Quantum Sequential Hypothesis Testing

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We introduce sequential analysis in quantum information processing, by focusing on the fundamental task of quantum hypothesis testing. In particular, our goal is to discriminate between two arbitrary quantum states with a prescribed error threshold \( \epsilon \) when copies of the states can be required on demand. We obtain ultimate lower bounds on the average number of copies needed to accomplish the task. We give a block-sampling strategy that allows us to achieve the lower bound for some classes of states. The bound is optimal in both the symmetric as well as the asymmetric setting in the sense that it requires the least mean number of copies out of all other procedures, including the ones that fix the number of copies ahead of time. For qubit states we derive explicit expressions for the minimum average number of copies and show that a sequential strategy based on fixed local measurements outperforms the best collective measurement on a predetermined number of copies. Whereas for general states the number of copies increases as \( \log 1/\epsilon \), for pure states sequential strategies require a finite average number of samples even in the case of perfect discrimination, i.e., \( \epsilon = 0 \).

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Introduction.—Statistical inference permeates almost every human endeavor, from science and engineering all the way through to economics, finance, and medicine. The perennial dictum in such inference tasks has been to optimize performance—often quantified by suitable cost functions—given a fixed number \( N \) of relevant resources [1,2]. This approach often entails the practical drawback that all \( N \) resources need to be batch processed before a good inference can be made. Fixing the number of resources ahead of time does not reflect the situation that one encounters in many real-life applications that might require an online, early, inference—such as change-point detection [3–6], or where additional data may be obtained on demand if the required performance thresholds are not met.

Sequential analysis [7] is a statistical inference framework designed to address these shortcomings. Resources are processed on the fly, and with each new measured unit a decision to stop the experiment is made depending on whether prescribed tolerable error rates (or other cost functions) are met; the processing is continued otherwise. Since the decision to stop is solely based on previous measurement outcomes, the size \( N \) of the experiment is not predetermined but is, instead, a random variable. A sequential protocol is deemed optimal if it requires the least average number of resources among all statistical tests that guarantee the same performance thresholds. For many classical statistical inference tasks it is known that sequential methods can attain the required thresholds with a substantially lower average number of samples than any statistical test based on a predetermined number of samples [7]. The ensuing savings in resources, and the ability to take actions in real time, have found applications in a wide range of fields [3,8]. Extending sequential analysis to the quantum setting is of fundamental interest, and with near-term quantum technologies on the verge of impacting the global market, the versatility and resource efficiency that sequential protocols provide for quantum information processing is highly desirable.

In this Letter, we consider the discrimination of two arbitrary finite dimensional quantum states [9], \( \rho \) (corresponding to the null hypothesis \( H_0 \)) and \( \sigma \) (corresponding to the alternative hypothesis \( H_1 \)), in a setting where a large number of copies can be used in order to meet a desired error threshold \( \epsilon \). A first step in this direction was taken in Ref. [10], which considers the particular case where \( \rho \) and \( \sigma \) are pure states and restricts the analysis to specific local measurement strategies. Here, we address the problem in full generality, including arbitrary states, weak and collective measurements. For collective strategies involving a large fixed number of copies the relation between this number and the error \( \epsilon \) is \( N \sim - (1/\xi) \log \epsilon \) [11], where the rate \( \xi \) depends on the pair of hypotheses and on the precise setting as we explain shortly. We show that one can significantly reduce the expected number of copies \( \langle N \rangle \) by considering sequential strategies where copies are
provided on demand. We give the ultimate lower bounds as a single-letter expression of the form
\[
\langle N \rangle_0 \geq - \frac{\log \epsilon}{D(\rho \| \sigma)} + O(1), \quad \langle N \rangle_1 \geq - \frac{\log \epsilon}{D(\sigma \| \rho)} + O(1)
\]
(1)
for \( \epsilon \ll 1 \), where \( \langle N \rangle_\nu \) is the mean number of copies given the true hypothesis is \( \nu \in \{0, 1\} \) and \( D(\rho \| \sigma) = \text{tr}\rho (\log \rho - \log \sigma) \) is the quantum relative entropy. In such cases it is imperative to minimize the mean probability of error \( \epsilon \) when approving an ineffective treatment. In medical trials, where the effect of approving an ineffective treatment can be generally met in a deterministic setting. Specifically, the classical sequential test, for both the strong error as well as the symmetric and asymmetric setting, is known to be the sequential probability ratio test (SPRT) [23] which we now review.

After \( n \) measurements have been performed, we have a string of outcomes \( x_n = \{x_1, x_2, \ldots, x_n\} \), where each element has been sampled effectively from a probability distribution determined by the positive operator-valued measure (POVM) \( E = \{E_x\} \) and the true state of the system, i.e., either \( p(x) := \text{tr}(E_x \rho) \), or \( q(x) := \text{tr}(E_x \sigma) \). For given error thresholds \( \epsilon_0, \epsilon_1 \), the strong condition demands that for each conclusive sequence the conditional probabilities obey either
\[
P(\rho| \sigma) = \frac{\eta_0 p(x_n)}{\eta_0 p(x_n) + \eta_1 q(x_n)} \geq 1 - \epsilon_0, \quad \text{or} \quad (2)
\]
\[
P(\sigma|x_n) = \frac{\eta_1 q(x_n)}{\eta_0 p(x_n) + \eta_1 q(x_n)} \geq 1 - \epsilon_1, \quad \text{or} \quad (3)
\]
where \( p(x_n) = \prod_{k=1}^n p(x_k) \) since the copies are identical and independent (the same holds for \( q \)). If neither condition is met, a new copy needs to be requested and we continue measuring. That is, starting at \( n = 1 \) at every step \( n \) we check whether (1) \( P(\rho| x_n) \geq 1 - \epsilon_0 \), then stop and accept \( H_0 \), with guaranteed probability of success \( s_0 = 1 - \epsilon_0 \); (2) \( P(\sigma| x_n) \geq 1 - \epsilon_1 \), then stop and accept \( H_1 \), with guaranteed probability of success \( s_1 = 1 - \epsilon_1 \); (3) if neither 1 nor 2 hold, continue sampling.

Using (2) and (3), the condition to continue sampling can be written in terms of a single sample statistic, the log-likelihood ratio
\[
Z_n = \log \frac{q(x_n)}{p(x_n)} = \sum_{k=1}^{n} z_k \quad \text{with} \quad z_k = \log \frac{q(x_k)}{p(x_k)}
\]
(4)
as \( b := \log B \leq Z_n \leq \log A = a \), where \( A = (\eta_0/\eta_1)(1 - \epsilon_1/\epsilon_0) \), \( B = (\eta_1/\eta_0)(1 - \epsilon_0/\epsilon_1) \).

It is convenient to interpret \( Z_n \) as a random walk (see Fig. 1) that at every instance performs a step of
FIG. 1. Random walk describing the likelihood function $Z_n$ under $H_0$ (green) and $H_1$ (orange). When the value of $Z_n$ crosses $b \sim \log \epsilon_0$ ($a \sim \log 1/\epsilon_1$) we decide in favor of $H_0$ ($H_1$). $N$ indicates the corresponding stopping time.

The mean position of the walker at step $n$ is given by $\langle Z_n \rangle = \sum_{k=1}^{n} \langle z_k \rangle_1 = n(z)_1 = nD(q||p) > 0$, where $D(q||p) = \sum_x q(x) \log(q(x)/p(x))$ is the relative entropy; while for $H_0$, $\langle Z_n \rangle = -nD(p||q) < 0$. That is, under $H_1$ the walker has a drift toward the positive axis, while under $H_0$ it drifts toward the negative axis. We define as the stopping time the first instance in which the walker steps out of the region $(a,b)$, i.e., $N := \inf \{ n : Z_n \notin (a,b) \}$, and note that it is a stochastic variable that only depends on the current as well as the past measurement record. The stochastic variable $Z = Z_N$ is the position of the walker at $N$. The mean value of this position can be related to the mean number of steps by Wald’s identity [24],

$$\langle Z \rangle = \sum_{k=1}^{n} z_k = \langle z \rangle_1 \langle N \rangle_1 = D(q||p) \langle N \rangle_1 \tag{5}$$

under hypothesis $H_1$, and likewise $\langle Z \rangle = -D(p||q) \langle N \rangle_0$. In order to estimate $\langle N \rangle$ from (5) we need to provide a good estimate for $\langle Z \rangle$. For this purpose let us first define $X_1$ as the set of strings $x$ such that $b < x_j < a$ for all $j < n$ and $X_0$ as the set of strings $x$ such that $b < x_j < a$ for all $j < n$ and $Z_n \leq b$. Then, the following relations hold:

$$\alpha = P_0(\langle Z \rangle \geq a) = \sum_{x \in X_1} p(x) \leq \sum_{x \in X_1} \frac{q(x)}{A} = \frac{1 - \beta}{A},$$

$$\beta = P_1(\langle Z \rangle \leq b) = \sum_{x \in X_0} q(x) \leq \sum_{x \in X_0} p(x)B = (1 - \alpha)B, \tag{6}$$

where in the first (second) inequality we used that $q(x)/p(x) \geq A$ for strings in $X_1$ ($q(x)/p(x) \leq B$ for strings in $X_2$), and in the last equality we have used that $\lim_{n \to \infty} P[Z_n \in (b,a)] = 0$ [23], i.e., the walker eventually stops. The above equations are an instance of so-called Wald’s likelihood ratio identity [25]. We note that the above inequalities can be taken to be approximate equalities if we assume that the process ends close to the prescribed boundary, i.e., there is no overshooting. In particular, this will be valid in our asymptotically small error settings where the boundaries are far relative to the (finite) step size $z_k$. This allows us to establish a one-to-one correspondence between the thresholds $A$, $B$ and the type I and II errors: $\alpha \approx 1 - B/A - B = e_1(\eta_1 - \epsilon_0)/(1 - \epsilon_0 - \epsilon_1)\eta_0$, and $\beta \approx B(A - 1)/A - B = e_0(\eta_0 - \epsilon_1)/(1 - \epsilon_0 - \epsilon_1)\eta_1$ [26,27]. Neglecting the overshooting also allows us to consider $Z$ as a stochastic variable that takes two values $Z \in \{a,b\}$. Under hypothesis $H_0$, $a$ occurs with probability $P_0(Z = a) = a$ and $b$ with $P_0(Z = b) = 1 - a$; while under hypothesis $H_1$, $a$ and $b$ occur with probabilities $P_1(Z = a) = 1 - \beta$ and $P_1(Z = b) = \beta$.

$$\langle Z \rangle = aa + b(1 - a) \text{ and } \langle Z \rangle = a(1 - \beta) + b\beta. \tag{7}$$

Making use of (5) one can now write a closed expression for $\langle N \rangle_0$ and $\langle N \rangle_1$ in terms of $e_0$, $e_1$ and the priors. A remarkable property of the SPRT with error probabilities $\alpha$ and $\beta$ is that it minimizes both $e_1$, $e_0$ and the priors. A remarkable property of the SPRT with error probabilities $\alpha$ and $\beta$ is that it minimizes both $\epsilon_1$, $\epsilon_0$ and the priors. A remarkable property of the SPRT with error probabilities $\alpha$ and $\beta$ is that it minimizes both $\epsilon_1$, $\epsilon_0$ and the priors.

$$\langle N \rangle_0 \sim -\frac{\log \epsilon_0}{D(p||q)} \text{ and } \langle N \rangle_1 \sim -\frac{\log \epsilon_0}{D(q||p)} \tag{8}$$

The same expressions hold at leading order in the asymmetric scenario when the type I and II errors are vanishingly small, replacing $\log \epsilon_1$ and $\log \epsilon_0$ by $\log \alpha$ and $\log \beta$, respectively—and in the symmetric scenario replacing both quantities by $\log \bar{\epsilon}$. If one of the error thresholds, say $\alpha$, is kept finite while the second is made vanishingly small $\beta \ll 1$, $\langle N \rangle_1$ remains finite, while the other conditional mean scales as $\langle N \rangle_0 \sim -((1 - \alpha) \log \beta/D(p||q))$.

In the Supplemental Material [29] we apply these results to the discrimination of qubit states using projective measurements and give closed expressions for the optimal Bayesian mean number of copies $\langle N \rangle = \eta_0 \langle N \rangle_0 + \eta_1 \langle N \rangle_1$.

Figure 2 also shows that in the symmetric setting these restricted sequential strategies already require on average between 25%-50% fewer resources than the best deterministic strategy that uses a fixed number of copies $N_{00} \sim -\log \bar{\epsilon} / \bar{C}_2$ [12,21], and requires nontrivial collective measurements [35].
Ultimate quantum limit.—Quantum mechanics allows for much more sophisticated strategies. For a start, performing a nonprojective generalized measurement already gives important advantages (see below). One can also adapt the measurements depending on the previous measurement outcomes and, importantly, measurements may be weak so that each new measurement acts on a fresh copy but also on the preceding, already measured, copies. Without loss of generality we can assume that at every step $k$ we perform a measurement with three outcomes $x_k \in \{0, 1, 2\}$: the first two must fulfill conditions (2) and (3) and trigger the corresponding guess ($H_0$ or $H_1$, respectively), while the third outcome signals to continue measuring having an additional fresh copy available. The measurement at step $k$ is characterized by a quantum operator $\mathcal{M}_k = \{\mathcal{M}_k^0, \mathcal{M}_k^1, \mathcal{M}_k^2\}$, and the sequential strategy is given by a sequence of instruments $\mathcal{M} = \{\mathcal{M}_k\}_{k=1}^\infty$. With this, given hypothesis $\nu = \{0, 1\}$, the probability of getting outcome $x_k$ at step $k$ can be written as

$$P_\nu(x_k) := \text{tr}[\mathcal{M}_k^0 \circ \mathcal{M}_k^0 \cdots \circ \mathcal{M}_k^0 (\rho^\otimes k)] = \text{tr}(E^k_\nu \rho^\otimes k),$$

where we have used that in order to arrive to step $k$ a “continue” outcome must be triggered in all previous steps, and in the last equality we have defined the effective POVM $E^k = \{E^k_i\}_{i=0}^4$. Making use of the indicator function $\mathbb{1}_{\nu \leq N}$, the mean number of steps under hypothesis $\nu$ can be computed as

$$\langle N \rangle_\nu := \sum_{k=1}^N \mathbb{1}_{\nu \leq N} = \sum_{k=1}^\infty \mathbb{1}_{\nu \leq N} = \sum_{n=0}^\infty \mathbb{1}_{\nu \leq N} = \sum_{n=0}^\infty T^\nu_n,$$

where $T^\nu_n = P_\nu(n < N)$ is the probability that the sequence does not stop at step $n$, which from (9) is given by $T^\nu_n = P_\nu(x_n = 2)$. Optimizing $\langle N \rangle_\nu$ over all quantum sequential strategies $\mathcal{M}$ is daunting, as all terms $T^\nu_n$ are strongly interrelated through the intricate structure of $E^n$. However, a lower bound to each $T^\nu_n$ can be found by relaxing such a structure and only imposing minimal requirements on the effective POVM; namely the error bounds (6), positivity and completeness:

$$\text{min } \text{tr}(E^\nu_i \rho^\otimes n) \text{ such that } E^\nu_i \geq 0, \quad \sum_{i=0}^2 E^\nu_i = 1, \quad \text{and } \text{tr}[E^\nu_1 (\sigma^\otimes n - A \rho^\otimes n)] \geq 0, \quad \text{tr}[E^\nu_0 (\rho^\otimes n - B^{-1} \sigma^\otimes n)] \geq 0.$$  

This semidefinite program, which can be considered a two-sided version of the quantum Neyman-Pearson test [20], is an interesting open problem in its own right. Our focus, however, is the asymptotic regime of small error bounds. In these asymptotic scenarios we are able to show, exploiting some recent strong converse results in hypothesis testing [33,36], that for all $n < n^* = \log \epsilon_0 / 2 (1 - A^{-1} / D(\rho||\sigma))$, $T^\nu_n \geq 1 - O(\epsilon^n)$ for some $\epsilon \in (0, 1)$ [29], which leads to the desired bound:

$$\langle N \rangle_0 \geq \sum_{n=0}^{n^*} T^\nu_n \geq \frac{-\log \epsilon_0 (1 - A^{-1})}{D(\rho||\sigma)} + O(1).$$

An analogous bound holds for $\langle N \rangle_1$. The bounds for asymmetric (symmetric) scenarios (see [29]) take the same form, replacing $\log \epsilon_0$ by $\log \beta$ (log $\epsilon$) and $A^{-1}$ by $\alpha^{-1}$ (log $\beta$). In the asymmetric scenario where $\epsilon_1 < \alpha$ is kept finite, it also holds that $\langle N \rangle_1 = O(1)$ and $\langle N \rangle_0$ is given by the appropriate version of (12).

Attainability and upper bounds.—Consider a sequential strategy that involves a fixed, collective measurement $K = \{K_i\}$, acting on consecutive blocks of $\ell'$ copies, yielding two possible distributions $f'_{\ell'} q_{\ell'}$. Using the classical SPRT we get that

$$\langle N \rangle_0 = \ell' \text{inf}_K \langle M \rangle_0 \sim \ell' \text{inf}_K \frac{-\log \epsilon_0}{D(p_{\ell'}||q_{\ell'})} \sim \frac{-\log \epsilon_0}{D(\rho||\sigma)},$$

where $M$ is the number of blocks used at the stopping time. In the last relation of (13) we have used the fact that we are in the asymptotic setting where $\epsilon_0 \ll 1$ and therefore we can take arbitrarily long block lengths $\ell' \gg 1$. We also exploit the following property of the measured relative entropy [14,37]: $\text{sup}_p D(q_{\ell'}||p_{\ell'}) \sim \ell' D(\sigma||p)$.

 Notice, however, that for arbitrary states $\rho$ and $\sigma$ block sampling can attain either $\langle N \rangle_0$ or $\langle N \rangle_1$, but it is unknown whether one can attain in general both bounds simultaneously, i.e., whether a measurement achieving the
supremum of \( \lim_{\ell \to \infty} 1/\ell D(q_\ell^k || p_\ell^k) \) can also attain the supremum of \( \ell \lim_{\ell \to \infty} 1/\ell D(p_\ell^k || q_\ell^k) \). For instance, if we wish to optimize the Bayesian mean number of copies \( \langle N \rangle \), we can use block sampling to attain

\[
\langle N \rangle_{\text{block}} \sim \lim_{\ell \to \infty} \inf_k \left( \frac{-\ell \eta_0 \log \epsilon_0 - \ell \eta_1 \log \epsilon_1}{D(p_\ell^k || q_\ell^k)} \right).
\]

(14)

However, this strategy might be suboptimal and hence it only provides an upper bound to the optimal Bayesian mean \( \langle N \rangle \leq \langle N \rangle_{\text{block}} \). This notwithstanding, there are at least two cases when this upper bound coincides with the lower bound provided by (12): when \( \rho \) and \( \sigma \) commute, and when the two states do not have common support. If, say, \( \text{supp} \sigma \cap \ker \rho \neq 0 \), one can use block sampling to attain (12) for \( \langle N \rangle_0 \) and always detect \( \rho \) with a finite number of copies—note that since \( D(\sigma || \rho) = \infty \), the lower bound \( \langle N \rangle_1 = O(1) \) is also attained.

We can also give achievable lower bounds for a worst-case type figure of merit \( N_{\text{wc}} \) := \max \{ \langle N \rangle_0, \langle N \rangle_1 \}. \) If, say, \( \langle N \rangle_0 > \langle N \rangle_1 \), then in [29] we give some instances of qubit pairs where a specific block-sampling strategy [37] saturates (12) for \( \langle N \rangle_0 \), while at the same time \( \lim_{\ell \to \infty} 1/\ell D(q_\ell^k || p_\ell^k) \geq D(\rho || \sigma) \), and hence (12) provides the ultimate attainable limit for \( N_{\text{wc}} \). In Fig. 2 we compare \( N_{\text{wc}} \) with \( N_{\text{Ch}} \) for several pairs of states, highlighting the achievable cases, and show a consistent advantage of sequential protocols over deterministic ones [38].

Finally, we note that, in an asymmetric scenario where \( \langle N \rangle_1 \) is finite and the value of \( \langle N \rangle_0 \) achieves the lower bound (12), sequential protocols provide a strict advantage over Stein’s limit for deterministic protocols by a factor \((1 - \alpha)\).

The curious case of pure states.—If the two states are pure, the behavior of \( \langle N \rangle \) changes drastically: it is possible to reach a decision with guaranteed zero error using a finite average number of copies. To see this, consider again Eq. (10). Under a zero-error condition, the minimal (unrestricted) \( T_0^\alpha \) is achieved by a global unambiguous three-outcome POVM [39–41] on \( n \) copies, which identifies the true state with zero error when the first or the second outcome occurs—at the expense of having a third, inconclusive outcome. For a single-copy POVM over pure states, the probabilities \( c_\nu \) of the inconclusive outcome under \( H_\nu \) are subject to the tradeoff relation \( c_0 c_1 \geq \text{tr} \rho \sigma \) [6], where equality can always be attained by suitable POVM that maximizes the probability of a successful identification. Likewise, for a global measurement on \( n \) copies we have \( T_0^\alpha T_1^\alpha \geq (\text{tr} \rho \sigma)^\alpha \). Now, it is evident that a sequence of \( n \) locally optimal unambiguous POVMs applied on every copy, for which \( T_0^\alpha = \nu_0 \), also fulfills the global optimality condition. Hence, we have

\[
\langle N \rangle_\nu \geq \sum_{n=0}^{\infty} T_\nu^n = \sum_{n=0}^{\infty} c_\nu^n = \frac{1}{1 - c_\nu} = : \langle N \rangle_{\text{local}}^\nu.
\]

This shows that, for pure states, it suffices to perform local unambiguous measurements to attain the optimal (finite) average number of copies with zero error under hypothesis \( H_\nu \). Note that because of the tradeoff \( c_0 c_1 \geq \text{tr} \rho \sigma \) one cannot attain the minimal values of \( \langle N \rangle_{\text{local}}^\nu \) and \( \langle N \rangle_{\text{local}}^1 \) for general states \( \rho, \sigma \), simultaneously. For instance, one can reach the minimal value \( c_0 = \text{tr} (\rho \sigma) \) for one hypothesis, but then having a maximal value \( c_1 = 1 \) for the second; or choose the optimal symmetric setting, \( c_0 = c_1 = \sqrt{\text{tr} \rho \sigma} \), that achieves the minimum value of both the worst-case \( N_{\text{wc}} \) and the Bayesian mean \( \langle N \rangle \) with equal priors (see [29]). This is in stark contrast with the behavior found in [10], where all strategies considered were based on two-outcome projective measurements, for which the average number of copies scaled as \( \langle N \rangle \propto -\log \epsilon \).

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[11] By $f(\epsilon) \sim g(\epsilon)$ we mean asymptotic equivalence $\lim_{\epsilon \to 0} f(\epsilon)/g(\epsilon) = 1$.
[29] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.126.180502 where we provide the proof of the lower bound for the mean number of copies under each hypothesis, we apply our general results to the case of qubit states, we compute the exact optimal mean number of copies (worst-case and Bayesian) required for the perfect discrimination of pure states, and which includes [26,27,30–34].
[38] Note that the comparison with $N_{Ch}$ is unfavorable to sequential strategies. Substituting $\epsilon_0$ and $\epsilon_1$ by $\bar{\epsilon}$ in Eq. (12) implies that each type of error is independently constrained, whereas $N_{Ch}$ refers to a deterministic (symmetric) protocol where the mean error is $\bar{\epsilon}$ and thus to a weaker version of the problem. In spite of this, the sequential scenario displays a significant advantage.