomes inadequate at the quantum scale, where a richer spectrum of causal relations is accessible. Here we show that quantum strategies can greatly speed up the identification of causal relations. We analyse the task of identifying the effect of a given variable, and we show that the optimal quantum strategy beats all classical strategies by running multiple equivalent tests in a quantum superposition. The same working principle leads to advantages in the detection of a causal link between two variables, and in the identification of the cause of a given variable.

INTRODUCTION

Identifying causal relations is a fundamental primitive in a variety of areas, including machine learning, medicine, and genetics [1–3]. A canonical approach is to formulate different hypotheses on the cause-effect relations characterising a given phenomenon, and test them against each other. For example, in a drug test some patients are administered the drug, while others are administered a placebo, with the scope of determining whether or not the drug causes recovery. Traditionally, causal discovery techniques have been based on classical statistics, which effectively describes the behaviour of macroscopic variables. However, classical techniques become inadequate when dealing with quantum systems, whose response to interventions can strikingly differ from that of classical random variables [4, 5].

Recently, there has been a growing interest in the extension of causal reasoning to the quantum domain. Several quantum generalizations of the notion of causal network have been proposed [6–15] and new algorithms for quantum causal discovery have been designed [16–20]. Besides its foundational relevance, the study of quantum causal discovery algorithms is expected to have applications in the emerging area of quantum machine learning [21, 22], in the same way as classical causal discovery algorithms have previously impacted classical artificial intelligence.

An intriguing possibility is that quantum mechanics may provide enhanced ways to identify causal links. A clue in this direction comes from Refs. [17, 18], where the authors show that certain quantum correlations are witnesses of causal relationships, in apparent violation of the classical tenet correlation does not imply causation. This observation suggests that quantum setups for testing causal relationships could overcome some of the limitations of existing classical setups. However, the type of advantage highlighted in [17, 18] only concerns a limited class of setups, where the experimenter is constrained to a subset of the possible interventions. If arbitrary interventions are allowed, this particular type of advantage disappears. A fundamental open question is whether quantum setups can offer an advantage over all classical setups, without any restriction on the experimenter’s interventions.

Here we answer the question in the affirmative, proving that quantum features like superposition and entanglement can significantly speed up the identification of causal relations. We start from the task of deciding which variable, out of a list of candidates, is the effect of a given variable. We first analyze the problem in the classical setting, determining the performance of the best classical strategy. Then, we construct a quantum strategy that reduces the error probability by an exponential amount, doubling the decay rate of the error probability with the number of accesses to the relevant variables. Remarkably, the decay rate of our strategy is the highest achievable rate allowed by quantum mechanics, even if one allows for exotic setups where the order of operations is indefinite [23, 24].

The key ingredient of the quantum speedup is the ability to run multiple equivalent experiments in a quantum superposition. The same working principle enables quantum speedups in a broader set of tasks, including, e.g., the task of deciding whether there exists a causal link between two given variables, and the task of identifying the cause of a given variable.

RESULTS

Theory-independent framework for testing causal hypotheses. Here we outline a framework for testing causal hypotheses in general physical theories [25–30]. In this
framework, variables are represented as physical systems, each system with its set of states. The framework applies to theories satisfying the Causality Axiom [28], stating that the probability of an event at a given time should not depend on choices of settings made at future times.

A causal relation between variable $A$ and variable $B$ is represented by a map describing how the state of $B$ responds to changes in the state of $A$. If the map discards $A$ and outputs a fixed state of $B$, then no causal influence can be observed. In all the other cases, some change of $A$ will lead to an observable change of $B$. Hence, we say that $A$ is a cause for $B$.

In general, the set of allowed causal relationships depends on the physical theory, which determines which maps can be implemented by physical processes. In classical physics, cause-effect relations can be represented by conditional probability distributions of the form $p(b|a)$, where $a$ and $b$ are the values of the random variables $A$ and $B$, respectively. In quantum theory, cause-effect relations are described by quantum channels, i.e. completely positive trace-preserving maps transforming density matrices of system $A$ into density matrices of system $B$.

Given a set of variables, one can formulate hypotheses on the causal relationships among them. For example, consider a three-variable scenario, where variable $A$ may cause either variable $B$ or variable $C$, but not both. The causal relation is described by a process $C$, with input $A$ and outputs $B$ and $C$. Here we consider two alternative causal hypotheses: either $A$ causes $B$ but not $C$, or $A$ causes $C$ but not $B$. The problem is to distinguish between these two hypotheses without having further knowledge of the physical process responsible for the causal relation. This means that the process $C$ is unknown, except for the fact that it must compatible with one and only one of the two hypotheses. Mathematically, the two hypotheses correspond to two sets of physical processes, and the problem is to determine which set contains the process $C$.

In order to decide which hypothesis is correct, we assume that the experimenter has black box access to the physical process $C$. The experimenter can probe the process for $N$ times, intervening between one instance and the next, as illustrated in Figure 1. In the end, a measurement is performed and its outcome is used to guess the correct hypothesis.

An important question is how fast the probability of error decays with $N$. The decay is typically exponential, with an error probability vanishing as $p_{\text{err}}(N) \approx 2^{-RN}$ for some positive constant $R$, which we call the discrimination rate. The operational meaning of the discrimination rate is the following. Given an error threshold $\epsilon$, the error probability can be made smaller than $\epsilon$ using approximately $N > \log \epsilon^{-1}/R$ calls to the unknown process. The bigger the rate, the smaller the number of calls needed to bring the error below the desired threshold.

Since the explicit form of the process $C$ is unknown, we take $p_{\text{err}}(N)$ to be the worst-case probability over all processes compatible with the two given causal hypotheses. If prior information over $C$ is available, one may also consider a weaker performance measure, based on the average with respect to some prior. In the following we stick to the worst case scenario, as it provides a stronger guarantee on the performance of the test.

**FIG. 1. Testing causal hypotheses in the black box scenario.** The unknown process $C$ induces a causal relation between one input variable and two output variables. The experimenter probes the process for $N$ times, intervening on the relevant variables at each time step. The first intervention is the preparation of a state $\Psi$, involving the input of the black box and, possibly, an additional reference system (top wire). The subsequent interventions $U_i$ manipulate the output variables and prepare the inputs variables for the next steps. In the end, the output variables and the reference system are measured, and the measurement outcome is used to infer the causal relation.

**FIG. 2. Spacetime picture of a causal intermediary.** Variable $A$ is localized at a point in spacetime, and its causal influences propagate within its future light cone. Variable $B$ is distributed over a section of the light cone of $A$ and intercepts all the influences of $A$. Every other variable $B'$ that is affected by $A$ and comes after $B$ must be obtained from variable $B$ through some physical process.

Identifying causal intermediaries. A variable $B$ is a causal intermediary for variable $A$ if all the influences of $A$ propagate through $B$. Physically, one can think of $B$ as a slice of the future light cone of $A$, so that all causal influences of $A$ must pass through $B$, as illustrated in Figure 2. Mathematically, the fact that $B$ is a causal intermediary means that there exist a process $C$ from $A$ to $B$ such that for every other variable $B'$ and for every process $C'$ with input $A$ and output $B'$ one can decompose $C'$ as $C' = R \circ C$, where $R$ is a suitable process from $B$ to $B'$.

The condition that a variable is a causal intermediary of another has a simple characterisation in all phys-
cal theories where processes are fundamentally reversible, meaning that they can be modeled as the result of a reversible evolution of the system and an environment [28]. The reversibility condition is captured by the expression $C = (I_{\rho} \otimes Tr_{E'}) U (I_A \otimes \eta_E)$, where variables $E$ and $E'$ represent the environment (before and after the interaction), $\eta$ is the initial state of the environment, $Tr_{E'}$ is the operation of discarding system $E'$ [28], and $U$ is a reversible process from $AE$ to $BE'$.

When the reversibility condition is satisfied, the variable $A$ can be recovered from variables $B$ and $E'$. If variable $B$ is to be a causal intermediary of $A$, then the process $C$ must be correctable, in the sense that its action can be undone by another process $R$. In addition, if the state spaces of variables $A$ and $B$ are finite dimensional and of the same dimension, then the process $C$ must be reversible. In classical theory, this means that $C$ is an invertible function. In quantum theory, this means that $C$ is a unitary channel, of the form $C(\rho) = U \rho U^\dagger$ for some unitary operator $U$.

In the following, we will consider the task of identifying which variable, out of a given set of candidates, is the causal intermediary of a given variable $A$. An important feature of this task is that it admits a complete analytical treatment, allowing us to rigorously prove a quantum advantage over all classical strategies. Besides its fundamental interest, this advantage could have applications to the task of monitoring the information flow in future quantum communication networks, allowing an experimenter to determine which node of a quantum network receives information from a given source node.

**Optimal classical strategy.** Suppose that $A$, $B$, and $C$ are random variables with the same alphabet of size $d < \infty$. In this case, the fact that $X \in \{B,C\}$ is a causal intermediary for $A$ means that the map from $A$ to $X$ is a permutation. The first (second) causal hypothesis is that $B$ ($C$) is a permutation of $A$, while $C$ ($B$) is uniformly random. Other than this, no information about the functional relation between the variables is known to the experimenter. In particular, the experimenter does not know which permutation relates the variable $A$ to its causal intermediary $X$.

Let us determine how well one can distinguish between the two hypotheses with a finite number of experiments. In principle, we should examine all sequential strategies as in Figure 1. However, in classical theory the problem can be greatly simplified: the optimal discrimination rate can be achieved by a parallel strategy, wherein the $N$ input variables are initially set to some prescribed set of values [31].

The possibility of an error arises when the randomly fluctuating variable accidentally takes values that are compatible with a permutation, so that the outcome of the test gives no ground to discriminate between the two hypotheses. The probability of such inconclusive scenario is equal to $P(d,v)/d^N$, where $v$ is the number of distinct values of $A$ probed in the experiment and $P(d,v) = d!/(d-v)!$ is the number of injective functions from a $v$-element set to a $d$-element set. The probability of confusion is minimal for $v = 1$, leading to the overall error probability

$$ p_{\text{err}} = \frac{1}{2d^{N-1}}. \quad (2) $$

As a consequence, the rate at which the two causal hypotheses can be distinguished from each other is

$$ R_C = \log d. \quad (3) $$

A first quantum advantage. Classical systems can be regarded quantum systems that lost coherence across the states of a fixed basis, consisting of the classical states. But what if coherence is preserved? Could a coherent superposition of classical states be a better probe for the causal structure?

If the causal relations are restricted to reversible gates that permute the classical states, coherence offers an immediate advantage. The experimenter can prepare $N$ probes, each in the superposition $|\psi_0\rangle = \sum_{i=0}^{d-1} |i\rangle/\sqrt{d}$. Since the superposition is invariant under permutations, the unknown process will produce either $N$ copies of the state $|\psi_0\rangle \otimes I/d$ or $N$ copies of the state $I/d \otimes |\psi_0\rangle$, depending on which causal hypothesis holds. Using Helstrom’s minimum error measurement [32], the error probability is reduced to

$$ p_{\text{err}}^{\text{coh}} = \frac{1}{2d^N}. \quad (4) $$

Compared with the classical error probability (2), the error probability of this simple quantum strategy is reduced by a factor $d$, which does not change the rate, but could be significant when the size of the alphabet is large.

Let us consider the full quantum version of the problem. Three quantum variables $A$, $B$, and $C$, corresponding to $d$-dimensional quantum systems, are promised to satisfy one of two causal hypotheses: either (i) the state of $B$ is obtained from the state of $A$ through an arbitrary unitary evolution and the state of $C$ is maximally mixed, or (ii) the state of $C$ is obtained from the state of $A$ through an arbitrary unitary evolution and the state of $B$ is maximally mixed.

Despite the fact that now the cause-effect relation can be one of infinitely many unitary gates, it turns out that the error probability (4) can still be attained. A universal quantum strategy, working for arbitrary unitary gates, is to prepare $d$ particles in the singlet state

$$ |S_d\rangle = \frac{1}{\sqrt{d!}} \sum_{k_1,k_2,\ldots,k_d} \epsilon_{k_1,k_2,\ldots,k_d} |k_1\rangle|k_2\rangle\cdots|k_d\rangle \quad (5) $$

where $\epsilon_{k_1,k_2,\ldots,k_d}$ is the totally antisymmetric tensor and the sum ranges over all vectors in the computational basis. Then, each of the $d$ particles is used as an input to one use of the channel. Repeating the experiment for $t$ times, and performing Helstrom’s minimum error measurement one can attain the error probability $p_{\text{err}}^{\text{coh}} = (2d^N)^{-1}$, with
$N = td$, independently of the unitary gate representing the cause-effect relationship. In summary, the quantum error probability is at least $d$ times smaller than the best classical error probability, even if the cause-effect relationship is described by an arbitrary unitary gate.

**Optimality among simple parallel strategies.** We now show that the value (4) is optimal among all simple strategies where the unknown process is applied $N$ times in parallel on $N$ identical input systems, as in Figure 3.

Optimality follows from a complementarity relation between the information about the causal structure and the information about the functional dependence between cause and effect. Suppose that the cause-effect dependence amounts to a unitary gate $U$ in some finite set $U$. The ability of a state $|\Psi\rangle$ to probe the cause-effect dependence can be quantified by the probability $p_{\text{guess}}^U$ of correctly guessing the unitary $U$ from the state $U^\otimes N |\Psi\rangle$. When the set of possibly unitaries has sufficient symmetry, we find that the probability of error in identifying the causal structure satisfies the lower bound

$$p_{\text{err}} \geq \frac{1}{2d^N} \left\{ 1 + \frac{1}{2(d^N - 1)} \left( \frac{p_{\text{guess}}^U - 1}{|U|} \right)^2 \right\}$$

(6)

(Appendix A). The higher the probability of success in guessing the cause-effect dependence, the higher the probability of error in identifying the causal structure. A consequence of the bound (6) is that the minimum error probability in identifying the causal intermediary is $(2d^N)^{-1}$, and is attained when the success probability $p_{\text{guess}}^U$ is equal to the random guess probability $1/|U|$.

**Exponential reduction of the error probability.** The bound (6) shows that the discrimination rate of simple parallel strategies cannot exceed the classical discrimination rate $\log d$. We now show that the rate can be doubled by entangling the $N$ probes with an additional reference system.

The working principle of our strategy is to build a quantum superposition of equivalent experimental setups. If no reference system is used, we know that the optimal strategy is to divide the $N$ probes into $N/d$ groups (assuming for simplicity that $N$ is a multiple of $d$), and to entangle the probes within each group. Clearly, different ways of dividing the $N$ inputs into groups of $d$ are equally optimal: it does not matter which particle is entangled with which, as long as each particle is part of a singlet state. Still, we can imagine a machine that partitions the particles according to a certain configuration $i$ if a control system is in the state $|i\rangle$. When the control system is in a superposition, the machine will probe the unknown process in a superposition of configurations, as pictorially illustrated in Figure (4). Explicitly, the optimal input state is

$$|\Psi\rangle = \frac{1}{\sqrt{G_{N,d}}} \sum_{i=1}^{G_{N,d}} (|S_i\rangle^\otimes N/d) \otimes |i\rangle,$$

(7)

where $i$ labels the different ways to partition $N$ identical objects into groups of $d$ elements, $G_{N,d}$ is the number of such ways, $(|S_i\rangle^\otimes N/d)$ is the product of $N/d$ singlet states arranged according to the $i$-th configuration, and $\{ |i\rangle, i = 1, \ldots, G_{N,d} \}$ are orthogonal states of the reference system.

Classically, there would be no point in randomizing optimal configurations, because mixtures cannot reduce the error probability. But in the quantum case, the coherent superposition of equivalent configurations brings the
The ultimate quantum limit. So far, we examined strategies where the unknown process is applied in parallel to a large entangled state. Could a general sequence of interventions achieve an even better rate?

Finding the optimal sequential strategy is generally a hard problem. To address this problem, we introduce the fidelity divergence of two quantum channels $C_1$ and $C_2$, defined as

$$\partial F(C_1, C_2) = \inf_{R} \inf_{\rho_1, \rho_2} \frac{F([C_1 \otimes I_R](\rho_1), [C_2 \otimes I_R](\rho_2))}{F(\rho_1, \rho_2)},$$

where $\rho_1$ and $\rho_2$ are joint states of the channel’s input and of the reference system $R$. It is understood that the infimum in the right hand side is taken over pairs of states $(\rho_1, \rho_2)$ for which the fidelity $F(\rho_1, \rho_2)$ is non-zero, so that the expression on the right hand side of Equation (10) is well-defined.

The fidelity divergence quantifies the ability of channels $C_1$ and $C_2$ to move two states apart from each other. In the Methods section, we show that the error probability in distinguishing between $C_1$ and $C_2$ with $N$ queries is lower bounded as

$$p_{\text{err}}^{\text{coh}}(C_1, C_2; N) \geq \frac{\partial F(C_1, C_2)^N}{4}.$$  

In particular, suppose that the two channels $C_1$ and $C_2$ have the form $C_1 = I \otimes I/d$ and $C_2 = I/d \otimes U$, where $U$ is a fixed unitary channel. In this case, we find that the fidelity divergence is $1/d^2$. Hence, the error probability satisfies the bound

$$p_{\text{err}}^{\text{coh}}(C_1, C_2; N) \geq \frac{1}{4d^2 N}.$$  

In the causal intermediary problem, the unitary gate $U$ is unknown, and therefore the error probability can only be larger than $p_{\text{err}}^{\text{coh}}(C_1, C_2; N)$. Hence, the identification of the causal intermediary cannot occur at a rate faster than $2 \log d$.

Equation (12) limits all sequential quantum strategies. But in fact quantum theory is also compatible with scenarios where physical processes take place in an indefinite order [23, 24]. Could the rate be increased if the experimenter had access to exotic phenomena involving indefinite order?

The answer is negative. In the Methods section we develop the concepts and methods needed to answer this question, and we show that the minimum error probability in distinguishing between the two channels $C_1 = I \otimes I/d$ and $C_2 = I/d \otimes I$ using arbitrary setups with indefinite order satisfies the bound

$$p_{\text{err}}^{\text{ind}}(C_1, C_2; N) \geq \frac{1 - \sqrt{1 - 1/d^2}}{2}.$$  

Clearly, this bound applies to the causal intermediary problem, which is harder than the discrimination of the two specific channels $C_1 = I \otimes I/d$ and $C_2 = I/d \otimes I$. Hence, the rate $R_Q = 2 \log d$ represents the ultimate quantum limit to the identification of a causal intermediary.

Extension to arbitrary numbers of hypotheses. The quantum advantage demonstrated in the previous sections can be extended to the identification of the causal intermediary among an arbitrary number $k$ of candidate variables. The best classical strategy still consists in initializing all variables to the same value. Erors arise when the values of two or more output variables are compatible with an invertible function. In the limit of many repetitions, the minimum error probability is $p_{\text{err}}^{\text{k coh}} = (k - 1)/(2d^{N-1}) + O(d^{-2N})$. (Appendix C). For quantum strategies, the best option among simple parallel strategies is still to divide the input particles into $N/d$ groups of $d$ particles and to initialize each group in the singlet state. In Appendix D, we show that this strategy reduces the error probability to $p_{\text{err}}^{\text{k coh}} = (k - 1)/(2d^N) + O(d^{-2N})$, for causal relations represented by arbitrary unitary gates.

An exponentially smaller error probability can be achieved using the input state (7). The evaluation of
the error probability is more complex than in the two-

hypothesis case, but the end result is the same: when the
causal dependency is probed \(N\) times, the quantum error
probability decays at the exponential rate \(R_Q = 2 \log d\),
twice the rate of the best classical strategy (see Appendix
E for the technical details).

Applications to other tests of causal hypotheses. The
strategies developed in the previous sections can be ap-
plied to the identification of causal relations in a variety of
scenarios. For example, they can be used to decide
whether there is a causal link between two variables \(A\) and \(B\). More specifically, they can be used to determine
whether variable \(B\) is a causal intermediary for variable
\(A\) or whether \(B\) fluctuates at random independently of
\(A\). Also in this case, the error probability of the best
classical strategy is \(1/(2d^{N-1})\), whereas preparing \(N/d\)
copies of the singlet yields error probability \(1/(2d^\frac{N}{d})\).

By superposing all possible partitions of the \(N\) inputs
into groups of \(d\), one can boost the discrimination rate
from \(\log d\) to \(2\log d\). One could speculate that, in the fu-
ture, such a fast identification could be useful as a quan-
tum version of the ping protocol, capable of establishing
whether there exists a quantum communication link be-
tween two nodes of a quantum internet [34].

Another application of our techniques is in the prob-
lem of identifying the cause of a given variable. Suppose
that one of \(k\) variables \(A_1, A_2, \ldots, A_k\) is the cause for a
given variable \(B\). An example of this situation arises in
genetics, when trying to identify the gene responsible for
a certain characteristic. Here, the interesting scenario is
when the number of candidate causes is large.

Classically, the problem is to find the variable \(A_x\) such
that \(B\) is a function of \(A_x\). For simplicity, we first as-
sume that all variables have the same \(d\)-dimensional al-
phabet, and that the function from \(A_x\) to \(B\) is the iden-
tity, namely \(b = a_x\). In this case, the cause can be iden-
tified without any error by probing the unknown process
for \(\lceil \log_d k \rceil\) times. The identification is done by a simple
search algorithm, where one divides the candidate vari-
bles in \(d\) groups and initializes the input variables in
the \(i\)-th group to the value \(i\). In this way, \(d - 1\) groups
can be ruled out, and one can iterate the search in the
remaining group. Using a decision tree argument [35], it
is not hard to see that \(\lceil \log_d k \rceil\) is the minimum number of
queries needed to identify the unknown process in the
worst case scenario.

In the quantum version of the problem, we find that
the number of queries can be cut down by approximately
half when the number of hypotheses is large. The trick
is to prepare \(k\) maximally entangled states, and to apply
the unknown process to the first system of each pair.
Repeating this procedure for \(N\) times and using results
on port-based teleportation [36] we find that the error
probability is \(p_{err} = (k - 1)/(d^{2N} + k - 1)\). Hence, \(N =
\lceil (1 + \epsilon)(\log_d k)/2 \rceil\) queries are sufficient to identify the
cause with vanishing error probability in the large \(k\) limit.

In Appendix F we consider the more complex scenario
where the functional dependence between the cause and
effect is unknown, and the only assumption is that the
effect is a causal intermediary of the cause. Despite the
lack of information about the functional dependence, we
show that the correct cause can be still identified with
high probability using \(N = \lceil (1 + \epsilon)(\log_d k)/2 \rceil\) calls to
the unknown process. The fast identification of the cause
is achieved by dividing the \(N\) copies of each input vari-
able \(A_i\) into groups of \(d\) copies, preparing each group in
the singlet state, and entangling the configuration of the
groupings with an external reference system. Once again,
the superposition of multiple equivalent setups leads to
a quantum speedup over the best classical strategy.

DISCUSSION

We showed that quantum mechanics enhances our abil-
ity to detect direct cause-effect links. This finding moti-
vates the exploration of more complex networks of causal
relations, including intermediate nodes and global causal
dependences between groups of variables [1–3]. The de-
velopment of new techniques for testing causal relations
could find applications to future quantum communica-
tion networks, providing a fast way to test the presence
of communication links. It could also assist the design of
intelligent quantum machines, in a similar way as classi-
cal causal discovery algorithms have been useful in clas-
sical artificial intelligence. In view of such applications,
it is important to go beyond the noiseless scenario con-
sidered in this paper, and to address scenarios where the
cause-effect relationships are obfuscated by noise. The
techniques developed in our work already provide some
insights in this direction. Quite Interestingly, one can
show that the quantum advantage persists in the pres-
ence of depolarizing noise, provided that the noise level
is not too high (see Appendix G). A complete study of
the noisy scenario, however, remains an open direction of
future research.

Another direction of future investigation is founda-
tional. Given the advantage of quantum theory over
classical theory, it is tempting to ask whether alterna-
tive physical theories could offer even larger advantages.
Interesting candidates are theories that admit more pow-
erful dense coding protocols than quantum theory [37],
as one might expect super-quantum advantages to arise
from the presence of stronger correlations with the refe-
rence system. In a similar vein, one could explore phys-
ical theories with higher dimensional state spaces, such
as Zyczkowski’s quartic theory [38], or quantum theory
on quaternionic Hilbert spaces [39]. Indeed, it is intrigu-
ing to observe that the classical rate \(R_C = \log d\) and the
quantum rate \(R_Q = 2 \log d\) are equal to the logarithms of
the dimensions of the classical and quantum state spaces,
respectively. In general, one may expect a relationship
between the dimension of the state space and the rate.
Should super-quantum advantages emerge, it would be
natural to ask which physical principle determines the
causal identification power of quantum mechanics. An
intriguing possibility is that one of the hidden physical principles of quantum theory could be a principle on the ability to distinguish alternative causal hypotheses.

METHODS

Properties of the fidelity divergence. Here we derive two properties of the fidelity divergence defined in Equation (10). First, the fidelity divergence provides a lower bound on the probability of misidentifying a channel with another:

**Proposition 1.** The probability of error in distinguishing between two quantum channels \( C_1 \) and \( C_2 \) with \( N \) queries is lower bounded as:

\[
p_{\text{err}}(C_1, C_2; N) \geq \frac{1}{4} \left( 1 - \frac{1}{2} \left\| \rho_1^{(N)} - \rho_2^{(N)} \right\|_1 \right)
\]

The bound can be obtained in the following way. Let \( \rho_x^{(N)} \) be the output state of a circuit as in Figure 1. Then, we have the bound:

\[
p_{\text{err}}(C_1, C_2; N) = \frac{1}{2} \left( 1 - \frac{1}{2} \left\| \rho_1^{(N)} - \rho_2^{(N)} \right\|_1 \right)
\]

The first line follows from Helstrom’s theorem [32], and the second line follows from the Fuchs-Van De Graaf Inequality [40]. The third line follows from the definition of the fidelity divergence (10), which implies that the fidelity between the states right after the \((t+1)\)-th use of the unknown channel \( C_x \), denoted by \( \rho_{x,t+1} \), satisfies the bound:

\[
F(\rho_{1,t+1}, \rho_{2,t+1}) \geq \frac{1}{2} \left( 1 - \frac{1}{2} \left\| \rho_1^{(N)} - \rho_2^{(N)} \right\|_1 \right)
\]

Another important property is that the fidelity divergence can be evaluated on pure states. The proof is simple: let \( \rho_1 \) and \( \rho_2 \) be two arbitrary states of the composite system \( AR \), where \( R \) is an arbitrary reference system. By Uhlmann’s theorem [41], there exists a third system \( E \) and two purifications \( |\Psi_1\rangle, |\Psi_2\rangle \in \mathcal{H}_A \otimes \mathcal{H}_R \otimes \mathcal{H}_E \), such that:

\[
F(|\Psi_1\rangle, |\Psi_2\rangle) = F(\rho_1, \rho_2).
\]

Fidelity divergence for the identification of the causal intermediary. Let us see how the fidelity divergence can be applied to our causal identification problem. The two channels are of the form:

\[
C_{1,U}(\rho) = U \rho U^\dagger \otimes I/\mathcal{d} \text{ and } C_{2,V} = I/\mathcal{d} \otimes V \rho V^\dagger,
\]

where \( U \) and \( V \) are two unknown unitary gates. Since we are interested in the worst case scenario, every choice of \( U \) and \( V \) will give an upper bound to the discrimination rate. In particular, we pick \( U = V \).

**Proposition 2.** The fidelity divergence for the two channels \( C_{1,U} \) and \( C_{2,V} \) is:

\[
\partial F(C_{1,U}, C_{2,V}) = 1/\mathcal{d}^2.
\]

By the unitary invariance of the fidelity, \( \partial F(C_{1,U}, C_{2,U}) \) is independent of \( U \). Without loss of generality, let us pick \( U = I \). For a generic reference system \( R \) and two generic pure states \( |\Psi_1\rangle, |\Psi_2\rangle \in \mathcal{H}_A \otimes \mathcal{H}_R \), the two output states are:

\[
\rho_1' = (C_{1,I} \otimes I_R)(|\Psi_1\rangle) = (\Psi_1)_{BR} \otimes I_C,
\]

\[
\rho_2' = (C_{2,I} \otimes I_R)(|\Psi_2\rangle) = I_R \otimes (\Psi_2)_{CR},
\]

up to reordering of the Hilbert spaces. The fidelity can be computed with the relation:

\[
F(\rho_1', \rho_2') = \frac{\text{Tr} \left( \sqrt{\rho_1' |\Psi_2\rangle \langle \Psi_2| |\Psi_1\rangle \rho_2'} \right)^2}{d^2},
\]

where we omitted the identity operators for the sake of brevity. Let us expand the input states as:

\[
|\psi_x\rangle = \sum_n \langle \phi_{xn} | \otimes |n\rangle, \quad x \in \{0,1\}
\]

where \( \{|n\rangle\} \) is an orthonormal basis for the reference system, and \( \{|\psi_{xn}\rangle\} \) is a set of unnormalized vectors. Inserting Equation (18) into Equation (17), we obtain the expression:

\[
F(\rho_1', \rho_2') = \frac{\text{Tr} \left( \sqrt{C^\dagger C} \right)^2}{d^2} = \frac{\text{Tr} |C|^2}{d^2},
\]

with \( C = \sum_n \langle \phi_1 | \langle \phi_2 | \). On the other hand, the fidelity between the input states is:

\[
F(\rho_1, \rho_2) = |\langle \Psi_1 | \Psi_2 \rangle|^2 = |\text{Tr} |C|^2|.
\]

Hence, the fidelity divergence satisfies the bound:

\[
\partial F(C_1, C_2) = \inf_{R} \inf_{\rho_1, \rho_2} \frac{F(\rho_1', \rho_2')}{F(\rho_1, \rho_2)} = \frac{1}{d^2} \inf_{C} \left| \frac{\text{Tr} |C|^2}{\text{Tr} |C|} \right| \geq \frac{1}{d^2},
\]
having used the inequality $|\text{Tr}[C]| \leq \text{Tr}[|C|]$, valid for every operator $C$. The inequality holds with the equality sign whenever $C$ is positive. This condition is satisfied, e.g. when the input states $|\Psi_1\rangle$ and $|\Psi_2\rangle$ are identical.

Quantum strategies with indefinite causal order. In principle, quantum mechanics is compatible with situations where multiple processes are combined in indefinite order [23, 24]. This suggests that an experimenter could devise new ways to probe quantum channels, allowing the relative order among different uses of the same channel to be indefinite. We call such strategies indefinite testers.

Consider the problem of identifying a channel $C_x$ from $N$ uses. The input resource is the channel $C_x^{\otimes N}$, representing $N$ identical black boxes that can be arranged in any desired order. Besides the product of $N$ independent channels, the most general class of channels with this property is the class of no-signalling channels with $N$ pairs of input/output systems.

Mathematically, an indefinite tester is a linear map from the set of no-signalling channels to the set of probability distributions over a given set of outcomes. Equivalently, the tester can be described by a set of operators $\{T_x\}$, where each operator $T_x$ acts on the Hilbert space $\bigotimes_i (\mathcal{H}^{in}_i \otimes \mathcal{H}^{out}_i)$, where $\mathcal{H}^{in}_i$ and $\mathcal{H}^{out}_i$ are the Hilbert spaces of the input and output system in the $i$-th pair, respectively. When the test is performed on a no-signalling channel $C$, the probability of the outcome $x$ is given by the generalized Born rule $p_x = \text{Tr}[T_x C]$, where $C$ is the Choi operator of the channel $C$ [43]. The normalization of the probabilities

$$\sum_x \text{Tr}[T_x C] = 1 \quad (22)$$

is required to hold for every no-signalling channel $C$.

Consider the problem of distinguishing between a set of no-signalling channels $\{C_x\}$ using an indefinite tester. For every probability distribution $\{p_x\}$, the worst-case probability of error satisfies the bound

$$p_{err}^{\text{ind}} \geq 1 - \sum_x p_x \text{Tr}[T_x C_x] \quad (23)$$

Now, suppose that there exists a constant $\lambda$ and a no-signalling channel $C$ such that

$$\lambda C \geq p_x C_x \quad (24)$$

for every $x$. Substituting Equation (24) into Equation (23) one obtains the bound

$$p_{err}^{\text{ind}} \geq 1 - \lambda \sum_x \text{Tr}[T_x C] = 1 - \lambda, \quad (25)$$

having used the normalization condition (22). The bound (25) can be seen as a generalization of the classical Yuen-Kennedy-Lax bound for quantum state discrimination [44].

We now apply the bound (25) to the task of distinguishing between the two channels $C_{1,t} = (U \otimes I/d)^{\otimes N}$ and $C_{2,t} = (I/d \otimes U)^{\otimes N}$. To this purpose, we consider the universal cloning channel [45]

$$C_\pm := \frac{2}{d^N+1} P_+ (\rho \otimes I^{\otimes N}) P_+, \quad (26)$$

and the universal NOT channel [46]

$$C_\pm := \frac{2}{d^N-1} P_- (\rho \otimes I^{\otimes N}) P_-, \quad (27)$$

with $P_\pm = (I \pm \text{SWAP})/2$, and SWAP being the unitary operator that swaps between the even and odd output spaces. It is easy to verify that both channels are no-signalling. Moreover, we find that the convex combination $C = p_+ C_+ + p_- C_-$ with

$$p_\pm = \sqrt{\frac{d^N+1}{2d^N}} / \left( \sqrt{\frac{d^N+1}{2d^N}} + \sqrt{\frac{d^N-1}{2d^N}} \right)$$

(see Appendix H for technical details). Hence, the bound (25) becomes

$$p_{err}^{\text{ind}} \geq 1 - \lambda = \frac{1 - \sqrt{1 - \frac{1}{d^N}}}{2} \geq \frac{1}{4d^2 N}. \quad (28)$$

The above bound implies that the discrimination rate of quantum strategies with indefinite order cannot exceed $2 \log d$.

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Appendix A: Complementarity relation between tests of the causal structure and tests of the functional dependency between cause and effect.

Here we provide the proof of the complementarity relation (7) in the main text.

1. Bound on the error probability for parallel strategies with no reference system

The two causal hypotheses are that the quantum channel from $A$ to the composite system $B \otimes C$ is either of the form $C_{1,U_1} = U_{1,B} \otimes I_C / d$, or of the form $C_{2,U_2} = I_B / d \otimes U_{2,C}$, with $U_1(\cdot) := U_1 \cdot U_1^\dagger$, $U_2(\cdot) := U_2 \cdot U_2^\dagger$. Here, $U_1$ and $U_2$ are unitary operations, unknown to the experimenter but fixed throughout the $N$ rounds of the experiment.

Here we consider parallel strategies, where the channel $C_{x,U_x}$ (with $x = 1$ or $x = 2$) is applied in parallel on a multipartite input state, as in the following diagram

\[
\begin{array}{c}
\begin{tikzpicture}
\node (A1) at (0,0) {$A_1$};
\node (A2) at (0,-1) {$A_2$};
\node (A3) at (0,-2) {$A_N$};
\node (B1) at (1,0) {$B_1$};
\node (B2) at (1,-1) {$B_2$};
\node (B3) at (1,-2) {$B_N$};
\node (C1) at (2,0) {$C_1$};
\node (C2) at (2,-1) {$C_2$};
\node (C3) at (2,-2) {$C_N$};
\node (R) at (0,-3) {$R$};
\node (rho) at (-1,-3) {$\rho$};
\node (C_xU_x) at (1,-3) {$C_{x,U_x}^\otimes N$};
\node (P_x) at (2,-3) {$P_x$};
\end{tikzpicture}
\end{array}
\]

where $R$ is a reference system of fixed dimension.

The probability to obtain the outcome $\bar{x}$ when the channel is $C_{x,U_x}$ is equal to

\[ p(\bar{x}|x) = \text{Tr} \left[ P_\bar{x} \left( C_{x,U_x}^\otimes N \otimes I_R \right) (\rho) \right]. \quad (A2) \]

For fixed gates $U_1$ and $U_2$, the probability of error is

\[ p_{\text{err}}(U_1,U_2) = \frac{1}{2} \text{Tr} \left[ P_1 \left( C_{2,U_2}^\otimes N \otimes I_R \right) (\rho) \right] + \frac{1}{2} \text{Tr} \left[ P_2 \left( C_{1,U_1}^\otimes N \otimes I_R \right) (\rho) \right]. \quad (A3) \]
Since \( U_1 \) and \( U_2 \) are unknown, we consider the worst-case error probability, namely

\[
p_{\text{err}}^{\text{wc}} := \max_{U_1, U_2 \in \mathcal{U}} p_{\text{err}}(U_1, U_2),
\]

where \( \mathcal{U} \) is a set of unitary operators. For example, \( \mathcal{U} \) can be

1. the group of permutation operators of the form \( U_\pi = \sum_{d_i=1}^d |\pi(i)\rangle \langle i| \), where \( \pi \) is an element of the permutation group \( S_d \)
2. the group of all unitary operators in dimension \( d \).

In general, we assume that the set \( \mathcal{U} \) is a generalised \( N \)-design [47], meaning that (i) \( \mathcal{U} \) is a subset of a group representation \( \{U_g\}_{g \in \mathcal{G}} \) for some group \( \mathcal{G} \), and (ii) for every operator \( A \), one has the identity

\[
\frac{1}{|\mathcal{U}|} \sum_{U \in \mathcal{U}} U \otimes^N A U \otimes^N = \int_{\mathcal{G}} dg U_g \otimes^N A U_g^\dagger, \tag{A5}
\]

where \( dg \) denotes the normalized invariant measure over \( \mathcal{G} \) (for finite groups, it is understood that the integral \( \int_{\mathcal{G}} dg \) has to be replaced by the sum \( \frac{1}{|\mathcal{G}|} \sum_g \)).

The worst-case error probability is lower bounded by the average error probability

\[
p_{\text{err}}^{\text{ave}} := \frac{1}{|\mathcal{U}|^2} \sum_{U_1, U_2} p_{\text{err}}(U_1, U_2). \tag{A6}
\]

By definition, the average error probability is equal to the error probability in distinguishing between the average channels

\[
C^{(N)}_1 := \frac{1}{|\mathcal{U}|} \sum_{U_1} C_{1,U_1}^{\otimes N} \quad \text{and} \quad C^{(N)}_2 := \frac{1}{|\mathcal{U}|} \sum_{U_2} C_{2,U_2}^{\otimes N}. \tag{A7}
\]

Now, suppose that the experimenter prepares an \( N \)-particle state \( |\Psi\rangle \in \mathcal{H} \otimes^N \), without using a reference system. The average error probability has the tight lower bound

\[
p_{\text{err}}^{\text{ave}} \geq \frac{1 - \frac{1}{2} \left\| C^{(N)}_1(|\Psi\rangle) - C^{(N)}_2(|\Psi\rangle) \right\|_1}{2} \tag{A8}
\]

achieved by Helstrom’s minimum error measurement [32]. The distance between the average output states can be expressed as

\[
\left\| C^{(N)}_1(|\Psi\rangle) - C^{(N)}_2(|\Psi\rangle) \right\|_1 = \left\| \langle \Psi \rangle \otimes \left( \frac{I}{d} \right)^{\otimes N} - \left( \frac{I}{d} \right)^{\otimes N} \otimes \langle \Psi \rangle \right\|_1
\]

\[
= \frac{1}{dN} \sum_{i,j=0}^{dN-1} |p_i - p_j|
\]

\[
= \frac{1}{dN} \sum_{k=1}^{dN-1} \left\| \langle \Psi \rangle - S^k \langle \Psi \rangle S^k \right\|_1
\]

\[
= \left( 1 - \frac{1}{dN} \right) \left\| \langle \Psi \rangle \otimes \omega - \Sigma \right\|_1, \tag{A9}
\]

with

\[
\omega := \frac{\sum_{k=1}^{dN-1} |k\rangle \langle k|}{dN - 1} \quad \text{and} \quad \Sigma := \frac{1}{dN - 1} \sum_{k=1}^{dN-1} S^k \langle \Psi \rangle S^k \otimes |k\rangle \langle k|. \tag{A10}
\]
Now, the pure states
\[
|\Gamma\rangle := \sum_{i=0}^{dN-1} \sum_{k=1}^{dN-1} \sqrt{\frac{p_i}{dN-1}} |i\rangle \otimes |i\rangle \otimes |k\rangle \otimes |k\rangle
\]
\[
|\Delta\rangle := \sum_{j=0}^{dN-1} \sum_{l=1}^{dN-1} \sqrt{\frac{p_j}{dN-1}} S^k |j\rangle \otimes S^k |j\rangle \otimes |l\rangle \otimes |l\rangle
\]
(A11)
are purifications of $\langle \Psi \rangle \otimes \omega$ and $\Sigma$, respectively. Hence, the monotonicity of the trace distance yields the bound
\[
\| C_1^{(N)}(\Psi) - C_2^{(N)}(\Psi) \|_1 \leq \left( 1 - \frac{1}{dN} \right) \| \Gamma - \Delta \|_1
\]
\[
= \left( 1 - \frac{1}{dN} \right) 2 \sqrt{1 - |\langle \Gamma | \Delta \rangle|^2}
\]
\[
\leq \left( 1 - \frac{1}{dN} \right) 2 \left( 1 - \frac{|\langle \Gamma | \Delta \rangle|^2}{2} \right).
\]
(A12)
Inserting this bound into Equation (A8), we then obtain
\[
p_{\text{ave}}^\text{err} \geq \frac{1}{2dN} \left[ 1 + (dN - 1) \frac{|\langle \Gamma | \Delta \rangle|^2}{2} \right]
\]
(A13)
Now, note that we have
\[
\langle \Gamma | \Delta \rangle = \frac{1}{dN-1} \sum_{i,j=0}^{dN-1} \sqrt{p_i p_j} \langle i | \left( \sum_{k=1}^{dN-1} S^k |j\rangle \langle k| \right) |i\rangle
\]
\[
= \frac{1}{dN-1} \sum_{i,j=0}^{dN-1} \sqrt{p_i p_j} \langle i | (I - |j\rangle \langle j|) |i\rangle
\]
\[
= \frac{1}{dN-1} \sum_{i,j=0}^{dN-1} \sqrt{p_i p_j} (1 - \delta_{ij})
\]
\[
= \frac{\Tr \left[ \sqrt{\langle \Psi \rangle} \right]^2 - 1}{dN-1}
\]
(A14)
Hence, the Equation (A13) yields the bound
\[
p_{\text{wc}}^\text{err} \geq p_{\text{ave}}^\text{err} \geq \frac{1}{2dN} \left\{ 1 + \frac{\left( \Tr \left[ \sqrt{\langle \Psi \rangle} \right]^2 - 1 \right)^2}{2(dN - 1)} \right\}.
\]
(A15)
It is clear that the minimum of the right-hand-side is obtained when the state $\langle \Psi \rangle$ is pure, in which case, the bound becomes $p_{\text{wc}}^\text{err} \geq 1/(2dN)$.

2. Bound on the success probability in the identification of a unitary gate

More generally, the bound (A15) can be interpreted as a complementarity relation between the estimation of the causal structure and the estimation of the functional dependence between cause and effect.

Lemma 1. Consider the task of guessing the gate $U \in U$ from the state $|\Psi_U\rangle := U^{\otimes N} |\Psi\rangle$. If $U$ is a generalised $N$-design for some group representation $\{U\}_{U \in G}$, then the probability of a correct guess satisfies the bound
\[
p_U^{\text{guess}} \leq \frac{\Tr \left[ \sqrt{\langle \Psi \rangle} \right]^2}{|U|}.
\]
(A16)
The bound is attained by the square-root measurement [48], with operators $P_U = (\Psi)^{-\frac{1}{2}} \Psi_U (\Psi)^{-\frac{1}{2}} / |U|$. 


Proof. Equation (A16) follows from the Yuen-Kennedy-Lax bound \[ p_{guess}^U \leq \text{Tr} [\Lambda] \] where \( \Lambda \) is a positive operator satisfying the inequalities \( \Lambda \geq \frac{1}{|U|} U^\otimes N \Psi U^\otimes N \) for all \( U \in U \). Equivalently, one has \( U^\otimes N \Lambda U^\otimes N \leq \Psi / |U| \) for all \( U \), which implies the condition

\[
\langle \Lambda \rangle \geq \frac{\Psi}{|U|}, \quad \langle \Lambda \rangle := \frac{1}{|U|} \sum U^\otimes N \Lambda U^\otimes N. \tag{A17}
\]

Then, the Yuen-Kennedy-Lax bound implies the inequality

\[
p_{guess}^U \leq \text{Tr} [\langle \Lambda \rangle]. \tag{A18}
\]

Since the unitaries \( U \) form a generalised \( N \)-design, the operator \( \langle \Lambda \rangle \) is invariant under the action of the group representation \( \{ U^\otimes N \}_{U \in G} \). Moreover, every invariant operator \( \Gamma \) can be written as \( \langle \Lambda \rangle \) for some suitable \( \Lambda \) (in fact, it suffices to take \( \Lambda = \Gamma \)). Hence, one has the bound

\[
p_{guess}^U \leq \text{Tr} [\Gamma], \quad \forall \Gamma : \langle \Gamma \rangle = \Gamma, \quad \Gamma \geq \frac{\Psi}{|U|}. \tag{A19}
\]

In particular, one can take \( \Gamma = c \sqrt{\langle \Psi \rangle} \) for some suitable constant \( c \). With this choice, the condition \( \Gamma \geq \Psi / |U| \) is equivalent to

\[
c I \geq \frac{\langle \Psi \rangle^{-\frac{1}{2}} \Psi \langle \Psi \rangle^{-\frac{1}{2}}}{|U|}, \tag{A20}
\]

which in turn is equivalent to

\[
c \geq \frac{\text{Tr} [\Psi \langle \Psi \rangle^{-\frac{1}{2}}]}{|U|} = \frac{\text{Tr} [\langle \Psi \rangle \langle \Psi \rangle^{-\frac{1}{2}}]}{|U|} = \frac{\text{Tr} [\langle \Psi \rangle^{\frac{1}{2}}]}{|U|}. \tag{A21}
\]

Then, the bound (A19) becomes \( p_{guess}^U \leq \text{Tr} [\sqrt{\langle \Psi \rangle}]^2 / |U| \). The bound is attained by the square-root measurement \( P_U = \langle \Psi \rangle^{-\frac{1}{2}} \Psi U \langle \Psi \rangle^{-\frac{1}{2}} / |U| \), which yields

\[
\text{Tr} [P_U \Psi_U] = \frac{1}{|U|} \text{Tr} [\langle \Psi \rangle^{-\frac{1}{2}} \Psi U \langle \Psi \rangle^{-\frac{1}{2}} \Psi_U]
\]

\[
= \frac{1}{|U|} \text{Tr} [\langle \Psi \rangle^{-\frac{1}{2}} \Psi \langle \Psi \rangle^{-\frac{1}{2}} \Psi]
\]

\[
= \frac{1}{|U|} \left| \langle \Psi \rangle^{-\frac{1}{2}} \langle \Psi \rangle^{-\frac{1}{2}} \right|^2
\]

\[
= \frac{1}{|U|} \left| \text{Tr} [\Psi \langle \Psi \rangle^{-\frac{1}{2}}] \right|^2
\]

\[
= \frac{1}{|U|} \left| \text{Tr} [\langle \Psi \rangle^{\frac{1}{2}}] \right|^2
\]

\[
= \frac{1}{|U|} \left| \text{Tr} [\langle \Psi \rangle^{\frac{1}{2}}] \right|^2, \tag{A22}
\]

for every \( U \).

Combining the above lemma with Equation (A15) we obtain the relation

\[
p_{wc \rightarrow err} \geq \frac{1}{2d^N} \left( 1 + \frac{1}{2(d^N - 1)} \left( \frac{p_{guess}^U - 1}{|U|} \right)^2 \right). \tag{A23}
\]

Appendix B: Optimal universal strategy

Here we derive the optimal strategy for identifying the causal intermediary when the cause-effect relationship is described by an arbitrary unitary gate.
1. Reduction to the minimisation of the average probability

The problem is to find the strategy that minimises the worst-case error probability. Thanks to the symmetry of the problem, the minimisation of the worst-case error probability can be reduced to the minimisation of the average error probability:

**Lemma 2.** For every fixed reference system $R$ and for every fixed $N$, minimum worst-case error probability in the discrimination of the channels $C_{1,U_1}$ and $C_{2,U_2}$ with $N$ uses is equal to the average error probability

\[
p_{\text{err}}^{\text{ave}} := \int_{U_1 \in SU(d)} dU_1 \int_{U_2 \in SU(d)} dU_2 p_{\text{err}}(U_1, U_2),
\]

where $dU$ is the normalised invariant measure. In turn, the average error probability is equal to the minimum error probability in the discrimination of the channels

\[
C^{(N)}_1 := \int dU_1 C^{\otimes N}_{1,U_1} \quad \text{and} \quad C^{(N)}_2 := \int dU_2 C^{\otimes N}_{2,U_2}.
\]

There exists a state $\rho$ and a measurement $\{P_1, P_2\}$ that are optimal for both problems.

We omit the proof, which is a simple adaptation of Holevo's argument on the optimality of covariant measurements [49], see also [50].

2. Optimal form of the input states

Let us search for the optimal quantum strategy. Note that the channels $C^{(N)}_1$ and $C^{(N)}_2$ satisfy the condition

\[
C^{(N)}_x = C^{(N)}_x \circ T^{(N)}_{\text{in}}, \quad \forall x \in \{1, 2\}.
\]

where $T^{(N)}_{\text{in}}$ is the twirling channel

\[
T^{(N)}_{\text{in}} := \int dW W^{\otimes N}.
\]

Eq. (B3) implies that the search of the optimal input state can be restricted to invariant states—i.e. states satisfying the condition

\[
T^{(N)}_{\text{in}}(\rho) = \rho.
\]

The structure of the invariant states can be made explicit using the Schur-Weyl duality [51], whereby the tensor product Hilbert space $\mathcal{H}^{\otimes N}$ is decomposed as

\[
\mathcal{H}^{\otimes N} = \bigoplus_{\lambda \in Y_{N,d}} (\mathcal{R}_\lambda \otimes \mathcal{M}_\lambda),
\]

where $Y_{N,d}$ is the set of Young diagrams of $N$ boxes arranged in $d$ rows, while $\mathcal{R}_\lambda$ and $\mathcal{M}_\lambda$ are representation and multiplicity spaces for the tensor action of $SU(d)$, respectively. Using the Schur-Weyl decomposition, every invariant state on $\mathcal{H}^{\otimes N} \otimes \mathcal{H}_R$ can be decomposed as

\[
\rho = \bigoplus_{\lambda} q_{\lambda} \left( \frac{P_\lambda}{d_\lambda} \otimes \rho_{\lambda R} \right),
\]

where $\{q_{\lambda}\}$ is a probability distribution, $P_\lambda$ is the identity operator on the representation space $\mathcal{R}_\lambda$, and $\rho_{\lambda R}$ is a density matrix on the Hilbert space $\mathcal{M}_\lambda \otimes \mathcal{H}_R$.

Note that the set of invariant states (B7) is convex. Since the (average) error probability is a linear function of $\rho$, the minimisation can be restricted to the extreme points of this convex set. Hence, we have the following

**Proposition 3.** Without loss of generality, the optimal input state for a parallel strategy with reference system $R$ can be taken of the form

\[
\rho = \frac{P_{\lambda_0}}{d_{\lambda_0}} \otimes \Psi_{\lambda_0 R},
\]

where $\lambda_0 \in Y_{N,d}$ is a fixed Young diagram and $\Psi_{\lambda_0 R}$ is a pure state on $\mathcal{M}_{\lambda_0} \otimes \mathcal{H}_R$. 
3. Error probability for states of the optimal form

The problem is to find the input state that makes the output states most distinguishable. To this purpose, it is convenient to label operators with the corresponding systems and to use the notation $A := A_1 A_2 \cdots A_N$, $B := B_1 B_2 \cdots B_N$, $C := C_1 C_2 \cdots C_N$, and $R := R$.

When applied to an invariant state of the composite system $A R$, the two channels $C_1^{(N)}$ and $C_2^{(N)}$ produce the output states

$$
(C_1^{(N)} \otimes I_R)(\rho_{AR}) = \rho_{BR} \otimes \left( I_\frac{N}{C} \right) \otimes N \quad \text{and} \quad (C_2^{(N)} \otimes I_R)(\rho_{AR}) = \left( I_\frac{N}{B} \right) \otimes \rho_{CR},
$$

up to a convenient reordering of the Hilbert spaces.

The minimum error probability in the discrimination of the output states is given by Helstrom’s theorem [32]. Specifically, one has

$$
p_{\text{err}} = \frac{1}{2} \left( 1 - \frac{1}{2} \| \Delta \|_1 \right), \quad \Delta := \rho_{BR} \otimes \left( I_\frac{N}{C} \right) \otimes N - \left( I_\frac{N}{B} \right) \otimes \rho_{CR}.
$$

In the following, we compute the trace norm explicitly for input states of the optimal form

$$
\rho = \frac{P_{\lambda_0}}{d_{\lambda_0}} \otimes \Psi_{\lambda_0 R},
$$

It is convenient to decompose the identity operator $I^{\otimes N}$ as

$$
I^{\otimes N} = \bigoplus_{\lambda \in \mathcal{N}, d} \left( P_\lambda \otimes Q_\lambda \right),
$$

where $P_\lambda$ is the identity operator on the representation space $R_\lambda$ and $Q_\lambda$ is the identity operator on the multiplicity space $\mathcal{M}_\lambda$. In the following, we denote by $m_\lambda = Tr(Q_\lambda)$ the dimension of $\mathcal{M}_\lambda$. Combining Eqs. (B9), (B11), and (B12), we obtain

$$
\| \Delta \|_1 = \frac{d_{\lambda_0} m_{\lambda_0}}{d^N} \left\| \frac{P_{\lambda_0}}{d_{\lambda_0}} \otimes \frac{P_{\lambda_0}}{d_{\lambda_0}} \left( \Psi_{\lambda_0 R} \otimes \frac{Q_{\lambda_0}}{m_{\lambda_0}} - \frac{Q_{\lambda_0}}{m_{\lambda_0}} \otimes \Psi_{\lambda_0 R} \right) \right\|_1 + 2 \sum_{\lambda \neq \lambda_0} \frac{d_{\lambda} m_{\lambda}}{d^N} \left\| \frac{P_{\lambda}}{d_{\lambda}} \otimes \frac{P_{\lambda}}{d_{\lambda}} \left( Q_{\lambda} \otimes \frac{Q_{\lambda}}{m_{\lambda}} \right) \right\|_1
\]
\[
= \frac{d_{\lambda_0} m_{\lambda_0}}{d^N} \left\| \Psi_{\lambda_0 R} \otimes \frac{Q_{\lambda_0}}{m_{\lambda_0}} - \frac{Q_{\lambda_0}}{m_{\lambda_0}} \otimes \Psi_{\lambda_0 R} \right\|_1 + 2 \left( 1 - \frac{d_{\lambda_0} m_{\lambda_0}}{d^N} \right)
\]

It remains to compute the trace norm in the first summand. To this purpose, it is convenient to define the states

$$
| \Phi_{m}^{\pm} := \frac{\Psi_{\lambda_0 R} \otimes |n\rangle \pm |n\rangle \otimes \Psi_{\lambda_0 R}}{\gamma_n^{\pm}}, \quad \gamma_n^{\pm} := \sqrt{2(1 \pm \langle n | \rho | n \rangle}},
$$

where $\rho$ is the marginal state of $\Psi_{\lambda_0 R}$ on the multiplicity space $\mathcal{M}_{\lambda_0}$, and $\{|n\rangle, n = 1, \ldots, m_{\lambda_0}\}$ are the eigenvectors of $\rho$. With this definition, the states

$$
\{| \Phi_{m}^{k} \rangle, k \in \{+,-\}, n \in \{1, \ldots, m_{\lambda_0}\}\}
$$

are mutually orthogonal. For example, one has

$$
\langle \Phi_{m}^{+} | \Phi_{m}^{+} \rangle = \text{Re}[\langle m | \rho | n \rangle] \gamma_{m,n}^{+} \gamma_{m,n}^{-} = 0,
$$

the second equality coming from the fact that $\rho$ is diagonal in the basis $\{|n\rangle\}$.

In terms of the vectors (B14), one can rewrite the relevant terms as

$$
\Psi_{\lambda_0 R} \otimes \frac{Q_{\lambda_0}}{m_{\lambda_0}} - \frac{Q_{\lambda_0}}{m_{\lambda_0}} \otimes \Psi_{\lambda_0 R} = \frac{1}{2 m_{\lambda_0}} \sum_{n} \gamma_{n}^{+} \gamma_{n}^{-} \left( |\Phi_{m}^{+} \rangle \langle \Phi_{n}^{+}| + |\Phi_{n}^{-} \rangle \langle \Phi_{m}^{-}| \right).
$$
Then, the trace norm is
\[
\left\| \psi_{\lambda \partial} R \otimes \frac{Q_{\lambda \partial}}{m_{\lambda \partial}} - \frac{Q_{\lambda \partial}}{m_{\lambda \partial}} \psi_{\lambda \partial} R \right\|_1 = \frac{1}{2m_{\lambda \partial}} \sum_{n} \gamma_{\lambda \partial}^{\langle \partial \partial \rangle} \left\| \phi_{\lambda \partial}^{\langle \partial \partial \rangle} \right\|_1
\]
\[
= \frac{2}{m_{\lambda \partial}} \sum_{n} \sqrt{1 - \langle n|\rho|n\rangle^2}.
\]
(B18)
The maximum trace norm is reached when the eigenvalues of \( \rho \) are all equal. In that case, one has
\[
\left\| \psi_{\lambda \partial} R \otimes \frac{Q_{\lambda \partial}}{m_{\lambda \partial}} - \frac{Q_{\lambda \partial}}{m_{\lambda \partial}} \psi_{\lambda \partial} R \right\|_1 = \frac{2}{m_{\lambda \partial}} \left( m_{\lambda \partial} - r + r \sqrt{1 - r^{-2}} \right),
\]
(B19)
where \( r \) is the rank of \( \rho \). Combining the above equation with Eqs. (B13) and (B10) we obtain the error probability
\[
pe_{\text{err}} = \frac{d_{\lambda \partial}}{2d_{\partial}} f(r)
\]
\[
f(r) := r \left( 1 - \sqrt{1 - r^{-2}} \right).
\]
(B20)
Note that the function \( f(r) \) is monotonically decreasing, and therefore the error probability is minimised by maximising the rank \( r \), i.e. by choosing
\[
r = \min\{m_{\lambda \partial}, d_R\},
\]
(B21)
where \( d_R \) is the dimension of the reference system.

### 4. Minimum error probability

The probability of error is given by Eq. (B20). When the reference system has dimension larger than the multiplicity \( m_{\lambda \partial} \), one has the equality
\[
r = m_{\lambda \partial}
\]
(B22)
and the error probability becomes
\[
pe_{\text{err}} = \frac{d_{\lambda \partial}}{2d_{\partial}} f(m_{\lambda \partial}),
\]
(B23)
with \( f \) defined as in Equation (B20).

The only way to beat the classical scaling \( 1/d^N \) is to make \( f(m_{\lambda \partial}) \) exponentially small. Since \( f \) is positive and monotonically decreasing, this means that \( m_{\lambda \partial} \) must be exponentially large. Note that, for large \( m_{\lambda \partial} \), the probability of error has the asymptotic expression
\[
pe_{\text{err}} = \frac{d_{\lambda \partial}}{4m_{\lambda \partial}d^N} \left[ 1 + O \left( m_{\lambda \partial}^{-2} \right) \right].
\]
(B24)
Asymptotically, the problem is reduced to the minimisation of the ratio \( d_{\lambda \partial}/m_{\lambda \partial} \).

To find the minimum, it is useful to apply the notion of majorisation Young diagrams. Given two diagrams \( \lambda \) and \( \mu \) of \( N \) boxes arranged in \( d \) rows, we say that \( \lambda \) majorises \( \mu \) if
\[
\sum_{i=1}^{s} \lambda_i \geq \sum_{i=1}^{s} \mu_i \quad \forall s \in \{1, \ldots, d\},
\]
(B25)
where \( \lambda_i (\mu_i) \) is the length of the \( i \)-th row of the diagram \( \lambda (\mu) \).

**Lemma 3.** If \( \lambda \) majorises \( \mu \), then \( d_\lambda/m_\lambda \geq d_\mu/m_\mu \).

**Proof.** For a generic Young diagram \( \lambda \in Y_{N+1,d} \), one has
\[
d_\lambda = \frac{\prod_{(i,j) \in \lambda} d - i + j}{\prod_{(i,j) \in \lambda} \text{hook}(i,j)} \quad \text{and} \quad m_\lambda = \frac{N!}{\prod_{(i,j) \in \lambda} \text{hook}(i,j)},
\]
(B26)
Choosing \( s = d \) and recalling Eq. (B27), one finally obtains \( d_\lambda/m_\lambda \geq d_\mu/m_\mu \).

**Proposition 4.** Define \( t := N - d[N/d] \). Then, the ratio \( d_\lambda/m_\lambda \) is

1. minimum when \( \lambda \) is the Young diagram with \( t \) rows of length \([N/d] \) and \( d - t \) rows of length \([N/d] \)
2. maximum when \( \lambda \) is the Young diagram with one row or length \( N \).

**Proof.** The Young diagram \( \lambda_0 = ([N/d], \ldots, [N/d], [N/d], \ldots, [N/d]) \) is majorised by any other Young diagram in \( \mathcal{Y}_{N,d} \). Hence, \( \lambda_0 \) minimises the ratio \( d_\lambda/m_\lambda \) (by Lemma 3). Similarly, the Young diagram \( \lambda_0 = (N, 0, \ldots, 0) \) majorises every other young diagram and therefore it maximises the ratio \( d_\lambda/m_\lambda \).

Summarising, we showed that

1. when \( N \) is a multiple of \( d \), the optimal Young diagram corresponds to the trivial representation of \( SU(d) \)
2. when \( N \) is not a multiple of \( d \), the optimal Young diagram corresponds to the totally antisymmetric representation acting on \( N - d[N/d] \) particles.
3. asymptotically, the symmetric subspace is the worst possible choice, leading to the classical rate \( R_C = \log d \).

In conclusion, we proved the following

**Proposition 5.** When \( N \) is a multiple of \( d \), the optimal input state is \( P_{\lambda_0}/d_{\lambda_0} \otimes |\Psi\rangle\langle\Psi|_{\lambda_0 R} \), where \( \lambda_0 \) is the trivial representation of \( SU(d) \) in the \( N \)-fold tensor product \( U^\otimes N \), \( d_R \geq m_{\lambda_0} \), and \( |\Psi\rangle_{\lambda_0 R} \in \mathcal{M}_{\lambda_0} \otimes \mathcal{H}_R \) is a maximally entangled state.

Since the trivial representation is one-dimensional, the error probability (B24) takes the form

\[
p_{\text{err}} = \frac{1}{4m_{\lambda_0} d^N} \left[ 1 + O\left( m_{\lambda_0}^{-2}\right) \right]. \tag{B29}
\]

Moreover, the trivial representation of \( SU(d) \) corresponds to the Young diagram with \( d \) rows, each of length \( N/d \). Hence, its multiplicity is given by

\[
m_{\lambda_0} = \frac{N!}{\prod_{i=1}^{d} \frac{(d - i)!}{(d - i)!}} \cdot \tag{B30}
\]
For fixed \( d \), the Stirling approximation yields the expression
\[
m_{\lambda_0} = d^N \left[ \frac{d^2 e^{d(d-1)} \prod_{i=1}^d(d-i)!}{(2\pi)^{d+1} N^{d^2-1}} \right] c(N),
\]
where \( c(N) \) is a function tending to 1 in the large \( N \) limit. Taking the logarithm on both sides, one obtains
\[
\log m_{\lambda_0} = N \log d + O(\log N).
\]
Inserting this value into the expression of the error probability (B24), we obtain the rate
\[
R = \lim_{N \to \infty} \frac{-\log \text{err}}{N} = \lim_{N \to \infty} \frac{\log(4m_{\lambda_0} d^N)}{N} = 2 \log d.
\]

5. Quantum superposition of equivalent setups

Here we prove that the optimal state can be realized as a coherent superposition of equivalent setups, where the \( N \) input variables are divided in groups of \( d \), and all the variables in the same group are initialized in the \( \text{SU}(d) \) singlet state.

**Proposition 6.** For \( N \) multiple of \( d \), consider the state
\[
|\Psi\rangle_{\text{AR}} = \frac{1}{\sqrt{G_{N,d}}} \sum_i \left( |S_i\rangle_A^{\otimes N/d} \right)_i \otimes |i\rangle_R,
\]
where \( \{|i\rangle_R\}_{i=1}^{G_{N,d}} \) is an orthonormal basis for the reference system, indexed by the possible ways to group \( N \) objects into groups of \( d \), and \( (|S_i\rangle^{\otimes N/d})_i \) is the product of \( N/d \) singlet states, distributed according to the grouping \( i \). Then,

1. the state \( |\Psi\rangle_{\text{AR}} \) is optimal for the identification of the causal intermediary
2. the number \( r \) of linearly independent vectors of the form \( (|S_i\rangle^{\otimes N/d})_i \) satisfies the equality
\[
r = d^N \left[ \frac{d^2 e^{d(d-1)} \prod_{i=1}^d(d-i)!}{(2\pi)^{d+1} N^{d^2-1}} \right] c(N),
\]
where \( c(N) \) is a function tending to 1 in the large \( N \) limit.

**Proof.** By definition, \( |\Psi\rangle_{\text{AR}} \) is invariant under the \( n \)-fold action of \( \text{SU}(d) \) on system \( A \), meaning that the corresponding density matrix has the optimal form \( |\Psi\rangle\langle\Psi|_{\text{AR}} = P_{\lambda_0/d\lambda_0} \otimes |\Psi\rangle\langle\Psi|_{\lambda_0 R} \), where \( \lambda_0 \) is the trivial representation of \( \text{SU}(d) \).

Now, the marginal state
\[
\rho_A := \text{Tr}_R [|\Psi\rangle\langle\Psi|_{\text{AR}}] = \frac{1}{G_{N,d}} \sum_i \left( |S_i\rangle\langle S_i|^{\otimes N/d} \right)_i
\]

is invariant under permutations. Hence, the Schur lemma implies the relation
\[
\rho_A = \frac{Q_{\lambda_0}}{m_{\lambda_0}}.
\]
Since \( |\Psi\rangle_{\text{AR}} \) is a purification of \( \rho_A \), we conclude that \( |\Psi\rangle_{\text{AR}} \) is a maximally entangled state between \( R \) and the multiplicity system \( M_{\lambda_0} \). Hence, \( |\Psi\rangle_{\text{AR}} \) coincides with the optimal input state of Proposition 5.

Moreover, comparing Equations (B36) and (B37) we obtain that the rank of \( \rho_A \) is equal to the multiplicity \( m_{\lambda_0} \). Since the rank of \( \rho_A \) is the number of linearly independent vectors of the form \( (|S_i\rangle^{\otimes N/d})_i \), we conclude that the number of such vectors is \( m_{\lambda_0} \). Finally, \( m_{\lambda_0} \) can be expressed as in Equation (B31). \( \Box \)
Appendix C: Optimal classical strategy for \( k \) causal hypotheses

Here we provide the optimal classical strategy for the case where exactly one out of \( k \) possible variables \( B_1, B_2, \ldots, B_k \) is the causal intermediary of \( A \). The result is stated in the following

Lemma 4. The minimum error probability in the identification of the causal intermediary among \( k \geq 2 \) alternatives is

\[
P_{\text{err}}^C = \frac{k-1}{2d^{N-1}} + O\left(\frac{1}{d^2N}\right).
\]

Proof. Suppose that the \( i \)-th output variable is not the causal intermediary. The probability that it takes values compatible with a permutation is

\[
P(d,v) = \frac{d!}{(d-v)!} \text{ for } v \text{ distinct values of } A \text{ probed in the experiment}
\]

and \( P(d,v) = d!/(d-v)! \) is the number of injective functions from a \( v \)-element set to a \( d \)-element set.

Hence, the probability that the \( i \)-th variable—and only the \( i \)-th variable—is confusable with the true causal intermediary is

\[
p_i = \frac{1}{d^N} \left[1 - \frac{P(d,v)}{d^N}\right]^{k-2}.
\]

Similarly, the probability that that variables \( i_1, i_2, \ldots, i_t \) (and only variables \( i_1, i_2, \ldots, i_t \)) are confusable with the true causal intermediary is

\[
p_{i_1i_2\ldots i_t} = \left[\frac{P(d,v)}{d^N}\right]^t \left[1 - \frac{P(d,v)}{d^N}\right]^{k-t-1}.
\]

When this situation arises, one has to resort to a random guess, with probability of error \( t/(t+1) \). In total, the probability of error is equal to

\[
P_{\text{err}}^C = \sum_{t=1}^{k-1} \frac{t}{t+1} \left[\frac{P(d,v)}{d^N}\right]^t \left[1 - \frac{P(d,v)}{d^N}\right]^{k-t-1}
\]

\[
= \frac{(k-1)P(d,v)}{2d^N} + O\left(\frac{1}{d^2N}\right).
\]

Since the coefficient \( P(d,v) \) is minimum when \( v = 1 \), the optimal strategy is to initialize all input variables in the same value, thus obtaining probability of error \( P_{\text{err}}^C = \frac{k-1}{2d^{N-1}} + O\left(\frac{1}{d^2N}\right) \).

Appendix D: Optimal quantum strategy for \( k \) hypotheses without reference system

Here we provide the best strategy among all quantum strategies that do not use a reference system.

Lemma 5. The best quantum strategy without reference system is to divide the \( N \) input variables into \( N/d \) groups of \( d \) elements each and, within each group, to prepare the singlet state

\[
|S_d\rangle = \frac{1}{\sqrt{d!}} \sum_{k_1, k_2, \ldots, k_d} \epsilon_{k_1k_2\ldots k_d} |k_1\rangle|k_2\rangle\cdots|k_d\rangle
\]

where \( \epsilon_{k_1k_2\ldots k_d} \) is the totally antisymmetric tensor and the sum ranges over all vectors in the computational basis. The corresponding error probability is

\[
P_{\text{err}}^{QC} = \frac{k-1}{2d^{N-1}} + O\left(\frac{1}{d^2N}\right).
\]

Proof. Let us denote by \( x \) the “true causal intermediary”, namely the quantum system \( B_x \) whose state depends on the state of \( A \), and by \( C_{x,U} \) the channel defined by the relation

\[
C_{x,U} = \mathcal{U}(\rho)\otimes\left(\frac{I}{d}\right)^{(k-1)},
\]

where \( \mathcal{U} \) is the universal unitary operator.
where the subscript $x$ indicates that the operator $\mathcal{U}(\rho)$ acts on the Hilbert space of system $B_x$ and the subscript $\lambda$ indicates that the operator acts on the Hilbert space of the remaining $k-1$ systems.

By the same arguments used in Lemma 2, the discrimination of the causal hypotheses can be reduced to the discrimination of the channels

$$C_x^{(N)} = \int dU C_{x,U} \quad x \in \{1, \ldots, k\}. \quad (D4)$$

Again, one can show that, for every reference system $R$, the optimal state can be chosen of the form

$$\rho = \frac{P_{\lambda_0}}{d_{\lambda_0}} \otimes \Psi_{\lambda_0 R}, \quad (D5)$$

where $P_{\lambda_0}$ is the projector on the SU($d$) representation space with Young diagram $\lambda_0$, $d_{\lambda_0} = \text{Tr}[P_{\lambda_0}]$, and $\Psi_{\lambda_0 R}$ is a pure state of the composite system $\mathcal{M}_{\lambda_0} \otimes \mathcal{H}_R$, $\mathcal{M}_{\lambda_0}$ being the SU($d$) multiplicity space associated to $\lambda_0$.

Here we consider the case where the reference system $R$ is trivial. In this case, the problem is to distinguish among the states

$$\rho_x := \left( \frac{P_{\lambda_0}}{d_{\lambda_0}} \otimes \Psi_{\lambda_0} \right)_x \otimes \left( I \right)_{\lambda}^{\otimes N(k-1)} \quad x \in \{1, \ldots, k\}. \quad (D6)$$

Using the Yuen-Kennedy-Lax formula [44], the maximum success probability in distinguishing among these states is

$$p_{\text{succ}} = \min \left\{ \text{Tr}[\Gamma] \mid \Gamma \geq \frac{1}{k} \rho_x, \quad \forall x \in \{1, \ldots, k\} \right\}.$$ 

Note that the states $\{\rho_x, k = 1, \ldots, k\}$ commute. Hence, they can be diagonalized in the same basis and the operator $\Gamma$ can be chosen to be diagonal in that basis without loss of generality. With a similar argument, one can restrict the search for the optimal $\Gamma$ over the operators of the form

$$\Gamma = \bigoplus_{\lambda_1, \lambda_2, \ldots, \lambda_k} P_{\lambda_1} \otimes P_{\lambda_2} \otimes \cdots \otimes P_{\lambda_k} \otimes \Gamma_{\lambda_1, \ldots, \lambda_k}, \quad (D7)$$

where $\Gamma_{\lambda_1, \ldots, \lambda_k}$ is an operator acting on the tensor product space $\mathcal{M}_{\lambda_1} \otimes \mathcal{M}_{\lambda_2} \otimes \cdots \otimes \mathcal{M}_{\lambda_k}$. Note that the operators $\Gamma_{\lambda_1, \ldots, \lambda_k}$ can be set to zero for all $k$-tuples $(\lambda_1, \ldots, \lambda_k)$ such that $\lambda_i \neq \lambda_0$ for every $i \in \{1, \ldots, k\}$. Now, suppose that $\lambda_i = \lambda_0$ and $\lambda_j \neq 0$ for the remaining $j \neq i$. In this case, we must have

$$\Gamma_{\lambda_1, \ldots, \lambda_i-1, \lambda_0, \lambda_i+1, \ldots, \lambda_k} \geq \frac{1}{kd_{\lambda_0} d^{N(k-1)}} Q_{\lambda_1} \otimes \cdots \otimes Q_{\lambda_i-1} \otimes \Psi_{\lambda_0} \otimes Q_{\lambda_i+1} \otimes \cdots \otimes Q_{\lambda_k}, \quad (D8)$$

where $Q_\lambda$ is the identity operator on the multiplicity space $\mathcal{M}_\lambda$. Taking the trace on both sides, we obtain the relation

$$\text{Tr} \left[ \Gamma_{\lambda_1, \ldots, \lambda_i-1, \lambda_0, \lambda_i+1, \ldots, \lambda_k} \right] \geq \frac{1}{kd_{\lambda_0} d^{N(k-1)}} m_{\lambda_1} \cdots m_{\lambda_i-1} m_{\lambda_i+1} \cdots m_{\lambda_k}. \quad (D9)$$

Similar bounds can be found for the operators $\Gamma_{\lambda_1, \ldots, \lambda_k}$ where two or more indices are equal to $\lambda_0$. For example, consider the terms where $\lambda_i = \lambda_j = \lambda_0$, while $\lambda_l \neq 0$ for the remaining values of $l$. In this case, we have the conditions

$$\Gamma_{\lambda_1, \ldots, \lambda_k} \geq \frac{1}{kd_{\lambda_0} d^{N(k-1)}} \left( \Psi_{\lambda_0} \otimes Q_{\lambda_0} \right)_{ij} \otimes \left( Q_{\lambda} \right)_{ij}, \quad (D10)$$

$$\Gamma_{\lambda_1, \ldots, \lambda_k} \geq \frac{1}{kd_{\lambda_0} d^{N(k-1)}} \left( Q_{\lambda_0} \otimes \Psi_{\lambda_0} \right)_{ij} \otimes \left( Q_{\lambda} \right)_{ij}, \quad (D11)$$

where we introduced the shorthand notation

$$\left( Q_{\lambda} \right)_{ij} := Q_{\lambda_1} \otimes \cdots \otimes Q_{\lambda_i-1} \otimes Q_{\lambda_i+1} \otimes \cdots \otimes Q_{\lambda_{i-1}} \otimes Q_{\lambda_{i+1}} \otimes \cdots \otimes Q_{\lambda_k}. \quad (D12)$$

We now combine conditions (D10) and (D11) can be combined into a single condition. To this purpose, we expand $Q_{\lambda_0}$ as

$$Q_{\lambda_0} = \Psi_{\lambda_0} + \Psi_{\lambda_0}^\perp,$$
which allows for rewriting (D10) and (D11) as

\[
\Gamma_{\lambda_1, \ldots, \lambda_k} \geq \frac{1}{kd\lambda_0 d^{N(k-1)}} \left( \psi_{\lambda_0} \otimes \psi_{\lambda_0} + \psi_{\lambda_0} \otimes \psi_{\lambda_0}^\perp \right)_{ij} \otimes \left( Q\lambda \right)_{ij},
\]

(D13)

\[
\Gamma_{\lambda_1, \ldots, \lambda_k} \geq \frac{1}{kd\lambda_0 d^{N(k-1)}} \left( \psi_{\lambda_0} \otimes \psi_{\lambda_0} + \psi_{\lambda_0}^\perp \otimes \psi_{\lambda_0} \right)_{ij} \otimes \left( Q\lambda \right)_{ij}. \tag{D14}
\]

Now, since \(\psi_{\lambda_0} \otimes \psi_{\lambda_0}^\perp\) and \(\psi_{\lambda_0}^\perp \otimes \psi_{\lambda_0}\) are orthogonal vectors, it is also true that

\[
\Gamma_{\lambda_1, \ldots, \lambda_k} \geq \frac{1}{kd\lambda_0 d^{N(k-1)}} \left( Q\lambda_0 \otimes Q\lambda_0 - \psi_{\lambda_0}^\perp \otimes \psi_{\lambda_0}^\perp \right)_{ij} \otimes \left( Q\lambda \right)_{ij},
\]

which can be rewritten as

\[
\Gamma_{\lambda_1, \ldots, \lambda_k} \geq \frac{1}{kd\lambda_0 d^{N(k-1)}} \left( Q\lambda_0 \otimes Q\lambda_0 - \psi_{\lambda_0}^\perp \otimes \psi_{\lambda_0}^\perp \right)_{ij} \otimes \left( Q\lambda \right)_{ij}. \tag{D15}
\]

Tracing on both sides, one obtains

\[
\text{Tr} [\Gamma_{\lambda_1, \ldots, \lambda_k}] \geq \frac{1}{kd\lambda_0 d^{N(k-1)}} \left( 2m_{\lambda_0} - 1 \right) \left( \prod_{t \neq 1, j} m_{\lambda_t} \right). \tag{D16}
\]

Likewise, a term with \(\lambda_{i_1} = \lambda_{i_2} = \cdots = \lambda_{i_t} = \lambda_0\) and all the remaining \(\lambda_t\) different from \(\lambda_0\) will satisfy the condition

\[
\Gamma_{\lambda_1, \ldots, \lambda_k} \geq \frac{1}{kd\lambda_0 d^{N(k-1)}} \left( Q\lambda_0^{\otimes t} - \psi_{\lambda_0}^\perp \otimes Q\lambda_0^t \right)_{i_1 \ldots i_t} \otimes \left( Q\lambda \right)_{i_1 \ldots i_t}, \tag{D17}
\]

leading to the inequality

\[
\text{Tr} [\Gamma_{\lambda_1, \ldots, \lambda_k}] \geq \frac{1}{kd\lambda_0 d^{N(k-1)}} [m_{\lambda_0}^{k} - (m_{\lambda_0} - 1)^t] \prod_{t \neq 1, \ldots, t} m_{\lambda_t}. \tag{D18}
\]

Note that one can choose the operator \(\Gamma\) in such a way that the equality holds in all bounds. With this choice, the probability of success is

\[
p_{\text{succ}} = \sum_{\lambda_1, \ldots, \lambda_k} d_{\lambda_1} \cdots d_{\lambda_k} \text{Tr}[\Gamma_{\lambda_1, \ldots, \lambda_k}]
\]

\[
= \sum_{t=1}^{k} \binom{k}{t} \frac{(d_{\lambda_0} m_{\lambda_0})^t}{kd\lambda_0 d^{N(k-1)}} \left[ 1 - \left( 1 - \frac{1}{m_{\lambda_0}} \right)^t \right] \quad \left( d^{N} - d_{\lambda_0} m_{\lambda_0} \right)^{k-t}
\]

\[
= \frac{d^{N}}{kd\lambda_0} \sum_{t=1}^{k} \binom{k}{t} \frac{d_{\lambda_0} m_{\lambda_0}^t}{p_{\lambda_0}^{t}} \left( 1 - p_{\lambda_0} \right)^{k-t} \left[ 1 - \left( 1 - \frac{1}{m_{\lambda_0}} \right)^t \right], \tag{D19}
\]

having defined the Schur-Weyl measure \(p_{\lambda} := d_{\lambda} m_{\lambda} / d^{N}\).

Expanding the term in square brackets, we obtain

\[
p_{\text{succ}} = \frac{d^{N}}{kd\lambda_0} \sum_{t=1}^{k} \binom{k}{t} \frac{d_{\lambda_0} m_{\lambda_0}^t}{p_{\lambda_0}^{t}} \left( 1 - p_{\lambda_0} \right)^{k-t} \left[ \sum_{s=1}^{t} \binom{t}{s} \frac{(-1)^{s+1}}{m_{\lambda_0}^s} \right]
\]

\[
= \frac{d^{N}}{kd\lambda_0} \sum_{s=1}^{k} \frac{(-1)^{s+1}}{m_{\lambda_0}^s} \left[ \sum_{t=1}^{k} \binom{k}{t} \frac{d_{\lambda_0} m_{\lambda_0}^t}{p_{\lambda_0}^{t}} \left( 1 - p_{\lambda_0} \right)^{k-t} \right]
\]

\[
= \frac{d^{N}}{kd\lambda_0} \sum_{s=1}^{k} \frac{(-1)^{s+1} p_{\lambda_0}^s}{m_{\lambda_0}^s} \binom{k}{s}
\]

\[
= \frac{d^{N}}{kd\lambda_0} \left[ 1 - \left( 1 - \frac{p_{\lambda_0}}{m_{\lambda_0}} \right)^k \right]
\]

\[
= 1 - \frac{(k-1)d_{\lambda_0}}{2d^{N}} + O \left( \left( \frac{d_{\lambda_0}}{d^{N}} \right)^2 \right). \tag{D20}
\]
Hence, the error probability is

\[ p_{\text{err}} = \left( \frac{k-1}{2d^{N}} \right) + O \left( \left( \frac{d_{\lambda_{0}}}{d^{N}} \right)^{2} \right). \]  

(D21)

Again, the optimal choice for \( N \) multiple of \( d \) is to pick \( \lambda_{0} \) to be the trivial representation of \( SU(d) \), in which case the error probability is

\[ p_{\text{err}} = \left( \frac{k-1}{2d^{N}} \right) + O \left( \frac{1}{d^{2N}} \right). \]  

(D22)

Note that, however, the choice of representation \( \lambda_{0} \) does not affect the asymptotic rate: indeed, for every \( \lambda_{0} \) we have

\[ R = -\lim_{N \to \infty} \frac{\log p_{\text{err}}}{N} = \log d - \lim_{N \to \infty} \frac{\log [(k-1)/2]}{N} = \log d \equiv R_{C}. \]  

(D23)

Note also that the rate is independent of the number of hypotheses, as in the case of the Chernoff bound for quantum states [52]. □

Appendix E: Optimal quantum strategy for \( k \) causal hypotheses with arbitrary reference system

Here we provide the optimal quantum strategy using a reference system. We will prove the following lemma:

**Lemma 6.** The optimal input state is

\[ |\rho\rangle = \frac{1}{\sqrt{G_{N,d}}} \sum_{i=1}^{G_{N,d}} \left( |S_{d}\rangle^{\otimes N/d} \right)_{i} \otimes |i\rangle, \]  

(E1)

where \( i \) labels the different ways to divide \( N \) identical objects into groups of \( d \) elements, \( G_{N,d} = \frac{N!}{(d!)^{N/d}(N/d)!} \) is the total number of such ways, \( \left( |S_{d}\rangle^{\otimes N/d} \right)_{i} \) is the product of \( N/d \) singlet states arranged according to the configuration \( i \), and \( \{ |i\rangle, i = 1, \ldots, G_{N,d} \} \) are orthogonal states of the reference system, chosen to be of dimension equal to or larger than \( G_{N,d} \). The corresponding error probability is upper bounded as

\[ p^{Q}_{\text{err}}(r) \leq \frac{k-1}{2d^{N}m(N,d)} \]  

(E2)

where \( m(N,d) \) is the dimension of the multiplicity space of the trivial representation, given by (for \( N/d \) being an integer)

\[ m(N,d) = d^{N} \left[ d^{\frac{d^{2}}{2}} \frac{e^{\frac{d(d-1)}{2}}}{(2\pi)^{\frac{d^{2}-1}{2}} N^{\frac{d^{2}-1}{2}}} \prod_{i=1}^{d} (d-i)! \right] c(N), \]  

(E3)

with \( \lim_{N \to \infty} c(N) = 1 \).

The proof consists of four steps:

**Step 1: reduction to the permutation register.** We apply \( N \) uses of the channel \( C_x \) to a state of the optimal form (B8), where the pure state \( |\Psi_{\lambda_{0}}\rangle \) is set to be the maximally entangled state \( |\Phi_{\lambda_{0}}\rangle = \sum_{i=1}^{m_{\lambda_{0}}} |i\rangle \otimes |i\rangle / \sqrt{m_{\lambda_{0}}} \). The output state is

\[ \rho^{\text{out}}_{x} = \left( P_{\lambda_{0}} \otimes \Phi_{\lambda_{0}} \right)_{x} \otimes \left( I_{N} \right)^{\otimes (N-1)} \]  

(E4)
where the subscript $x$ indicates that the corresponding operator acts on the $N$ Hilbert spaces with label $x$ (and on the reference), while the subscript $\overline{x}$ indicates that the corresponding operator acts on all systems except those with label $x$.

Breaking down the identity operator as $I = (P_{\lambda_0} \otimes Q_{\lambda_0}) \oplus (I - P_{\lambda_0} \otimes Q_{\lambda_0})$, we can decompose $\rho_{x_{\text{out}}}$ into orthogonal blocks where exactly $l$ output systems are in the sector $\lambda_0$. Explicitly, we have

$$\rho_{x_{\text{out}}} = \bigoplus_{l=1}^{k} \bigoplus_{A \in S_l} q(A|x) \left( \rho_{A,x} \otimes \chi_{\overline{x}} \right),$$

(E5)

where $S_l$ denotes the set of all $l$-element subsets of $\{1, 2, \ldots, k\}$, $\rho_{A,x}$ is the quantum state defined by

$$\rho_{A,x} = \begin{pmatrix} P_{\lambda_0} & \otimes & \Phi_{\lambda_0} \\ d_{\lambda_0} & \otimes & \chi_{\overline{x}} \end{pmatrix} \otimes \left( \bigotimes_{i \in A, i \neq x} \left( P_{\lambda_0} \otimes Q_{\lambda_0} / m_{\lambda_0} \right) \right),$$

(E6)

$\chi_{\overline{x}}$ is the quantum state defined by

$$\chi_{\overline{x}} = \bigotimes_{i \not\in A} \left( (I \otimes N) - P_{\lambda_0} \otimes Q_{\lambda_0} / (d_N - d_{\lambda_0} m_{\lambda_0}) \right),$$

(E7)

and $q(A|x)$ is the conditional probability distribution defined by

$$q(A|x) = \begin{cases} p_{\lambda_0}^{l-1} (1 - p_{\lambda_0})^{k-l} & \text{for } x \in A \\ 0 & \text{for } x \not\in A, \end{cases}$$

(E8)

$p_{\lambda} := d_{\lambda} m_{\lambda} / d_N$ being the Schur-Weyl measure.

From Eq. (E5) one can see that blocks with different values of $l$ and/or different subsets $A$ are orthogonal for every value of $x$. Hence, one can extract first the information about the block and then the information about $x$. Mathematically, this means performing a non-demolition measurement with outcomes $(l, A)$, which projects the state into the block labelled by $(l, A)$. When such a measurement is performed on the state $\rho_{x_{\text{out}}}$, the outcome $(l, A)$ can occur only if $A$ contains $x$—in which case the probability of occurrence is $q(A|x)$. Conditionally on the outcome, the system is left in the state $\rho_{A,x} \otimes \chi_{\overline{x}}$ and the problem is to identify $x$ within the set $A$. Hence, the probability of success for fixed $x$ is

$$p_{\text{succ}}(x) = \sum_{l=1}^{k} \sum_{A \in S_l} q(A|x) p_A^{(A)} p_{\text{succ}}(x),$$

(E9)

where $p_A^{(A)}$ is the probability of correctly identifying the state $\rho_{A,x} \otimes \chi_{\overline{x}}$.

Note that, for $x \in A$, the optimal success probability $p_A^{(A)}$ does not depend on the specific subset $A$, but only on its cardinality $l$: indeed, $p_A^{(A)}$ coincides with the probability $p_A^{(l)}$ of correctly identifying the label of the states

$$\sigma_x = \Phi_x \otimes \left( I_m / m \right)^{\otimes l-1}, \quad x \in \{1, 2, \ldots, l\},$$

(E10)

where we used the shorthand notation $\Phi_x := (\Phi_{\lambda_0})_x$, and used $I_m$ to denote the identity matrix in dimension $m$, with $m = m_{\lambda_0}$ (these are the states that arise from Eq. (E6) after discarding the representation spaces). We denote by $p^{(l)}_{\text{succ}}$ the average success probability

$$p^{(l)}_{\text{succ}} = \frac{1}{l} \sum_{x=1}^{l} p^{(l)}_{\text{succ}}(x),$$

(E11)
Averaging the success probability (E9) over \( x \), we obtain

\[
p_{\text{succ}} = \frac{1}{k} \sum_{x=1}^{k} p_{\text{succ}}(x)
\]

\[
= \frac{1}{k} \sum_{l=1}^{k} \sum_{x \in A} q(A|x) p_{\text{succ}}^{(A)}(x)
\]

\[
= \frac{1}{k} \sum_{l=1}^{k} \sum_{x \in A} p_{\lambda_0}^{l-1} (1 - p_{\lambda_0})^{k-l} p_{\text{succ}}^{(A)}(x)
\]

\[
= \frac{1}{k} \sum_{l=1}^{k} \sum_{x \in A} p_{\lambda_0}^{l-1} (1 - p_{\lambda_0})^{k-l} l p_{\text{succ}}^{(l)}
\]

\[
= \frac{1}{k} \sum_{l=1}^{k} \sum_{A \in S_l} \sum_{x \in A} p_{\lambda_0}^{l-1} (1 - p_{\lambda_0})^{k-l} l p_{\text{succ}}^{(l)}
\]

\[
= \frac{1}{k} \sum_{l=1}^{k} \left( \binom{k}{l} \right) p_{\lambda_0}^{l-1} (1 - p_{\lambda_0})^{k-l} l p_{\text{succ}}^{(l)}.
\]

(E12)

The next step is to compute \( p_{\text{succ}}^{(l)} \).

**Step 2: reduction to type states.** The state \( \sigma_x \) in Eq. (E10) is the product of a maximally entangled state and a \((l-1)\) copies of the maximally mixed state. The latter can be diagonalized as

\[
\left( \frac{I_m}{m} \right)^{\otimes(l-1)} = \frac{1}{m^{l-1}} \sum_{j} |j\rangle \langle j|,
\]

(E13)

where \(|j\rangle\) is the basis vector \(|j\rangle = |j_1\rangle \otimes |j_2\rangle \otimes \cdots \otimes |j_{l-1}\rangle\) corresponding to the sequence \(j = (j_1, j_2, \ldots, j_{l-1}) \in \{1, \ldots, m\}^{(l-1)}\).

Now, let us introduce the shorthand

\[
|\Phi_{x,j} \rangle := |\Phi\rangle_x \otimes |j\rangle_{\tau}.
\]

(E14)

Note that for \(x \leq y\) one has

\[
\langle \Phi_{x,j} | \Phi_{y,k} \rangle = \begin{cases} 
1 & \text{if } x = y, \ j = k \\
\frac{1}{m} & \text{if } x \neq y, \ j_i = k_i, \ \forall i < x, \ j_i = k_{i+1}, \ \forall x \leq i < y - 1, \ j_{y-1} = k_x, \ j_i = k_i, \ \forall i \geq y \\
0 & \text{otherwise}.
\end{cases}
\]

(E15)

Let \(n = (n_1, n_2, \ldots, n_m)\) be a partition of \(l - 1\) into \(m\) nonnegative integers. Recall that the sequence \(j = (j_1, j_2, \ldots, j_{l-1})\) is said to be of type \(n\) if it \(n_1\) entries of \(j\) are equal to 1, \(n_2\) entries are equal to 2, and so on. Eq. (E15) tells us that the vectors \( |\Phi_{x,j} \rangle\) and \( |\Phi_{y,k} \rangle\) are orthogonal whenever the sequences \(j\) and \(k\) are of different type. Using this fact, we can define the orthogonal subspaces

\[
\mathcal{H}_n = \text{Span}\left\{ |\Phi_{x,j} \rangle \mid x \in \{1, \ldots, l\}, \ j \in S_n \right\},
\]

(E16)

where \(S_n\) is the set of all sequences of length \(l - 1\) and of type \(n\). Hence, we can decompose the states \(\sigma_x\) in Eq. (E10) as

\[
\sigma_x = \bigoplus_n p(n) \sigma_{n,x},
\]

(E17)
with
\[
p(n) = \frac{C_n}{m^{l-1}} \quad \text{and} \quad \sigma_{n,x} = \frac{1}{C_n} \sum_{j \in S_n} |\Phi_{x,j}\rangle \langle \Phi_{x,j}| ,
\] (E18)

where \( C_n = (l-1)!/[n_1!n_2! \cdots n_m!] \) is the number of sequences of type \( n \).

Eq. (E17) tells us that, in order to distinguish the states \( \sigma_x \), one can perform an orthogonal measurement that projects on the subspaces \( \{ \mathcal{H}_n \} \) (E16). If the measurement outcome is \( n \), one is left with the task of distinguishing among the states \( \sigma_{n,x} \). The success probability of this strategy is
\[
p_s^{(l)} = \sum_{n} p(n) p_s^{(n)} ,
\] (E19)

where \( p_s^{(n)} \) is the probability of correctly distinguishing the states \( \{ \sigma_{n,x} \mid x \in \{1,\ldots,l\} \} \).

**Step 3: lower bound on the probability of success.** The probability of correctly distinguishing the states \( \{ \sigma_{n,x} \mid x \in \{1,\ldots,l\} \} \) is lower bounded by the probability of correctly distinguishing among all their eigenstates
\[
\left\{ |\Phi_{x,j}\rangle \mid x \in \{1,\ldots,l\}, \ j \in S_n \right\} .
\] (E20)

Note that the total number of states is \( lC_n \).

We now construct a measurement that distinguishes these states with high success probability. The measurement is constructed through a Gram-Schmidt orthogonalization procedure. We define a first batch of \( C_n \) vectors as
\[
|\Psi_{1,j}\rangle := |\Phi_{1,j}\rangle \quad \text{\( j \in S_n \).}
\] (E21)

This definition is well-posed, because the above vectors are orthonormal, due to Eq. (E15).

A second batch of vectors is constructed from the vectors \( \{ |\Phi_{2,j}\rangle, \ j \in S_n \} \) via the Gram-Schmidt procedure, which yields
\[
|\Psi_{2,j}\rangle := \frac{|\Phi_{2,j}\rangle - \frac{1}{m} |\Phi_{1,j}^{12}\rangle}{\sqrt{1 - \frac{1}{m^2}}} ,
\] (E22)

where \( j^{12} \) is the sequence such that \( \langle \Phi_{1,j}^{12} | \Phi_{2,j} \rangle = 1/m \).

A third batch of vectors is constructed from the vectors \( \{ |\Phi_{2,j}\rangle, \ j \in S_n \} \). Now, the Gram-Schmidt procedure yields
\[
|\Psi_{3,j}\rangle := \frac{|\Phi_{3,j}\rangle - \frac{1}{m} |\Phi_{2,j}^{12}\rangle - \frac{1}{m} |\Phi_{1,j}^{13}\rangle}{\sqrt{1 - \frac{2}{m^2}}} + O\left( \frac{1}{m^2} \right) |\Gamma_{3,j}\rangle + O\left( \frac{1}{m^3} \right) |\text{Rest}_{3,j}\rangle ,
\] (E23)

where \( |\Gamma_{3,j}\rangle \) is a vector of the form \( |\Phi_{1,k}\rangle \) for some suitable \( k \) and \( |\text{Rest}_{3,j}\rangle \) is a suitable unit vector, which is irrelevant for computing the leading order of the success probability.

In general, the \( x \)-th batch of vectors is
\[
|\Psi_{x,j}\rangle := \frac{|\Phi_{x,j}\rangle - \frac{1}{m} \sum_{y=1}^{x-1} |\Phi_{y,j}^{y+1}\rangle}{\sqrt{1 - \frac{x-1}{m^2}}} + O\left( \frac{1}{m^2} \right) |\Gamma_{x,j}\rangle + O\left( \frac{1}{m^3} \right) |\text{Rest}_{x,j}\rangle ,
\] (E24)

where \( |\Gamma_{x,j}\rangle \) is a normalized combination of vectors of the form \( |\Phi_{z,k}\rangle \), \( z < x - 2 \), while \( |\text{Rest}_{x,j}\rangle \) is a suitable unit vector.

Note that one has
\[
\langle \Phi_{x,j} | \Psi_{x,j} \rangle = \sqrt{1 - \frac{x-1}{m^2}} + O\left( \frac{1}{m^3} \right) , \quad \forall x \in \{1,\ldots,l\}, \ \forall j \in S_n ,
\] (E25)

having used the fact that the product \( \langle \Phi_{x,j} | \Gamma_{x,j} \rangle \) is \( O(1/m) \).
Using Eq. (E25), we can now evaluate the probability of correctly distinguishing the states \{|\Phi_{x,j}\rangle\}. On average over all possible states, the probability of success is

\[
p_{\text{succ}}^{(n)} = \frac{1}{lC_n} \sum_{x=1}^{l} \sum_{j \in S_n} \left| \langle \Psi_{x,j} | \Phi_{x,j} \rangle \right|^2
\]

\[
= \frac{1}{lC_n} \sum_{x=1}^{l} \sum_{j \in S_n} \left[ 1 - \frac{x-1}{m^2} + O\left(\frac{1}{m^3}\right) \right]
\]

\[
= \frac{1}{l} \sum_{x=1}^{l} \left[ 1 - \frac{x-1}{m^2} + O\left(\frac{1}{m^3}\right) \right]
\]

\[
= 1 - \frac{l-1}{2m^2} + O\left(\frac{1}{m^3}\right).
\]

(E26)

Since measuring on the basis \{|\Psi_{x,j}\rangle\} is not necessarily the optimal strategy, we arrived at the lower bound

\[
p_{\text{succ}}^{(n)} \geq 1 - \frac{l-1}{2m^2} + O\left(\frac{1}{m^3}\right).
\]

(E27)

Note that the (leading order of the) r.h.s. is independent of the type \(n\).

**Step 4: putting everything together.** Combining the results obtained so far, we can lower bound the success probability in distinguishing among \(k\) causal structures. Inserting the lower bound (E27) into Eq. (E19), we obtain

\[
p_{\text{succ}}^{(l)} = \sum_{n} p(n) \ p_{\text{succ}}^{n}
\]

\[
\geq 1 - \frac{l-1}{2m^2} + O\left(\frac{1}{m^3}\right).
\]

Then, we can insert the above bound into Eq. (E12). Reverting to the full notation \(m_{\lambda_0} \equiv m\), we obtain

\[
p_{\text{succ}} = \frac{1}{k} \sum_{l=1}^{k} \binom{k}{l} \left( p_{\lambda_0}^{l-1} (1 - p_{\lambda_0})^{k-l} \right) p_{\text{succ}}^{(l)}
\]

\[
\geq \frac{1}{k} \sum_{l=1}^{k} \binom{k}{l} \left( p_{\lambda_0}^{l-1} (1 - p_{\lambda_0})^{k-l} \right) \left[ 1 - \frac{l-1}{2m_{\lambda_0}} + O\left(\frac{1}{m_{\lambda_0}^3}\right) \right]
\]

\[
= 1 - \frac{(k-1)p_{\lambda_0}}{2m_{\lambda_0}^2} + O\left(\frac{1}{m_{\lambda_0}^3}\right)
\]

\[
= 1 - \frac{k-1}{2dN} \frac{d_{\lambda_0}}{m_{\lambda_0}} + O\left(\frac{1}{m_{\lambda_0}^3}\right).
\]

(E28)

Hence, the error probability of the optimal quantum strategy is upper bounded as

\[
p_{\text{err}} \leq \frac{k-1}{2dN} \frac{d_{\lambda_0}}{m_{\lambda_0}} + O\left(\frac{1}{m_{\lambda_0}^3}\right).
\]

(E29)

Recalling that the ratio \(d_{\lambda}/m_{\lambda}\) is minimised by the representation with “minimal” Young diagram (in the majorisation order), we conclude that, when \(N\) is a multiple of \(d\), the optimal error probability satisfies the bound

\[
p_{\text{err}} \leq \frac{k-1}{2dN} \frac{d_{\lambda_0}}{m_{\lambda_0}} + O\left(\frac{1}{m_{\lambda_0}^3}\right), \quad \text{with} \quad m(N, d) = d^N \left[ \frac{d^2 e^{d(d-1)/2} \prod_{i=1}^{d} (d-i)!}{(2\pi)^{d-1} d^{d^2/2} N^{d(d-1)/2}} \right] c(N) \quad \text{and} \quad c(N) \to 1.
\]

(E30)

Hence, the asymptotic decay rate is lower bounded as

\[
R_Q = -\lim_{N \to \infty} \frac{\log p_{\text{err}}}{N} \geq 2 \log d.
\]

(E31)
On the other hand, the r.h.s. is equal to the decay rate for \( k = 2 \), which is a lower bound for the decay rate for \( k \geq 2 \). In conclusion, we obtained that the optimal decay rate is equal to \( R_Q = 2 \log d \).

\[ \square \]

**Appendix F: Quantum speedup in the identification of a cause**

We consider the scenario where \( k \) quantum variables \( A_1, \ldots, A_k \) are candidate causes of a given effect \( B \). For simplicity, we assume that all variables are quantum systems of dimension \( d < \infty \). The causal relation is described by a quantum channel \( C_x, \mathcal{U} \) of the form \( C_x, \mathcal{U}(\rho) = \mathcal{U}(\text{Tr}_x[\rho]) \), where \( \text{Tr}_x \) denotes the partial trace over all input systems except \( A_x \), with \( x \in \{ 1, \ldots, k \} \), and \( \mathcal{U} \) is a generic unitary channel, acting on the remaining system \( A_x \). The problem is to identify the value of \( x \).

1. **Fixed unitary gates**

Suppose first that the unitary gate \( \mathcal{U} \) is fixed. Without loss of generality, we can assume \( \mathcal{U} = \mathcal{I} \), so that the channel \( C_x, \mathcal{I} \) is simply the partial trace over all systems except \( x \). The distinguishability of the channels \( \{ C_x, \mathcal{I} \}_{x=1}^k \) has been studied extensively in the optimization of port-based teleportation [36]. A simple strategy is to entangle each input system with a reference system, obtaining the output state \( \rho_x := \Phi^+_{BR_x} \otimes \left( \frac{1}{d} \right)^{k-1} \), where \( \Phi^+ \) is the maximally entangled state, \( R_x \) is the \( x \)-th reference system, and the subscript \( \pi \) indicates that the operator \( (I/d)^{\otimes(k-1)} \) acts on the Hilbert space of all reference systems except \( R_x \).

For \( k \geq d \), the optimal probability of success in distinguishing between the states \( \{ \rho_x \}_{x=1}^k \) is \( p_{\text{suc}} = d^2/(k-1+d^2) \) [36]. If the unknown process is probed for \( N \) times, the output state is \( \rho_x^\otimes N \) and the probability of success is \( p_{\text{suc}} = d^{2N}/(k-1+d^{2N}) \).

2. **Unknown unitary gates**

Let us consider the scenario where the unitary gate \( \mathcal{U} \) is completely unknown. By the same argument as in Appendix 1, the minimum worst-case error probability is equal to the minimum error probability in distinguishing between the average channels

\[
C^{(N)}_x = \int d\mathcal{U}_1 d\mathcal{U}_2 \cdots d\mathcal{U}_k \; C^{\otimes N}_x \circ (\mathcal{U}_1 \otimes \mathcal{U}_2 \cdots \otimes \mathcal{U}_k)^\otimes N.
\]  

(F1)

The symmetry of the problem implies that the optimal input states are of the form

\[
\rho_{AR} = \frac{P_{\lambda_1}}{d_{\lambda_1}} \otimes \frac{P_{\lambda_2}}{d_{\lambda_2}} \otimes \cdots \otimes \frac{P_{\lambda_k}}{d_{\lambda_k}} \otimes \Psi_{M_{\lambda_1},M_{\lambda_2} \cdots M_{\lambda_k} R},
\]  

(F2)

where \( P_{\lambda_i} \) is the projector on the representation space \( R_{\lambda_i} \) in the tensor product \( (\mathcal{H}^\otimes N)_i \) of the \( N \) systems corresponding to variable \( A_i \), and the subscript \( M_{\lambda_i} \) denotes the multiplicity space in \( (\mathcal{H}^\otimes N)_i \).

When the input variables are initialized in the state \( \rho_{AR} \), the output is

\[
\rho_{BR,x} = \frac{P_{\lambda_x}}{d_{\lambda_x}} \otimes \text{Tr}_{M_{\lambda_x}} \left[ \Psi_{M_{\lambda_1},M_{\lambda_2} \cdots M_{\lambda_k} R} \right],
\]  

(F3)

where \( \text{Tr}_{M_{\lambda_x}} \) is the trace over all multiplicity spaces except \( M_{\lambda_x} \).

We now show that the true cause can be perfectly identified using at \( O(\log d k) \) queries to the unknown process. We first provide an exact strategy using \( \log d k \) queries (at the leading order), and then show that the number of queries can be reduced to \( 1/2 \log d k \) (at the leading order) if a small error, vanishing in the large \( k \) limit, is tolerated.

Our exact strategy disregards the reference system \( R \). In this strategy, we prepare the multiplicity systems in the product state

\[
|\Psi\rangle_{M_{\lambda_1}M_{\lambda_2} \cdots M_{\lambda_k}} = |\psi_1\rangle_{M_{\lambda_1}} \otimes |\psi_2\rangle_{M_{\lambda_2}} \otimes \cdots \otimes |\psi_k\rangle_{M_{\lambda_k}}.
\]  

(F4)

We divide the indices \( i \) into \( L \) groups, labelled as \( G_1, G_2, \ldots, G_L \) and assign a distinct Young diagram to each group, so that \( \lambda_i = \lambda_j \) for \( i, j \) in the same group. Within each group, we choose the states \( |\psi_i\rangle_{M_{\lambda_i}} \) to be orthogonal. This
choice constrains the number of indices in group $G_t$ to be at most the dimension of the multiplicity space $\mathcal{M}_{\lambda_{G_{t}}}$, where $\lambda_{G_{t}}$ is the Young diagram assigned to the group $G_t$. In turn, this implies that the condition

$$k \leq \sum_{l=1}^{L} m_{\lambda_{G_{l}}} \leq \sum_{\lambda} m_{\lambda}$$

must be satisfied. Both bounds can be saturated, as one can choose $L$ to be the number of Young diagrams in the decomposition of the tensor representation $U \otimes N$. On the other hand, the multiplicities are lower bounded as $m_{\lambda} \geq \binom{N}{\lambda} / ((N+1)^{d}-1)^{d-1}/2$ where $\binom{N}{\lambda} = N! / (\lambda_1! \lambda_2! \cdots \lambda_k!)$ is the multinomial coefficient [53, 54]. Hence, we have the bound $\sum_{\lambda} m_{\lambda} \geq d^{N} / ((N+1)^{d}-1)^{d-1}/2$, meaning that condition (F5) can be satisfied with $N \geq \log_{d} k + O(\log \log k)$. Hence, the unknown cause can be identified with zero error using approximately $\log_{d} k$ queries.

We now construct a strategy that identifies the correct cause with $1/2 \log_{d} k + O(\log \log k)$ queries and with vanishing error probability. In this strategy, all the input variables are initialized in the same sector, namely $\lambda_1 = \lambda_2 = \cdots = \lambda_k \equiv \lambda$. Specifically, we take $N$ to be a multiple of $d$ and choose $\lambda$ to be the Young diagram corresponding to the trivial representation of $SU(d)$. The strategy uses the reference system $R = M_{\lambda} \otimes \mathcal{E}$ and the input state

$$\rho_{AR} = \left(\frac{P_{\lambda}}{d_{\lambda}}\right) \otimes \left(\Phi_{\lambda}^{+}\right)^{\otimes k} \text{,}$$

where $\Phi_{\lambda}^{+}$ is the projector on the maximally entangled state of two identical copies of $M_{\lambda}$. Then, the output state is

$$\rho_{BR,x} = \left(\frac{P_{\lambda}}{d_{\lambda}}\right) \otimes \left(\Phi_{\lambda}^{+}\right)_{x} \otimes \left(\frac{Q_{\lambda}}{m_{\lambda}}\right)_{\tau}^{\otimes (k-1)} \text{,}$$

where the maximally entangled state $(\Phi_{\lambda}^{+})_{x}$ involves the output system $B$ and the $x$-th reference system, while all the remaining reference systems are in the maximally mixed state $Q_{\lambda}/m_{\lambda}$. Distinguishing among the states $\rho_{BR,x}$ is equivalent to distinguishing the states $(\Phi_{\lambda}^{+})_{x} \otimes \left(\frac{Q_{\lambda}}{m_{\lambda}}\right)_{\tau}^{\otimes (k-1)}$. This problem has been solved in the context of port-based teleportation, and the minimum error probability is known to be $p_{\text{err}} = (k-1)/(m_{\lambda}^{2} + k - 1)$ [36]. Using Equation (E3), we then obtain

$$p_{\text{err}} \leq \frac{k - 1}{m_{\lambda}^{2}} = k - 1 \left[ \frac{(2\pi)^{d-1} \pi^{d-1}}{d^{2d}} \sum_{l=1}^{d} \prod_{i=1}^{d} c(N) \right] \text{,}$$

with $\lim_{N \to \infty} c(N) = 1$. Hence, a vanishing error probability can be obtained by setting $N = \left[ (\log_{d} k)(1+\epsilon)/2 \right]$ with $\epsilon > 0$.

**Appendix G: A quantum advantage in the presence of noise**

Here we consider the task of identifying causal intermediaries when the cause-effect relation is obfuscated by depolarizing noise, corresponding to the channel $\mathcal{D}_{\rho} = (1-p)I + pf/d$, where $p$ is the probability of depolarization.

For simplicity, consider the case of one input variable $A$ and two output variables $B$ and $C$. Suppose that the experimenter prepares $N$ copies of the maximally entangled state and sends half of each entangled state through one instance of the unknown process. With this choice, the output state consists of $N$ copies of the state $\Sigma_{x}$, $x \in \{1, 2\}$, with

$$\Sigma_{1} = \left[ (1-p)\Phi + pI \otimes I \right]_{BR} \otimes \frac{I}{d} \otimes \left[ (1-p)\Phi + pI \otimes I \right]_{CR} \text{,}$$

$$\Sigma_{2} = \left[ \frac{I}{d} \right]_{B} \otimes \left[ (1-p)\Phi + pI \otimes I \right]_{CR} \text{,}$$

where $\Phi$ is the projector on the canonical maximally entangled state. Then, the quantum Chernoff bound [55] yields the rate

$$R = -\log \min_{0 \leq s \leq 1} \text{Tr}[\Sigma_{1}^{s} \Sigma_{2}^{1-s}] = -\log \min_{0 \leq s \leq 1} \frac{1}{d^{2}} \left[ \left(1 - \frac{p}{d^{2}}\right)^{s} + \left(d^{2} - 1\right) \left(\frac{p}{d^{2}}\right)^{s} \right] \left[ \left(1 - \frac{p}{d^{2}}\right)^{1-s} + \left(d^{2} - 1\right) \left(\frac{p}{d^{2}}\right)^{1-s} \right] = 2 \log d - 2 \log \left[ \sqrt{1 - \frac{p}{d^{2}}} + \sqrt{\frac{p}{d^{2}}} \right] \text{.}$$
When $p$ is small enough, the rate can be larger than $\log d$, the best classical rate in the noiseless scenario. Since noise can only increase the error probability, this implies a quantum-over-classical advantage in the noisy scenario. The same result holds for the discrimination of $k \geq 2$ hypotheses, as the quantum Chernoff bound for multiple states is equal to the worst-case Chernoff bound among all pairs [52].

We now provide a partial discussion of the scenario where the functional dependence between cause and effect is unknown. This scenario can be modelled by concatenating the depolarizing channel with a completely unknown unitary gate acting on the input variable. The full analysis of the probability of error is substantially more complex, and we leave it as a topic of future research. Here we evaluate the error probability in the simplified scenario where the depolarization is heralded, meaning that when the system is depolarized to the maximally mixed state, the unitary gate acting on the input variable. The full analysis of the probability of error is substantially more complex, is unknown. This scenario can be modelled by concatenating the depolarizing channel with a completely unknown unitary gates is $\rho_{\text{in}} = \bigoplus_{\lambda} p_{\lambda} \frac{P_{\lambda} \otimes P_{\lambda}}{d_{\lambda}^{2}} \otimes \Phi_{\lambda}$, (G3)

where $p_{\lambda} = d_{\lambda} m_{\lambda}/d^{N}$ is the Schur-Weyl measure, and $\Phi_{\lambda}$ is the maximally entangled state in $M_{\lambda} \otimes M_{\lambda}$.

The two output states corresponding to the two hypotheses are

$$
\rho_{\text{out},1} = (\rho_{\text{in}})_{\text{BR}} \otimes \left(\frac{I}{d}\right)^{\otimes k}_{\text{C}} \quad \text{and} \quad \rho_{\text{out},2} = \left(\frac{I}{d}\right)^{\otimes k}_{\text{B}} \otimes (\rho_{\text{in}})_{\text{CR}}.
$$

(G4)

The distance between them is

$$
\|\rho_{\text{out},1} - \rho_{\text{out},2}\|_{1} = \left\| \bigoplus_{\lambda,i,\mu} \frac{(P_{\lambda})_{\text{B}} \otimes (P_{\mu})_{\text{R}} \otimes (P_{\nu})_{\text{C}}}{d_{\lambda} d_{\mu} d_{\nu}} \otimes \left[ \frac{p_{\lambda} p_{\nu} \delta_{\lambda \mu} (\Phi_{\lambda})_{\text{BR}} \otimes \left( \frac{Q_{\nu}}{m_{\nu}} \right)_{\text{C}} - p_{\lambda} p_{\nu} \delta_{\mu \nu} \left( \frac{Q_{\lambda}}{m_{\lambda}} \right)_{\text{B}} \otimes (\Phi_{\nu})_{\text{CR}} \right] \right\|_{1}
$$

$$
= 2 \left( 1 - \sum_{\lambda} p_{\lambda}^{2} \right) + \sum_{\lambda} p_{\lambda}^{2} \left\| (\Phi_{\lambda})_{\text{BR}} \otimes \left( \frac{Q_{\lambda}}{m_{\lambda}} \right)_{\text{C}} - \left( \frac{Q_{\lambda}}{m_{\lambda}} \right)_{\text{B}} \otimes (\Phi_{\lambda})_{\text{CR}} \right\|_{1}
$$

$$
= 2 \left( 1 - \sum_{\lambda} p_{\lambda}^{2} \right) + 2 \sum_{\lambda} p_{\lambda}^{2} \sqrt{1 - m_{\lambda}^{-2}}.
$$

where the second term in the sum has been evaluated through Equation \((B19)\).

Hence, we have the approximate expression

$$
\|\rho_{\text{out},1} - \rho_{\text{out},2}\|_{1} = 2 \left( 1 - \sum_{\lambda} p_{\lambda}^{2} \right) + 2 \sum_{\lambda} p_{\lambda}^{2} \left[ 1 - \frac{1}{2m_{\lambda}^{2}} + O(m_{\lambda}^{4}) \right]
$$

$$
= 2 - \frac{1}{d^{2k}} \sum_{\lambda} d_{\lambda}^{2} + O(d^{-4k})
$$

$$
= 2 - \frac{\text{Poly}(k,d)}{d^{2k}} + O(d^{-4k}),
$$

(G5)

having used the fact that the dimensions and the number of Young diagrams grow at most polynomially in $k$ and $d$ (see e.g. [53, 54]). Using the above expression, we obtain the expression $p_{\text{err},k} = \frac{\text{Poly}(k,d)}{d^{2k}} + O(d^{-4k})$. Summing over $k$ and averaging with the Bernoulli distribution we finally obtain $p_{\text{err}} = \text{Poly}(N,d) \left( \frac{1-p}{d^2} + p \right)^{N}$ at the leading order.

In conclusion, the discrimination rate is $R = -\log \left( \frac{1-p}{d^2} + p \right)$, which is larger than the noiseless classical rate $\log d$ when $p$ is smaller than $1/(d+1)$. The rate $R = -\log \left( \frac{1-p}{d^2} + p \right)$ provides an upper bound to the achievable rate without heralding, for the simple strategy consisting in preparing $N$ copies of the maximally entangled state. When the probability of depolarisation exceeds $1/(d+1)$ this simple quantum strategy cannot beat the noiseless classical rate, and comparison between quantum and classical strategies requires a more detailed analysis.

It is worth noting the above derivation provides an alternative strategy for the identification of the causal intermediary in the noiseless case ($p = 0$). This strategy achieves the same rate of our universal strategy, although with a polynomially worse error probability. While suboptimal, the present strategy is practically interesting because it does not require input states with large-scale multipartite entanglement.
Appendix H: Proof of Equation (29) in the main text

Step 1. Observe that the channels $C_{\pm} = \frac{2}{d^2+1} P_{\pm} (\rho \otimes I \otimes N) P_{\pm}$ are no-signalling. Indeed, for every subset $S \subseteq \{1, \ldots, N\}$ one has that the input system $A(S) := \bigotimes_{i \in S} A_i$ cannot signal to the output system $BC(S) := \bigotimes_{i \in S} (B_i \otimes C_i)$. To check the no-signalling condition, we use the relation

$$P_{\pm} = \frac{I \pm \text{SWAP}}{2} = \left( \bigotimes_{i \in S} I_{B_i C_i} \right) \otimes \left( \bigotimes_{i \in S} I_{B_i C_i} \right) \pm \left( \bigotimes_{i \in S} \text{SWAP}_{B_i C_i} \right) \otimes \left( \bigotimes_{i \in S} \text{SWAP}_{B_i C_i} \right),$$

where $I_{B_i C_i}$ is the identity operator on the composite system $B_i C_i$, and $\text{SWAP}_{B_i C_i}$ is the unitary operator that swaps systems $B_i$ and $C_i$. The state of the output system $BC(S)$ is

$$(\bigotimes_{i \in S} \text{Tr}_{B_i C_i} \left[ C_{\pm}(\rho) \right]) \propto (\bigotimes_{i \in S} \text{Tr}_{B_i} \left[ \rho \right]) \otimes (\bigotimes_{i \in S} I_{C_i}) \pm (\bigotimes_{i \in S} \text{SWAP}_{B_i C_i} \left[ \rho \right]) \otimes (\bigotimes_{i \in S} I_{C_i}),$$

and depends only on the state of the input system $A(S)$.

Step 2. Show that there exist coefficients $a$ and $b$ such that the maps $aC_+ + bC_- - 1/2 C_{1, I}$ and $aC_+ + bC_- - 1/2 C_{2, I}$ are completely positive.

Let us consider the $N = 1$ case first. By definition, one has

$$aC_+ + bC_- - 1/2 C_{1, I} = M \circ (I \otimes I) \quad \text{and} \quad aC_+ + bC_- - 1/2 C_{2, I} = M \circ (I \otimes I),$$

where $M$ is the linear map defined by

$$M(A) := m_{00} A + m_{01} (\text{SWAP}) A + m_{10} (\text{SWAP}) A + m_{11} (\text{SWAP}) A (\text{SWAP})$$

with

$$m_{00} = \frac{a}{2(d+1)} + \frac{b}{2(d-1)} - \frac{1}{2d}, \quad m_{10} = \frac{a}{2(d+1)} - \frac{b}{2(d-1)} - \frac{1}{2d}, \quad m_{11} = \frac{a}{2(d+1)} + \frac{b}{2(d-1)}.\quad (H5)$$

Now, if the matrix $M$ is positive, then the map $M$ is completely positive. Defining

$$\alpha := \frac{a}{2(d+1)} \quad \text{and} \quad \beta := \frac{b}{2(d-1)},$$

the positivity condition becomes

$$\alpha + \beta \geq 1/(2d) \quad (H7)$$

$$4\alpha \beta \geq (\alpha + \beta)/(2d). \quad (H8)$$

As an ansatz, we choose $\alpha = \sqrt{d-1} x$ and $\beta = \sqrt{d+1} x$, for some $x > 0$. Then, condition (H8) becomes

$$x \geq \frac{1}{8d} \left( \frac{1}{\sqrt{d+1}} + \frac{1}{\sqrt{d-1}} \right) =: x_0. \quad (H9)$$

Note that the choice $x = x_0$ satisfies both conditions (H8) and (H7). Finally, note that the above derivation holds for arbitrary $N$, by replacing $d$ with $d^N$. 
Step 3. Define the constant $\lambda := a + b$ and the no-signalling channel $C := (aC_+ + bC_-)/\lambda$. By construction, the maps $\lambda C - 1/2 C_{1,I}$ and $\lambda C - 1/2 C_{2,I}$ are completely positive. Explicit evaluation yields

$$\lambda = \left( \frac{\sqrt{dN} + 1 + \sqrt{dN} - 1}{4dN} \right)^2.$$

Finally, observe that the maps $\lambda C - 1/2 C_{1,I}$ and $\lambda C - 1/2 C_{2,I}$ are completely positive if and only if the Choi operators $C, C_{1,I},$ and $C_{2,I}$ corresponding to $C, C_{1,I},$ and $C_{2,I}$ satisfy the inequalities $\lambda C \geq 1/2 C_{1,I}$ and $\lambda C \geq 1/2 C_{2,I}$. Inserting the expression of $\lambda$ into Equation (26) of the main text, we then obtain the desired bound

$$p_{err}^{ind} \geq 1 - \lambda = \frac{1 - \sqrt{1 - \frac{1}{d^2N}}}{2}.$$

(H11)