Upper bounds on error probabilities and asymptotic error exponents in quantum multiple state discrimination

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Abstract

We consider the multiple hypothesis testing problem for symmetric quantum state discrimination between $r$ given states $σ_1, \ldots, σ_r$. By splitting up the overall test into multiple binary tests in various ways we obtain a number of upper bounds on the optimal error probability in terms of the binary error probabilities. These upper bounds allow us to deduce various bounds on the asymptotic error rate, for which it has been hypothesised that it is given by the multi-hypothesis quantum Chernoff bound (or Chernoff divergence) $C(σ_1, \ldots, σ_r)$, as recently introduced by Nussbaum and Szkoła in analogy with Salikhov’s classical multi-hypothesis Chernoff bound. This quantity is defined as the minimum of the pairwise binary Chernoff divergences $\min_{j<k} C(σ_j, σ_k)$. It was known already that the optimal asymptotic rate must lie between $C/3$ and $C$, and that for certain classes of sets of states the bound is actually achieved. It was known to be achieved, in particular, when the state pair that is closest together in Chernoff divergence is more than 6 times closer than the next closest pair. Our results improve on this in two ways. Firstly, we show that the optimal asymptotic rate must lie between $C/2$ and $C$. Secondly, we show that the Chernoff bound is already achieved when the closest state pair is more than 2 times closer than the next closest pair. We also show that the Chernoff bound is achieved when at least $r - 2$ of the states are pure, improving on a previous result by Nussbaum and Szkoła. Finally, we indicate a number of potential pathways along which a proof (or disproof) may eventually be found that the multi-hypothesis quantum Chernoff bound is always achieved.

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1 Introduction

Consider a communication scenario where a sender (say, Alice) wishes to send one of \( r \) possible messages to a receiver (Bob). To achieve this goal, Alice has a device at her disposal that can prepare \( r \) quantum states \( \rho_1, \ldots, \rho_r \), one for each possible message, which she can then send through a quantum channel \( \Phi \), resulting in the states \( \sigma_i = \Phi(\rho_i) \) at Bob’s side. Bob then has to make a quantum measurement to identify which message was sent. His measurement is described by a set of positive semidefinite operators \( E_1, \ldots, E_r \), one corresponding to each possible message, that form an incomplete POVM (positive operator-valued measure), i.e., they satisfy \( E_1 + \ldots + E_r \leq I \). The operator \( E_0 := I - (E_1 + \ldots + E_r) \) corresponds to not making a decision on the identity of the received state. The probability of making an erroneous decision when the message \( i \) was sent is then given by \( \text{Tr} \sigma_i (I - E_i) \). If we also assume that Alice sends each message \( i \) with a certain probability \( p_i \) then Bob’s task is to minimise the Bayesian error probability

\[
P_e (\{E_1, \ldots, E_r\}) := \sum_{i=1}^{r} p_i \text{Tr} \sigma_i (I - E_i),
\]

We assume here that a complete mathematical description of the output states and the prior probabilities are known to Bob.

In the classical case, i.e., when the \( \sigma_i \) are probability distributions on some finite set, the optimal success probability is known to be reached by the so-called maximum likelihood measurement, and the optimal success probability is given by \( \text{Tr} \max_{i} \{p_i \sigma_i\} \). In the general quantum case, no explicit expression is known for the optimal error probability, or for the measurement achieving it, unless \( r = 2 \), in which case these optimal quantities are easy to find [19, 24]. Moreover, the maximum of a set of positive semidefinite operators on a Hilbert space is not well-defined, and hence a straightforward generalization of the classical results is not possible. In Section 2.3, we define a generalized notion of maximum for a set of self-adjoint operators, which we call the least upper bound (LUB). This notion reduces to the usual maximum in the classical case, and the optimal success probability can be expressed as \( \text{Tr} \text{LUB}(p_1 \sigma_1, \ldots, p_r \sigma_r) \) giving a direct generalization of the classical expression. We explore further properties of the least upper bound, and its dual, the greatest lower bound (GLB), in Appendix C.

An obvious way to reduce the error probability is to send the same message multiple times. For \( n \) repetitions, the optimal error probability is given by

\[
P_e^* (A_1, \ldots, A_r, n) := \min \left\{ \sum_{i=1}^{r} \text{Tr} A_{i,n} (I - E_i) : \{E_1, \ldots, E_r\} \text{ POVM} \right\},
\]

where \( A_{i,n} := p_i \sigma_i^{\otimes n} \). These error probabilities are known to decay exponentially fast in the number of repetitions in various special cases, and hence we are interested in the exponents

\[
P_e (\tilde{A}_1, \ldots, \tilde{A}_r) := \liminf_{n \to \infty} \frac{1}{n} \log P_e^* (A_1, \ldots, A_r, n) \quad \text{and} \quad \bar{P}_e (\tilde{A}_1, \ldots, \tilde{A}_r) := \limsup_{n \to \infty} \frac{1}{n} \log P_e^* (A_1, \ldots, A_r, n),
\]
where $\vec{A}_i := \{A_{i,n}\}_{n \in \mathbb{N}}$.

In the case of two possible messages, the theorem for the quantum Chernoff bound [4, 5, 38] states that

$$P_e(\vec{A}_1, \vec{A}_2) = p_e(\vec{A}_1, \vec{A}_2) = \min_{0 \leq t \leq 1} \log \text{Tr} \sigma_1^t \sigma_2^{1-t} =: -C(\sigma_1, \sigma_2),$$

(4)

where $C(\sigma_1, \sigma_2)$ is the Chernoff divergence of $\sigma_1$ and $\sigma_2$. According to a long-standing conjecture,

$$P_e(\vec{A}_1, ..., \vec{A}_r) = p_e(\vec{A}_1, ..., \vec{A}_r) = -\min_{(i,j): i \neq j} C(\sigma_i, \sigma_j),$$

(5)

i.e., the multi-hypothesis exponent is equal to the worst-case pairwise exponent. Following [39], we call $C(\sigma_1, ..., \sigma_r) := \min_{(i,j): i \neq j} C(\sigma_i, \sigma_j)$ the multi-Chernoff bound. The above conjecture is known to be true for commuting states [15] and when the states $\sigma_i$ have pairwise disjoint supports [11]. A special case of the latter is when all the states $\sigma_i$ are pure [10].

Our aim here is to establish decoupling bounds on the single-shot error probabilities, which in turn yield bounds on the exponents (2)–(3) in terms of the corresponding pairwise exponents. It has been shown in [15] that, for any choice of $\sigma_1, ..., \sigma_r$, and priors $p_1, ..., p_r$, we have

$$P^*_e(A_1, ..., A_r) \geq \frac{1}{r-1} \sum_{(i,j): i < j} P^*_e(A_i, A_j),$$

(6)

where $A_i := p_i \sigma_i$. Taking then $r$ sequences of states $\sigma_{i,n}, n \in \mathbb{N}$, and $\vec{A}_i := \{p_i \sigma_{i,n}\}_{n \in \mathbb{N}}$, we get

$$P_e(\vec{A}_1, ..., \vec{A}_r) \geq \max_{(i,j): i \neq j} P_e(\vec{A}_i, \vec{A}_j).$$

(7)

Note that this is true for arbitrary sequences of states $\{\sigma_{i,n}\}_{n \in \mathbb{N}}$, with no special assumption on the correlations. In the i.i.d. case the RHS of (7) is exactly $-\min_{(i,j): i \neq j} C(\sigma_i, \sigma_j)$, solving half of the conjecture in [4].

Hence, here we will focus on upper decoupling bounds. The main results of the paper are the following converses to (6) and (7):

**Single-shot upper decoupling bounds:** For $A_i := p_i \sigma_i, i = 1, ..., r$,

$$P^*_e(A_1, ..., A_r) \leq \sum_{(i,j): i \neq j} \sqrt{P^*_e(A_i, A_j)}.$$

(8)

It has been shown in Appendix A of [15] that if $A_i$ is rank one for all $i$ then the square root can be removed from the pairwise errors in the above formula; more precisely, the following inequality holds:

$$P^*_e(A_1, ..., A_r) \leq \frac{1}{\min_i p_i} \sum_{(i,j): i \neq j} P^*_e(A_i, A_j).$$

(9)

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We give several alternative proofs of this fact along the way of proving \( \mathbf{(8)} \).

These single-shot bounds immediately yield the following

**Asymptotic upper decoupling bounds:** For \( \vec{A}_i := \{ p_i \sigma_{i,n} \}_{n \in \mathbb{N}}, i = 1, \ldots, r \),

\[
\overline{p}_e \left( \vec{A}_1, \ldots, \vec{A}_r \right) \leq \frac{1}{2} \max_{(i,j): i \neq j} \overline{p}_e (\vec{A}_i, \vec{A}_j).
\]  

(10)

If \( A_{i,n} \) is rank one for all \( i \) and \( n \) then

\[
\overline{p}_e \left( \vec{A}_1, \ldots, \vec{A}_r \right) \leq \max_{(i,j): i \neq j} \overline{p}_e (\vec{A}_i, \vec{A}_j).
\]

(11)

Note that again (10) and (11) are true for arbitrary sequences of states, and in the i.i.d. case we have \( \max_{(i,j): i \neq j} \overline{p}_e (\vec{A}_i, \vec{A}_j) = - \min_{(i,j): i \neq j} C(\sigma_i, \sigma_j) = -C(\sigma_1, \ldots, \sigma_r) \). In particular, by (7) and (11) we recover the result of \( \mathbf{(10)} \), i.e., that \( \mathbf{(5)} \) is true for pure states. In fact, we prove more: namely that (11) holds whenever \( A_{i,n} \) is pure for at least \( r - 2 \) of the hypotheses. This latter improvement is based on the recent techniques of \( \mathbf{[42]} \).

For mixed states, Theorem 3 in \( \mathbf{[41]} \) gives that \( \overline{p}_e \left( \vec{A}_1, \ldots, \vec{A}_r \right) \) is between \( -C(\sigma_1, \ldots, \sigma_r) \) and \( -\frac{1}{3} C(\sigma_1, \ldots, \sigma_r) \). Our result (10) improves the factor \( 1/3 \) in this upper bound to \( 1/2 \), which is the best general result known so far.

Analytical proofs for various special cases and extensive numerical simulations suggest that the square root in \( \mathbf{(8)} \) - and, consequently, the factor \( \frac{1}{2} \) in (10) - can be removed. Along the way of proving \( \mathbf{(8)} \)–\( \mathbf{(11)} \), we explore several possible approaches to prove this expected stronger result.

The structure of the paper is as follows. In Section 2 we summarize the necessary preliminaries and review the known results that are relevant for the rest of the paper. In particular, we give a short proof of (6), and summarize the known results for the binary case. We also introduce the notion of the least upper bound for self-adjoint operators, and show how the optimal error probability can be expressed in this formalism.

In Section 3 we study a special binary problem where one of the hypotheses is i.i.d., while the other is averaged i.i.d., i.e., a convex mixture of i.i.d. states. In the setting of Stein’s lemma (with the averaged state being the null-hypothesis) the corresponding error exponent is known to be the worst-case pairwise exponent \( \mathbf{(7)} \) (see also \( \mathbf{[35]} \) for a simple proof), and we conjecture the same to hold in the symmetric setting of the Chernoff bound. Similarly to the case of multiple hypotheses, it is easy to show that the worst-case pairwise exponent cannot be exceeded (optimality). In Theorem 3.3 we show upper decoupling bounds on the error probability, analogous to (8) and (9), which in the asymptotics yield that \( 1/2 \) times the conjectured exponent is achievable. Moreover, when the i.i.d. state is pure then the \( 1/2 \) can be removed and we get both optimality and achievability. This problem is interesting in its own right, as it is arguably the simplest non-i.i.d. state discrimination problem and yet its solution is not yet known, despite considerable effort towards establishing non-i.i.d. analogs of the binary Chernoff bound theorem \( \mathbf{[22, 20, 21, 30, 31]} \). Moreover, it turns out that the solution of this binary non-i.i.d. problem would provide the solution of the general multi-state discrimination problem.
Indeed, in Section 4 we show that the exponential decay rate of the optimal error probability (1) is the same as that of another quantity, which we call the 
\textit{dichotomic error}. This is defined as the sum of the error probabilities of the binary state discrimination problems where we only want to decide whether hypothesis \(i\) is true or not, for every \(i = 1, \ldots, r\). In the i.i.d. case these binary problems are exactly of the type discussed in Section 3 and we can directly apply the bounds obtained there to get upper decoupling bounds on both the 
single-shot and the asymptotic error probabilities, which give the bounds (8)–(11).

In Section 5 we follow Nussbaum’s approach [42] to obtain a different kind of splitting of the optimal error probability. When applied recursively and combined with the bounds of Section 3, this approach provides an alternative way to obtain bounds of the type (8)–(9), which again yield (10)–(11) in the asymptotics.

Yet another approach is presented in Section 6, based on Tyson’s error bounds [50], which bound the optimal error probability by constant multiples of an explicitly computable quantity \(\Gamma^*\). Since the constants are universal, they don’t contribute to the exponential decay rate, and hence the optimal error probability and \(\Gamma^*\) have the same rate. We give single-shot upper bounds on \(\Gamma^*\) in terms of the pairwise Chernoff divergences. These in turn yield bounds of the form (10)–(11), with the pairwise exponents on the right replaced by the pairwise normalized Chernoff divergences. This approach is somewhat different from the other two in spirit, where the upper bounds themselves are in terms of error probabilities, and thus are somewhat stronger, but they yield the same asymptotic results in the i.i.d. case and, more generally, in any correlated scenario where the pairwise exponents are given by the regularized Chernoff divergences.

In Section 7 we show how the various single-shot bounds of the above described approaches translate into bounds for the error rates, i.e., we derive (10)–(11) for the most general scenario, and its variants for more specific settings, where the pairwise rates can be replaced by pairwise Chernoff divergences. We also give an improvement of Nussbaum’s asymptotic result [42], which says that (5) is true if there is a pair of states \((\sigma_i, \sigma_j)\) such that \(C(\sigma_i, \sigma_j) < \frac{1}{6}C(\sigma_k, \sigma_l)\) for any \((k, l) \neq (i, j)\). Here we show that the constant \(\frac{1}{6}\) can be replaced with \(\frac{1}{2}\).

Supplementary material is provided in a number of Appendices. In Appendix A, we show how our approaches work in the classical case, thus providing various alternative proofs for (5) in the classical case. In Appendix B we review the pure state case; we show an elementary way to derive the Chernoff bound theorem (4) for two pure states, and show how the combination of the single-shot bounds of [18] and [45] yield (5) for an arbitrary number of pure states. In Appendix C we explore some properties of the least upper bound and the greatest lower bound for self-adjoint operators, which further extend their analogy to the classical notions of minimum and maximum. In Appendix D we review the dual formulation of the optimal error probability due to [54]. For readers’ convenience, we provide a proof for Tyson’s error bounds in Appendix E.
2 Preliminaries

2.1 Notations

For a finite-dimensional Hilbert space $\mathcal{H}$, let $\mathcal{B}(\mathcal{H})$ denote the set of linear operators on $\mathcal{H}$, let $\mathcal{B}(\mathcal{H})_{\text{sa}}$ denote the set of self-adjoint (Hermitian) operators, $\mathcal{B}(\mathcal{H})_+$ the set of positive semidefinite (PSD) operators, and $\mathcal{S}(\mathcal{H})$ the set of density operators (states), i.e., the set of PSD operators with unit trace.

For $X$ a Hermitian operator, let $|X|$ denote its absolute value (or modulus), $|X| := \sqrt{X^2}$. The Jordan decomposition of $X$ into its positive and negative parts is given by $X = X_+ - X_-$, with $X_{\pm} = (|X| \pm X)/2$, and $|X| = X_+ + X_-$. It is clear that $X_+X_- = 0$. As the eigenvalues of $|X|$ are the absolute values of the eigenvalues of $X$, the eigenvalues of $X_+$ ($X_-$) are the positive (negative) eigenvalues of $X$. We denote the projections onto the support of $X_+$ and $X_-$ by $\{X > 0\}$ and $\{X < 0\}$, respectively.

We will follow the convention that powers of a positive semidefinite (PSD) operator are only taken on its support. That is, if $a_1, \ldots, a_r$ are the strictly positive eigenvalues of $A \geq 0$, with corresponding spectral projections $P_1, \ldots, P_r$, then $A^s := \sum_{i=1}^r a_i^s P_i$ for every $s \in \mathbb{R}$. In particular, $A^0$ denotes the projection onto the support of $A$.

By a POVM we will mean a set of PSD operators $E_1, \ldots, E_r$ such that $E_1 + \ldots + E_r \leq I$. On occasion we will also consider the underlying measurement operators $\{X_k\}_{k=1}^r$, which are sets of operators such that the products $X_k^\dagger X_k$ constitute a POVM.

We will normally not indicate the base of the logarithm, but we will always assume that it is larger than 1, and hence log is a strictly increasing function. We will use the conventions $\log 0 := -\infty$ and $\log +\infty := +\infty$.

2.2 The problem setting

We will consider a generalized state discrimination problem, where the hypotheses are represented by arbitrary non-zero PSD operators (i.e., not necessarily states). We consider such a generalized setting partly to absorb the priors into the states to make the formalism simpler, and partly because the formalism supports it, and all our results can be formulated and proved in this more general setting. More importantly, however, we need to treat such generalized setups even if we restrict our original hypotheses to be states; see, e.g., Lemma 5.2.

More in detail, in the single-shot case our hypotheses are represented by non-zero PSD operators $A_1, \ldots, A_r$. Occasionally, we will use the notations

$$p_k := \text{Tr} A_k, \quad \sigma_k := A_k/p_k, \quad k = 1, \ldots, r.$$

If $p_1 + \ldots + p_r = 1$ then we say that $\{A_k\}$ forms a set of weighted states.

For any POVM $E_1, \ldots, E_r$, we define the corresponding success- and error probabilities as

$$P_s(\{E_i\}) := \sum_{i=1}^r \text{Tr} A_i E_i, \quad P_e(\{E_i\}) := \sum_{i=1}^r \text{Tr} A_i (I - E_i).$$
These can indeed be interpreted as probabilities in the case of weighted states, whereas in the general case they might take values above 1. Since it will always be obvious what the hypotheses are, we don’t indicate them in the above notations. The optimal values of these quantities over all possible choices of POVMs are the optimal success- and error probability

\[
P_s^*(A_1, \ldots, A_r) := \max \left\{ \sum_{i=1}^r \text{Tr} A_i E_i : \{E_1, \ldots, E_r\} \text{ POVM} \right\},
\]

\[
P_e^*(A_1, \ldots, A_r) := \min \left\{ \sum_{i=1}^r \text{Tr} A_i (I - E_i) : \{E_1, \ldots, E_r\} \text{ POVM} \right\}.
\]

We will use the shorthand notations \(P_s^*\) and \(P_e^*\) when it is clear what the hypotheses are. Note that

\[
P_s^*(A_1, \ldots, A_r) + P_e^*(A_1, \ldots, A_r) = \text{Tr} A_0, \quad \text{where} \quad A_0 := \sum_{i=1}^r A_i.
\]

Again, these can be interpreted as probabilities if \(1 = \text{Tr} A_0 = \sum_i p_i\), i.e., in the case of weighted states. Note that any POVM that is optimal for \(P_s^*\) is also optimal for \(P_e^*\) and vice versa. Moreover, there always exists an optimal POVM \(\{E_i\}_{i=1}^r\) such that \(E_1 + \ldots + E_r = I\).

In the asymptotic setting, our hypotheses are going to be represented by sequences of PSD operators, \(\vec{A}_i := \{A_{i,n}\}_{n \in \mathbb{N}}, i = 1, \ldots, r\), and we will be interested in the exponents \(p_e\) and \(\bar{p}_e\), defined in (2) and (3), respectively. We say that the \(i\)-th hypothesis is \(i.i.d\). (for the classical analogy of independent and identically distributed) if \(p_{i,n} = \text{Tr} A_{i,n}\) is independent of \(n\) (and hence we can define \(p_i := p_{i,n}, n \in \mathbb{N}\), and \(A_{i,n}/p_i = \sigma_i^{\otimes n}\) for every \(i\), where \(\sigma_i := \sigma_{i,1}\). We say that the asymptotic state discrimination problem is \(i.i.d\). if all the hypotheses are \(i.i.d\).

When passing from single-shot error bounds to asymptotic error bounds, we will use the following standard lemma without further notice.

**Lemma 2.1.** Let \(a_{i,n}, n \in \mathbb{N}, i = 1, \ldots, r\), be sequences of positive numbers. Then

\[
\max_{i} \liminf_{n \to \infty} \frac{1}{n} \log a_{i,n} \leq \liminf_{n \to \infty} \frac{1}{n} \log \sum_{i=1}^r a_{i,n} \leq \limsup_{n \to \infty} \frac{1}{n} \log \sum_{i=1}^r a_{i,n} \leq \max_{i} \limsup_{n \to \infty} \frac{1}{n} \log a_{i,n}.
\]

**Proof.** The first inequality is straightforward from \(a_{i,n} \leq \sum_i a_{i,n}, \forall i\), and the second inequality is obvious. To prove the last inequality, let \(M := \max_i \limsup_{n \to \infty} \frac{1}{n} \log a_{i,n}\). If \(M = +\infty\) then the assertion is trivial, and hence we assume that \(M < +\infty\). By the definition of the limsup, for every \(M' > M\), there exists an \(N_{M'}\) such that for all \(n \geq N_{M'}\), \(a_{i,n} < \exp(M')\), \(i = 1, \ldots, r\), and hence \(\frac{1}{n} \log \sum_{i=1}^r a_{i,n} < \frac{1}{n} \log r + M'\). Thus \(\limsup_{n \to \infty} \frac{1}{n} \log \sum_{i=1}^r a_{i,n} \leq M'\). Since this is true for all \(M' > M\), the assertion follows. \(\square\)

### 2.3 The generalized maximum likelihood error

In the classical state discrimination problem, where the hypotheses are represented by non-negative functions \(A_i : \mathcal{X} \to \mathbb{R}_+\) on some finite set \(\mathcal{X}\), the optimal success probability is known to be \(\sum_i \max\{A_1, \ldots, A_r\}\), and it is achieved by the maximum likelihood measurement (see
Appendix A for details). If we consider the $A_i$ as diagonal operators in some fixed basis, then $P^*_s$ can be rewritten as

$$P^*_s(A_1, \ldots, A_r) = \text{Tr} \max\{A_1, \ldots, A_r\}, \tag{13}$$

where $\max\{A_1, \ldots, A_r\}$ is the operator with $\max_i A_i(x)$ in its diagonals. Note that this is not a maximum in the usual sense of PSD ordering; indeed, it is well-known that the PSD ordering does not induce a lattice structure \cite{3}, so in general the set of upper bounds to $r$ given self-adjoint operators $A_1, \ldots, A_r$, which is defined as $A := \{Y : Y \succeq A_k, k = 1, \ldots, r\}$, has no minimal element, not even when the $A_k$ mutually commute; see, e.g. Example C.1 in Appendix C. However, there is a unique minimal element within $A$ in terms of the trace ordering. We can therefore define a least upper bound in this more restrictive sense as

$$\text{LUB}(A_1, \ldots, A_r) := \arg \min_Y \{\text{Tr} Y : Y \succeq A_k, k = 1, \ldots, r\}. \tag{14}$$

For the proof of uniqueness, see Appendix C. In a similar vein we can define the greatest lower bound (GLB) as

$$\text{GLB}(A_1, \ldots, A_r) := \arg \max_Y \{\text{Tr} Y : Y \preceq A_k, k = 1, \ldots, r\}. \tag{15}$$

Clearly, we have

$$\text{GLB}(A_1, \ldots, A_r) = -\text{LUB}(-A_1, \ldots, -A_r). \tag{16}$$

For further properties of the above notions, see Appendix C.

Note that the set of $k$-outcome POVMs forms a convex set, and the optimal success probability in (12) is given as the maximum of a linear functional over this convex set. It was shown in \cite{53} that the duality of convex optimisation yields

$$P^*_s(A_1, \ldots, A_r) = \min \{\text{Tr} Y : Y \succeq A_k, k = 1, \ldots, r\} \tag{17}$$

(see also \cite{27} for a different formulation of the same result). Using the definition of the LUB above, this can be rewritten as

$$P^*_s(A_1, \ldots, A_r) = \text{Tr} \text{LUB}(A_1, \ldots, A_r), \tag{18}$$

in complete analogy with the classical case \cite{13}. For readers’ convenience, we provide a detailed derivation of (17) in Appendix D.

For an ensemble of PSD operators $\{A_i\}_{i=1}^r$, we define the complementary operator of $A_i$ as the operator given by the sum of all other operators in the ensemble: $\overline{A}_i := \sum_{j \neq i} A_j = A_0 - A_i$ where $A_0 = \sum_i A_i$. The optimal error probability can be expressed in terms of the GLB of the complementary density operators:

$$P^*_e(A_1, \ldots, A_r) = \text{Tr} \text{GLB}(\overline{A}_1, \ldots, \overline{A}_r). \tag{19}$$

This is easy to show:

$$P^*_e = \min_{\{E_l\}} \sum_k \text{Tr} A_k \sum_{l \neq k} E_l = \min_{\{E_k\}} \sum_l \text{Tr} E_l \sum_{k \neq l} A_k = \min_{\{E_k\}} \sum_l \text{Tr} E_l \overline{A}_l = -\max_{\{E_k\}} \sum_l \text{Tr} E_l(-\overline{A}_l)
= \text{Tr} \text{GLB}(\overline{A}_1, \ldots, \overline{A}_r),$$
where we used that an optimal POVM can be chosen so that $E_1 + \ldots + E_r = I$. Note that this is in general different from $\text{Tr} \, \text{GLB}(A_1, \ldots, A_r)$, which is the minimal i.e. worst-case success probability $P_{s, \text{min}} = \min_{\{E_k\}} \sum_k \text{Tr} \, A_k E_k$.

In the binary case, i.e., when $r = 2$, we have

$$P^*_e(A, A_2) = \max \{ \text{Tr} \, A_1 I + \text{Tr} \, A_2 (I - E) : 0 \leq E \leq I \} = \text{Tr} \, A_2 + \max_{0 \leq E \leq I} \text{Tr} \,(A_1 - A_2)E$$

and the maximum is attained at $E = \{ A_1 - A_2 > 0 \}$; this is the so-called Holevo-Helström measurement [24, 19]. Consequently, we have

$$P^*_e(A_1, A_2) = \min \{ \text{Tr} \, A_1 (I - E) + \text{Tr} \, A_2 E : 0 \leq E \leq I \}$$

Comparing these with (18) and (19), and noting that in the binary case $\bar{A}_1 = A_2, \bar{A}_2 = A_1$, we obtain

$$\text{Tr} \, \text{LUB}(A_1, A_2) = \frac{1}{2} \text{Tr} \,(A_1 + A_2) + \frac{1}{2} \| A_1 - A_2 \|_1,$$

$$\text{Tr} \, \text{GLB}(A_1, A_2) = \frac{1}{2} \text{Tr} \,(A_1 + A_2) - \frac{1}{2} \| A_1 - A_2 \|_1.$$

For a more straightforward way to derive these identities, see Appendix C.

In the rest of the paper, we will use the notations $P^*_e(A, B)$, $\text{Tr} \, \text{GLB}(A, B)$ and $\frac{1}{2} \text{Tr}(A + B) - \frac{1}{2} \| A - B \|_1$ interchangeably for PSD operators $A, B$.

### 2.4 Chernoff bound for binary state discrimination

For PSD operators $A, B$ on the same Hilbert space, define

$$Q_s(A \| B) := \text{Tr} \, A^s B^{1-s}, \quad s \in \mathbb{R},$$

$$Q_{\text{min}}(A, B) := \min_{0 \leq s \leq 1} Q_s(A \| B),$$

$$C(A, B) := - \log Q_{\text{min}}(A, B).$$

The last quantity, $C(A, B)$ is the Chernoff divergence of $A$ and $B$. As it was shown in Theorem 1 in [4] (see also [5, 6]),

$$\frac{1}{2} \text{Tr}(A + B) - \frac{1}{2} \| A - B \|_1 \leq Q_s(A \| B), \quad s \in [0, 1]. \quad (22)$$

Consider now the generalized asymptotic binary hypothesis testing problem with hypotheses $\bar{A}_1, \bar{A}_2$. By [22], we have

$$P^*_e(A_1, n, A_2, n) = \frac{1}{2} \text{Tr}(A_1, n + A_2, n) - \frac{1}{2} \| A_1, n - A_2, n \|_1 \leq Q_s(A_1, n \| A_2, n) \quad (23)$$
for every $n \in \mathbb{N}$ and $s \in [0,1]$, and hence,

$$
\overline{e}(\vec{A}_1, \vec{A}_2) = \limsup_{n \to \infty} \frac{1}{n} \log P_e^*(A_{1,n}, A_{2,n}) \leq -C(\vec{A}_1, \vec{A}_2),
$$

(24)

where

$$
C(\vec{A}_1, \vec{A}_2) := -\limsup_{n \to \infty} \frac{1}{n} \log Q_{\min}(A_{1,n}, A_{2,n}) = \liminf_{n \to \infty} \frac{1}{n} C(A_{1,n}, A_{2,n})
$$

(25)

is the regularized Chernoff divergence.

In the i.i.d. case, i.e., when $A_{1,n} = p_1 \sigma_1^{\otimes n}$ and $A_{2,n} = p_2 \sigma_2^{\otimes n}$ for every $n \in \mathbb{N}$, we have $Q_s(A_{1,n}||A_{2,n}) = p_1^s p_2^{1-s} Q_s(\sigma_1||\sigma_2)^n \leq \max\{p_1, p_2\} Q_s(\sigma_1||\sigma_2)^n$, and (23) yields

$$
P_e^*(p_1 \sigma_1^{\otimes n}, p_2 \sigma_2^{\otimes n}) \leq \max\{p_1, p_2\} Q_{\min}(\sigma_1, \sigma_2)^n = \max\{p_1, p_2\} \exp(-nC(\sigma_1, \sigma_2))
$$

for every $n \in \mathbb{N}$. In particular,

$$
\limsup_{n \to \infty} \frac{1}{n} \log P_e^*(p_1 \sigma_1^{\otimes n}, p_2 \sigma_2^{\otimes n}) \leq -C(\sigma_1, \sigma_2).
$$

(Note that in this case $C(\vec{A}_1, \vec{A}_2) = C(\sigma_1, \sigma_2)$).

The above argument shows that the asymptotic Chernoff divergence (which is equal to the single-shot Chernoff divergence in the i.i.d. case) is an achievable error rate. Optimality means that no faster exponential decay of the optimal error is possible, i.e., that

$$
\overline{e}(\vec{A}_1, \vec{A}_2) = \liminf_{n \to \infty} \frac{1}{n} \log P_e^*(A_{1,n}, A_{2,n}) \geq -C(\vec{A}_1, \vec{A}_2).
$$

This was shown to be true in the i.i.d. case in [38]. Optimality for various correlated scenarios was obtained in [20 21 22 30 31]; the classes of states covered include Gibbs states of finite-range translation-invariant interactions on a spin chain, and thermal states of non-interacting bosonic and fermionic lattice systems.

### 2.5 Pairwise discrimination and lower decoupling bounds

Consider the generalized state discrimination problem with hypotheses $A_1, \ldots, A_r$. In this section we review a lower bound on the optimal error probability for discriminating between $r$ given states in terms of the optimal pairwise error probabilities, originally given in [45]. Let us thereto define the following quantities:

$$
P_{e,2}^* := P_{e,2}^*(A_1, \ldots, A_r) := \frac{1}{r-1} \sum_{k,l, k < l} P_e^*(A_k, A_l) = \frac{1}{r-1} \sum_{k,l, k < l} \text{Tr LUB}(A_k, A_l)
$$

$$
= \frac{1}{r-1} \sum_{k,l, k < l} \frac{1}{2} \left( \text{Tr}(A_k + A_l) + \|A_k - A_l\|_1 \right).
$$

(26)

and

$$
P_{e,2}^* := P_{e,2}^*(A_1, \ldots, A_r) := \frac{1}{r-1} \sum_{k,l, k < l} P_e^*(A_k, A_l) = \frac{1}{r-1} \sum_{k,l, k < l} \text{Tr GLB}(A_k, A_l)
$$

$$
= \frac{1}{r-1} \sum_{k,l, k < l} \frac{1}{2} \left( \text{Tr}(A_k + A_l) - \|A_k - A_l\|_1 \right).
$$

(27)
Note that

\[ P_{s,2}^*(A_1, \ldots, A_r) + P_{e,2}^*(A_1, \ldots, A_r) = \sum_i \text{Tr} A_i = P_{s}^*(A_1, \ldots, A_r) + P_{e}^*(A_1, \ldots, A_r), \]

explaining the choice \( 1/(r-1) \) for the normalization.

In the case of weighted states, i.e., when \( \text{Tr} A_k = 1 \), we can interpret these quantities as optimal success and error probabilities in a very special setting, whereby the receiver can make use of a particular kind of side information. We shall assume that this side information has been provided by an oracle. The oracle knows the correct value of each symbol sent out by the source, but in the best of oracular traditions, does not quite reveal this information to the receiver. Rather, the oracle provides the receiver with a choice of two symbols, one of which is the correct one and the other is chosen from the remaining values at random, with uniform probability \( 1/(r-1) \). It is intuitively plausible that the receiver should only try to discriminate between the two options provided.

The optimal success probability in this setup can easily be calculated. From the receiver’s viewpoint, the probability that the values of the symbols provided by the oracle are \( k \) and \( l \) (with \( k \neq l \)) is \( p_k (r-1)^{-1} + (r-1)^{-1} p_l \), and the conditional probability that \( k \) is the correct one is \( p_k / (p_k + p_l) \). Hence, the receiver’s optimal success probability will be

\[ P_{s,2}^* = \sum_{k,l: k < l} \frac{p_k + p_l}{r-1} \left( 1 + \frac{\| p_k \sigma_k - p_l \sigma_l \|_1}{p_k + p_l} \right), \]

which simplifies to (26).

It is intuitively clear that this oracle-assisted success probability should never be smaller than the unassisted optimal success probability, whereby the receiver needs to discriminate between all \( r \) possible symbols. The following Theorem, first given in [45], shows that this is indeed the case. Here we give a detailed and slightly simplified proof for readers’ convenience.

**Theorem 2.2.** For any \( A_1, \ldots, A_r \in B(H)_+ \),

\[ P_{s}^*(A_1, \ldots, A_r) \leq P_{s,2}^*(A_1, \ldots, A_r), \quad \text{and} \quad P_{e}^*(A_1, \ldots, A_r) \geq P_{e,2}^*(A_1, \ldots, A_r). \]

**Proof.** First notice that

\[ \sum_{(k,l): k \neq l} (\text{Tr} A_k E_k + \text{Tr} A_l E_l) = 2(r-1) \sum_{k=1}^r \text{Tr} A_k E_k \]

and

\[ \text{Tr} A_k E_k + \text{Tr} A_l E_l \leq \text{Tr} A_k E_k + \text{Tr} A_l (I - E_k) + \text{Tr} A_l (I - E_k) = \text{Tr} A_l + \text{Tr} (A_k - A_l) E_k \leq \text{Tr} A_l + \text{Tr} (A_k - A_l)_+ \leq \frac{1}{2} (\text{Tr} (A_k + A_l) + \| A_k - A_l \|_1). \]
Hence,
\[
\sum_{k=1}^{r} \text{Tr} A_k E_k = \frac{1}{2(r-1)} \sum_{(k,l) : k \neq l} \left( \text{Tr} A_k E_k + \text{Tr} A_l E_l \right) \\
\leq \frac{1}{4(r-1)} \sum_{(k,l) : k \neq l} \left( \text{Tr}(A_k + A_l) + \| A_k - A_l \|_1 \right),
\]
which yields the first assertion. The second assertion, \( P_e^* \geq P_{e,2}^* \), is now obvious.

We conjecture that for any choice of signal states and source probabilities the oracle-assisted error probability can not be arbitrarily smaller than the unassisted one. In particular, we believe:

**Conjecture 2.3.** There exists a constant \( c \), only depending on the number of hypotheses \( r \), such that for all \( A_1, \ldots, A_r \geq 0 \)
\[
P_e^*(A_1, \ldots, A_r) \leq cP_{e,2}^*(A_1, \ldots, A_r).
\]

We have ample numerical evidence for this conjecture, and this evidence suggests that \( c = 4(r-1) \). Several approaches towards a proof will be provided in the next sections.

### 3 Binary state discrimination: i.i.d. vs. averaged i.i.d

Consider the binary state discrimination problem where one of the hypotheses is i.i.d., i.e., for \( n \) copies it is represented by \( \rho^\otimes n \) for some state \( \rho \), while the other hypothesis is averaged i.i.d., i.e., for \( n \) copies it is of the form \( \sum_{i=1}^{r} q_i \sigma_i^\otimes n \) for some states \( \sigma_1, \ldots, \sigma_r \), and a probability distribution \( q_1, \ldots, q_r \). This represents a situation where we have a further uncertainty about the identity of the true state when the second hypothesis is true. Alternatively, this can be considered as a state discrimination problem with \( r + 1 \) i.i.d. hypotheses, where we only want to know whether one of the hypotheses is true or not. If the state \( \rho \) has prior probability \( p > 0 \) then the optimal error probability for \( n \) copies is
\[
P_e^* \left( p\rho^\otimes n, (1-p)\sum_{i=1}^{r} q_i \sigma_i^\otimes n \right) = 1 - \left\| p\rho^\otimes n - (1-p)\sum_{i=1}^{r} q_i \sigma_i^\otimes n \right\|_1.
\]
Convexity of the trace-norm implies that
\[
P_e^* \left( p\rho^\otimes n, (1-p)\sum_{i=1}^{r} q_i \sigma_i^\otimes n \right) \geq \sum_{i=1}^{r} q_i \left( 1 - \left\| p\rho^\otimes n - (1-p)\sigma_i^\otimes n \right\|_1 \right)
\]
\[
= \sum_{i=1}^{r} q_i P_e^* \left( p\rho^\otimes n, (1-p)\sigma_i^\otimes n \right),
\]
and hence,
\[
P_e \left( \{ p\rho^\otimes n \}_n, \left\{ (1-p)\sum_{i=1}^{r} q_i \sigma_i^\otimes n \right\}_n \right) \geq \max_{1 \leq i \leq r} \left[ p_e \left( \{ p\rho^\otimes n \}_n, \left\{ (1-p)\sigma_i^\otimes n \right\}_n \right) \right] = - \min_i C(\rho, \sigma_i).
\]
Based on analytical proofs for various special cases as well extensive numerical search, we conjecture that the following converse decoupling inequality is also true:
Theorem 3.3.

which are the main results of this section: These will follow from the following single-shot decoupling bounds,

If \( A \) is pure then we have

\[
\rho = \frac{A}{\|A\|}
\]

is rank one then we also have

\[
\rho = \frac{1}{\|\rho\|} \rho
\]

This conjecture would immediately yield

Conjecture 3.1.

\[
\mathbb{P}_e \left( \{ pp \otimes^n \} \right) \leq \max_{1 \leq i \leq r} \mathbb{P}_e \left( \{ pp \otimes^n \} \right) = - \min_i C(\rho, \sigma_i).
\]

Below we will prove Conjecture 3.1 in the case where \( \rho \) is a pure state, and prove a weaker version in the general case. These will follow from the following single-shot decoupling bounds, which are the main results of this section:

Theorem 3.3. Let \( A, B_1, \ldots, B_r \in \mathcal{B}(\mathcal{H})_+ \). Then

\[
P_e^* \left( A, \sum_j B_j \right) \leq \sum_j \frac{\sqrt{\text{Tr}(A + B_j)}}{\sqrt{\text{Tr}(A, B_j)}}
\]

If \( A \) is rank one then we also have

\[
P_e^* \left( A, \sum_j B_j \right) \leq \left\{ \begin{array}{l}
\left( \sum_j \sqrt{1 + \frac{\text{Tr} B_j}{\text{Tr} A}} \right) \left( \frac{1}{\text{Tr} A} \right) \sum_j P_e^* (A, B_j), \\
\left( \sum_j \frac{\sqrt{\text{Tr} B_j}}{\sqrt{\text{Tr} A}} \right) \sum_j P_e^* (\frac{A}{\text{Tr} A}, B_j).
\end{array} \right.
\]

Theorem 3.3 immediately yields the following:

Corollary 3.4. For every \( n \in \mathbb{N} \), let \( A_n, B_{1,n}, \ldots, B_{r,n} \in \mathcal{B}(\mathcal{H}_n)_+ \), where \( \mathcal{H}_n \) is some finite-dimensional Hilbert space. If \( \lim_{n \to \infty} \text{Tr}(A_n + \sum_j B_{j,n}) < +\infty \) then

\[
\mathbb{P}_e \left( \frac{\bar{A}}{\|\bar{A}\|}, \sum_j \frac{\bar{B}_j}{\|\bar{B}_j\|} \right) \leq \frac{1}{2} \max_{1 \leq j \leq r} \mathbb{P}_e \left( \frac{\bar{A}}{\|\bar{A}\|}, \frac{\bar{B}_j}{\|\bar{B}_j\|} \right).
\]

If \( A_n \) is rank one for every large enough \( n \) and \( \lim_{n \to \infty} \text{Tr}(A_n + \sum_j B_{j,n})/\text{Tr} A_n < +\infty \) then

\[
\mathbb{P}_e \left( \frac{\bar{A}}{\|\bar{A}\|}, \sum_j \frac{\bar{B}_j}{\|\bar{B}_j\|} \right) \leq \max_{1 \leq j \leq r} \mathbb{P}_e \left( \frac{\bar{A}}{\|\bar{A}\|}, \frac{\bar{B}_j}{\|\bar{B}_j\|} \right).
\]

Applying Corollary 3.4 to the problem of i.i.d. vs. averaged state discrimination, we finally get the following

Theorem 3.5. In the i.i.d. case described at the beginning of the section,

\[
- \min_i C(\rho, \sigma_i) \leq \liminf_{n \to \infty} \frac{1}{n} \log P_e^* \left( pp \otimes^n, (1 - p) \sum_i q_i \sigma_i^{\otimes^n} \right)
\]

\[
\leq \limsup_{n \to \infty} \frac{1}{n} \log P_e^* \left( pp \otimes^n, (1 - p) \sum_i q_i \sigma_i^{\otimes^n} \right) \leq - \frac{1}{2} \min_i C(\rho, \sigma_i).
\]

If \( \rho \) is pure then we have

\[
\lim_{n \to \infty} \frac{1}{n} \log P_e^* \left( pp \otimes^n, (1 - p) \sum_i q_i \sigma_i^{\otimes^n} \right) = - \min_i C(\rho, \sigma_i).
\]
Remark 3.6. Note that the argument in (28) is not specific to the i.i.d. case, i.e., if we have two hypotheses, one represented by $A$ and the other by $\sum_{j=1}^{r} q_j B_j$, where $q_1, \ldots, q_r$ is a probability distribution, then
\[ P_e^*(A, \sum_{j} q_j B_j) \geq \sum_{j} q_j P_e^*(A, B_j). \quad (31) \]

It is clear from (20) that $P_e^*(A, q_j B_j) \leq P_e^*(A, B_j)$, and hence (31) combined with (29) yields
\[ \sum_{j} q_j P_e^*(A, B_j) \leq \sum_{j} \sqrt{\text{Tr}(A + B_j) \sqrt{P_e^*(A, B_j)}}. \]

and if $A$ is pure then the upper bound can be replaced by either of the bounds in (30). In the asymptotic setting, under the same conditions as in Corollary 3.4, we get
\[ \max_{j} p_e(\vec{A}, \vec{B}_j) \leq p_e(\vec{A}, \sum_{j} q_j \vec{B}_j) \leq \frac{1}{2} \max_{j} p_e(\vec{A}, \vec{B}_j), \]
and the factor $\frac{1}{2}$ can be removed in the last term when all the $A_n$ are pure.

To prove Theorem 3.3, we will need some properties of the fidelity, which we review below. Most of these properties are well-known, except maybe Lemma 3.10.

For positive semidefinite operators $A, B \in \mathcal{B}(\mathcal{H})_+$, their fidelity is defined as
\[ F(A, B) := \text{Tr}(A^{1/2} BA^{1/2})^{1/2}. \]

The following bounds between the fidelity and the trace-norm were shown in [14] for states, and extended to weighted states in [6], where also the sharpness of the inequalities (32) and (33) have been shown. The proof for the general case can be obtained exactly the same way as in the above cases.

**Lemma 3.7.** For any $A, B \in \mathcal{B}(\mathcal{H})_+$,
\[
\text{Tr GLB}(A, B) = \frac{1}{2} \text{Tr}(A + B) - \frac{1}{2} \| A - B \|_1 \\
\leq F(A, B) \\
\leq \sqrt{\frac{1}{4} (\text{Tr}(A + B))^2 - \frac{1}{4} \| A - B \|_1^2} \\
= \sqrt{\text{Tr LUB}(A, B) \text{Tr GLB}(A, B)} \\
\leq \sqrt{\text{Tr}(A + B) \text{Tr GLB}(A, B)}
\]

When $A$ is rank one, we also have the following inequality. This has been stated as an exercise in [37] for states; we provide a proof here for readers’ convenience.

**Lemma 3.8.** Let $A, B \in \mathcal{B}(\mathcal{H})_+$ and assume that $A$ has rank one. Then
\[
\text{Tr GLB}(A, B) = \frac{1}{2} \text{Tr}(A + B) - \frac{1}{2} \| A - B \|_1 \leq \frac{1}{\text{Tr} A} F(A, B)^2.
\]
Proof. The assumption that \( A \) is rank one yields that \( \text{Tr} A^2 = \text{Tr} A \) and \( F(A, B) = \sqrt{\text{Tr} AB} \). Let \( \tilde{A} := A / \text{Tr} A \). Using the representation (21), we get
\[
\frac{1}{2} \text{Tr}(A + B) - \frac{1}{2} \|A - B\|_1 = \min \{ A(I - E) + \text{Tr} BE : 0 \leq E \leq I \}
\leq \text{Tr} A(I - \tilde{A}) + \text{Tr} B\tilde{A} = \frac{1}{\text{Tr} A} \text{Tr} AB = \frac{1}{\text{Tr} A} F(A, B)^2. \quad \square
\]

Remark 3.9. Monotonicity of the fidelity yields that \( F(A, B) \leq (\text{Tr} A)^{1/2}(\text{Tr} B)^{1/2} \). If \( \text{Tr} B \leq \text{Tr} A \) then \( F(A, B) \leq \text{Tr} A \), or equivalently, \( \frac{1}{\text{Tr} A} F(A, B)^2 \leq F(A, B) \), and hence the upper bound in (34) is stronger than the bound in (32). This is the case, for instance, for states. In general, however, the two bounds are not comparable.

The function \( X \mapsto \text{Tr} \sqrt{X} \) is subadditive on PSD operators, i.e., if \( A, B \in \mathcal{B}(\mathcal{H})_+ \) then \( \text{Tr} \sqrt{A + B} \leq \text{Tr} \sqrt{A} + \text{Tr} \sqrt{B} \). Indeed,
\[
\text{Tr} \sqrt{A + B} - \text{Tr} \sqrt{A} = \int_0^1 \frac{d}{dt} \text{Tr} \sqrt{A + tB} dt = \int_0^1 \text{Tr} B \frac{1}{2}(A + tB)^{-1/2} dt \leq \text{Tr} \sqrt{B} \int_0^1 \frac{t^{-1/2}}{2} dt = \text{Tr} \sqrt{B},
\]
where we used the identity \( \frac{d}{dt} \text{Tr} f(A + tB) = \text{Tr} B f'(A + tB), \) and that the function \( x \mapsto x^{-1/2} \) is operator monotone decreasing. As a consequence, we have the subadditivity of the fidelity:

Lemma 3.10. Let \( A, B_1, \ldots, B_r \in \mathcal{B}(\mathcal{H})_+ \). Then
\[
F \left( A, \sum_i B_i \right) \leq \sum_i F(A, B_i). \quad (35)
\]

After this preparation, we are ready to prove Theorem 3.3.

Proof of Theorem 3.3:
\[
P_e^* \left( A, \sum_j B_j \right) = \text{Tr} \text{GLB} \left( A, \sum_j B_j \right) \leq F \left( A, \sum_j B_j \right) \leq \sum_j F(A, B_j)
\leq \sum_j \sqrt{\text{Tr}(A + B_j)} \sqrt{\text{Tr} \text{GLB}(A, B_j)} = \sum_j \sqrt{\text{Tr}(A + B_j)} \sqrt{P_e^*(A, B_j)},
\]
where we used Lemma 3.7 in the first inequality, the second inequality is due to Lemma 3.10 and the third inequality is again due to Lemma 3.7. This proves (24).

Assume now that \( A \) is rank one. Then the first inequality in the above chain can be replaced with \( P_e^* \left( A, \sum_j B_j \right) \leq \frac{1}{\text{Tr} A} F \left( A, \sum_j B_j \right)^2 \) due to Lemma 3.8. Continuing as above, we get
\[
P_e^* \left( A, \sum_j B_j \right) = \text{Tr} \text{GLB} \left( A, \sum_j B_j \right) \leq \frac{1}{\text{Tr} A} F \left( A, \sum_j B_j \right)^2 \leq \frac{1}{\text{Tr} A} \left( \sum_j F(A, B_j)^2 \right) \leq \frac{1}{\text{Tr} A} \left( \sum_j \sqrt{\text{Tr}(A + B_j)} \sqrt{P_e^*(A, B_j)} \right)^2
\leq \frac{1}{\text{Tr} A} \left( \sum_j \text{Tr}(A + B_j) \right) \sum_j P_e^*(A, B_j),
\]
15
where in the last line we used the Cauchy-Schwarz inequality. This proves the first bound in (30). Instead of the third inequality above, we may continue as

\[
\frac{1}{\text{Tr} A} \left( \sum_j F(A, B_j) \right)^2 = \left( \sum_j \sqrt{\text{Tr} B_j} F\left( \frac{A}{\text{Tr} A}, \frac{B_j}{\text{Tr} B_j} \right) \right)^2 \\
\leq \left( \sum_j \sqrt{\text{Tr} B_j} \sqrt{P_{e}^{*} \left( \frac{A}{\text{Tr} A}, \frac{B_j}{\text{Tr} B_j} \right)} \right)^2 \\
\leq \left( \sum_j \text{Tr} B_j \right) \sum_j P_{e}^{*} \left( \frac{A}{\text{Tr} A}, \frac{B_j}{\text{Tr} B_j} \right),
\]

where again in the last step we used the Cauchy-Schwarz inequality. This proves the second bound in (30).

We close this section with some discussion of the above results.

Let \( \rho, \sigma_1, \ldots, \sigma_r \) be states and \( q_1, \ldots, q_r \) be a probability distribution. Then we have

\[
\sum_i q_i F(\rho, \sigma_i) \leq F\left( \rho, \sum_i q_i \sigma_i \right) \leq \sum_i \sqrt{q_i} F(\rho, \sigma_i),
\]

where the first inequality is a special case of the joint concavity of the fidelity \[37\] Theorem 9.7, and the second inequality is due to Lemma \[3.10\] with the choice \( A = \rho \) and \( B_i = q_i \sigma_i \). Hence, Lemma \[3.10\] yields a complement to the concavity inequality \( \sum_i q_i F(\rho, \sigma_i) \leq F(\rho, \sum_i q_i \sigma_i) \). It is natural to ask whether the joint concavity inequality \( \sum_i q_i F(\rho_i, \sigma_i) \leq F(\sum_i q_i \rho_i, \sum_i q_i \sigma_i) \) can be complemented in the same way, but it is easy to see that the answer is no. Indeed, let \( \rho_1 = \sigma_2 = |x\rangle \langle x| \) and \( \rho_2 = \sigma_1 = |y\rangle \langle y| \) with \( x, y \) being orthogonal unit vectors in \( \mathbb{C}^2 \), and let \( q_1 = q_2 = 1/2 \). Then \( \sum_i q_i \rho_i = \frac{1}{2} I = \sum_i q_i \sigma_i \), and hence \( F(\sum_i q_i \rho_i, \sum_i q_i \sigma_i) = 1 \), while \( F(\rho_1, \sigma_1) = F(\rho_2, \sigma_2) = 0 \), and hence no inequality of the form \( F(\sum_i \rho_i, \sum_i \sigma_i) \leq c \sum_i F(\rho_i, \sigma_i) \) can hold with some \( c > 0 \).

One can ask the same questions about the quantity \( \text{Tr} \operatorname{GLB}(\ldots) \), which has very similar properties to the fidelity. Indeed, convexity of the trace-norm yields joint concavity of this quantity, i.e., \( \text{Tr} \operatorname{GLB}(\sum_i q_i \rho_i, \sum_i q_i \sigma_i) = 1 - \| \sum_i q_i \rho_i - \sum_i q_i \sigma_i \|_1 \geq \sum_i q_i (1 - \| \rho_i - \sigma_i \|_1) = \sum_i q_i \text{Tr} \operatorname{GLB}(\rho_i, \sigma_i) \), and the same example as above shows that this inequality cannot be complemented in general. On the other hand, one may hope that the weaker concavity inequality, where the first argument is a fixed \( \rho \), can be complemented the same way as for the fidelity, i.e., that there exists a constant \( c > 0 \), depending at most on \( r \), such that

\[
\text{Tr} \operatorname{GLB} \left( \rho, \sum_i q_i \sigma_i \right) = 1 - \| \rho - \sum_i q_i \sigma_i \|_1 \leq c \sum_i (1 - \| \rho - \sigma_i \|_1) = c \sum_i q_i \text{Tr} \operatorname{GLB}(\rho, \sigma_i).
\]

Alternatively, one could ask whether an analogy of the subadditivity inequality \[35\] holds for \( \text{Tr} \operatorname{GLB}(\ldots) \), i.e., if there exists a \( c > 0 \), depending at most on \( r \), such that

\[
\text{Tr} \operatorname{GLB} \left( A, \sum_j B_j \right) \leq c \sum_j \text{Tr} \operatorname{GLB}(A, B_j) \tag{36}
\]

for any PSD \( A, B_1, \ldots, B_r \). This would give an improvement over Theorem 3.3 and prove Conjecture 3.1.
It turns out that no such \( e \) exists. Counterexamples are as follows: for \( r = 2 \), take 
\[ A = \epsilon |\psi_1\rangle \langle \psi_1|, \quad B_1 = |\psi_2\rangle \langle \psi_2| \quad \text{and} \quad B_2 = |\psi_3\rangle \langle \psi_3| \]
with \( \epsilon \) small and \( \psi_2 \) and \( \psi_3 \) very close and almost orthogonal to \( \psi_1 \). For example, consider
\[ \psi_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \psi_2 = \begin{pmatrix} \sin \alpha \\ \cos \alpha \end{pmatrix}, \quad \psi_3 = \begin{pmatrix} -\sin \alpha \\ \cos \alpha \end{pmatrix}, \]
with \( \sin^2 \alpha = \epsilon/2 \). Then \( B_1 + B_2 = \text{Diag}(\epsilon, 2-\epsilon) \) and 
\[ \text{Tr GLB}(A, B_1 + B_2) = \frac{1}{2}(\epsilon + 2 - |2-\epsilon|) = \epsilon. \]
However, one can check that 
\[ \text{Tr GLB}(A, B_1) = \text{Tr GLB}(A, B_2) \approx \epsilon^2/2 \]
for very small \( \epsilon \). Thus, the LHS of (36) is linear in \( \epsilon \), whereas its RHS is quadratic, meaning that the RHS can be arbitrarily smaller than the LHS.

One might get the impression that this failure is due to the fact that \( A_1 \) has very small trace. Thus one could try to amend inequality (36) by dividing the RHS by that trace (making both sides linear in \( \epsilon \)):
\[ \text{Tr GLB} \left( A, \sum_j B_j \right) \leq \frac{1}{\text{Tr} A} \sum_j \text{Tr GLB}(A, B_j). \] (37)
This is a sensible amendment as it resonates with the appearance of the factor \( \frac{1}{\text{Tr} A} \) in (54) in our treatment of the pure state case, and furthermore, initial numerical simulations seemed to bolster the claim. However, this inequality is false too. We can use the direct sum trick based on Lemma 3.8 and replace \( A \) by \( A \oplus (1 - \text{Tr} A)|x\rangle \langle x| \) and \( B_j \) by \( B_j \oplus 0 \) in the counterexample of the previous paragraph, where \( x \) is a unit vector in some auxiliary Hilbert space. This does not change the Tr GLB terms but changes Tr A to 1, thereby eliminating its supposedly compensating effect. Thus inequality (37) is violated to arbitrarily high extent.

The problems presented by the above example could be eliminated if we allowed the cross-term \( \text{Tr GLB}(B_1, B_2) \) to appear (with some positive constant) on the RHS of (36), since the term \( \text{Tr GLB}(B_1, B_2) \) is close to 1 and swamps the distinction between \( \epsilon \) and \( \epsilon^2 \). Although such a bound is too weak for proving Conjecture 2.3, it would be just the right tool to prove Conjecture 2.3 as we will see in the next section.

4 Dichotomic discrimination

Consider the generalized state discrimination problem with hypotheses \( A_1, \ldots, A_r \). In this section we show an intermediate step towards proving Conjecture 2.3 in the form of a partial decoupling bound. Namely, we prove that the multiple state discrimination error is upper bounded by the dichotomic error, which is the sum of the error probabilities of discriminating one \( A_i \) from the rest of the hypotheses. Using then the bounds obtained in Section 3, we get full decoupling bounds.

Define the complementary operators as \( \bar{A}_i := \sum_{j \neq i} A_j = A_0 - A_i \), where \( A_0 := \sum_i A_i \). If we only want to decide whether the true hypothesis is \( A_i \) or not, i.e., we want to discriminate between \( A_i \) and \( \bar{A}_i \), then the corresponding optimal error is given by
\[ P_{e,\text{dich},i} := P_e^*(A_i, \bar{A}_i) = \text{Tr GLB}(A_i, \bar{A}_i) = \frac{1}{2}(\text{Tr} A_0 - \|A_i - \bar{A}_i\|_1). \] (38)
We will call this a *dichotomic discrimination*, and $P_{e,dich,i}^*$ the $i$-th optimal *dichotomic error*. Let us define $P_{e,dich}^*$ as the sum of the $r$ optimal dichotomic errors corresponding to each of the $A_i$:

$$P_{e,dich}(A_1, \ldots, A_r) := P_{e,dich}^* := \sum_{i=1}^r P_{e,dich,i}^*. \quad (39)$$

We first give a number of useful expressions for $P_{e,dich}^*$. Since $\text{Tr}(A_i - \bar{A}_i) = \text{Tr}(2A_i - A_0)$ we have $||A_i - \bar{A}_i||_1 = 2 \text{Tr}(2A_i - A_0)_+ + \text{Tr} A_0 - 2 \text{Tr} A_i$. Then

$$P_{e,dich}^* = 1/2 \sum_{i=1}^r (\text{Tr} A_0 - ||A_i - \bar{A}_i||_1)$$

$$= 1/2 \sum_{i=1}^r 2 \text{Tr} A_i - 2 \text{Tr}(2A_i - A_0)_+$$

$$= \text{Tr} A_0 - \sum_{i=1}^r \text{Tr}(2A_i - A_0)_+$$

$$= \text{Tr} A_0 - \sum_{i=1}^r \text{Tr}(A_i - \bar{A}_i)_+.$$  

The last two expressions show that the quantity $P_{e,dich}^*$ is a number between 0 and $\text{Tr} A_0$.

We now show that the optimal discrimination error $P_{e}^*$ between the $r$ states is well-approximated by $P_{e,dich}^*$. In particular, the bounds below, together with the fact that $P_{e,dich}^*$ is a number between 0 and $\text{Tr} A_0$, show that there exists a POVM $\{E_k\}_k$ for which $P_e^* \{E_k\} = P_{e,dich}^*$. Therefore, we can rightly call $P_{e,dich}^*$ the *dichotomic error*.

**Theorem 4.1.**

$$\frac{1}{2} P_{e,dich}^* \leq P_{e}^* \leq P_{e,dich}^*.$$  

**Proof.** Let us first prove the lower bound. Let $E_i$ be the optimal POVM element in the full $r$-state discrimination. Clearly, then, $E_i$ will in general be suboptimal in the dichotomic discrimination between $A_i$ and $\bar{A}_i$:

$$\text{Tr}(2A_i - A_0)_+ \geq \text{Tr}(2A_i - A_0)_{E_i} = 2 \text{Tr} A_i E_i - \text{Tr} A_0 E_i.$$  

Summing over $i$ yields

$$\sum_{i=1}^r \text{Tr}(2A_i - A_0)_+ \geq 2 \sum_{i=1}^r \text{Tr} A_i E_i - \text{Tr} A_0 \sum_{i=1}^r E_i = 2 \sum_{i=1}^r \text{Tr} A_i E_i - 1 = 2P_{s}^* - 1.$$  

This shows that

$$P_{e,dich}^* \leq \text{Tr} A_0 - (2P_{s}^* - \text{Tr} A_0) = 2P_{e}^*.$$  

Validity of the upper bound in the classical case is a simple consequence of the fact that in a list of positive numbers only the largest one can be bigger then half their sum. Hence, for diagonal states

$$\sum_{i}(2A_i - A_0)_+ = \text{LUB} \{((2A_i - A_0)_+)\} = 2 \text{LUB} \{\{A_i\}\} - A_0 \leq \frac{r \text{LUB}(\{A_i\}) - A_0}{r - 1}.$$
Taking the trace then yields
\[ 1 - P^*_{\text{e,dich}} = \sum_i \text{Tr}(2A_i - A_0)_+ \leq \frac{r \text{Tr LUB}\{A_i\} - \text{Tr} A_0}{r - 1} = \frac{r P^* - \text{Tr} A_0}{r - 1} = \text{Tr} A_0 - \frac{r}{r - 1} P^*_{\text{e}}, \]
which is slightly stronger than what we needed to prove.

To show that this is true in general, we will use Lemma 4.2 proven below. The trace of the positive part \( X_+ \) of a hermitian operator \( X \) can be expressed as \( \text{Tr} XP \) with \( P \) the projector on the support of \( X_+ \). In particular, if \( P_i \) is the projector on the support of \( (A_i - \bar{A}_i)_+ \), we have
\[ r \sum_i \text{Tr}(A_i - \bar{A}_i)_+ = \sum_i \text{Tr}(A_i - \bar{A}_i)P_i. \]
Defining \( P_0 := \sum_i P_i \), the summation on the right-hand side can be rewritten in the following way:
\[ \sum_i \text{Tr}(A_i - \bar{A}_i)P_i = \sum_i \text{Tr}(2A_i - A_0)P_i = 2 \sum_i \text{Tr} A_i P_i - \text{Tr} A_0 P_0 = \sum_i \text{Tr}(2P_i - P_0)A_i. \]
Now, because the \( A_i \) are PSD, \( \text{Tr}(2P_i - P_0)A_i \leq \text{Tr}(2P_i - P_0)_+ A_i \) so that
\[ \sum_i \text{Tr}(A_i - \bar{A}_i)P_i \leq \sum_i \text{Tr}(2P_i - P_0)_+ A_i. \]
By Lemma 4.2 the set of operators \( \{(2P_i - P_0)_+\} \) forms an (incomplete) POVM, so that the right-hand side is bounded above by the optimal success probability \( P^*_e \). Hence
\[ P^*_{\text{e,dich}} = \text{Tr} A_0 - \sum_i \text{Tr}(A_i - \bar{A}_i)P_i \geq P^*_e. \]

As it was pointed out in [43, Lemma 5], the map \( f : X \mapsto X^*X \) is operator convex on \( \mathcal{B}(\mathcal{H}) \). Indeed, For any \( X_1, X_2 \in \mathcal{B}(\mathcal{H}) \) and any \( t \in [0, 1] \), we have
\[ tf(X_1) + (1 - t)f(X_2) - f(tX_1 + (1 - t)X_2) = t(1 - t)(X_1 - X_2)^*(X_1 - X_2) \geq 0. \]
In particular, for \( X_1, \ldots, X_r \in \mathcal{B}(\mathcal{H}) \), we have \( (\sum_i X_i)^* (\sum_i X_i) \leq r \sum_i X_i^* X_i \), and operator monotony of the square root yields
\[ \left| \sum_i X_i \right| \leq \sqrt{r} \left( \sum_i |X_i|^2 \right)^{1/2}. \tag{40} \]
We will use this in the proof of the following Lemma:

**Lemma 4.2.** Let \( \{P_i\}_{i=1}^r \) be a set of \( r \) projectors. Define \( P_0 = \sum_{i=1}^r P_i \). Then
\[ 0 \leq \sum_i (2P_i - P_0)_+ \leq I, \]
i.e. the set of operators \( \{(2P_i - P_0)_+\} \) forms an (incomplete) POVM.
Proof. Let \( X_i := |2P_i - P_0| \), with \( P_i \) and \( P_0 \) as defined in the statement of the lemma. By (40),
\[
\sum_i |2P_i - P_0| \leq \sqrt{r} \left( \sum_i (2P_i - P_0)^2 \right)^{1/2}.
\]

Considering the facts that the \( P_i \) are projectors, i.e. \( P_i^2 = P_i \), and that \( P_0 \) is equal to their sum, the expression \( \sum_i (2P_i - P_0)^2 \) simplifies to
\[
\sum_i (2P_i - P_0)^2 = \sum_i (4P_i^2 + P_0^2 - 2P_iP_0 - 2P_0P_i) = 4P_0 + rP_0^2 - 4P_0^2 = 4P_0 + (r - 4)P_0^2.
\]

Now note the following:
\[
r(4P_0 + (r - 4)P_0^2) \leq r(4P_0 + (r - 4)P_0^2) + 4(I - P_0)^2
\]
\[
= 4rP_0 + (r^2 - 4r)P_0^2 + 4I - 8P_0 + 4P_0^2
\]
\[
= 4I + 4(r - 2)P_0 + (r - 2)^2 P_0^2
\]
\[
= (2I + (r - 2)P_0)^2.
\]

Thus, we get
\[
\sum_i |2P_i - P_0| \leq 2I + (r - 2)P_0.
\]

To rewrite this in terms of the positive parts, we use the relation \( |X| = 2X_+ - X \). This gives
\[
\sum_i |2P_i - P_0| = 2 \sum_i (2P_i - P_0)_+ - \sum_i (2P_i - P_0) = 2 \sum_i (2P_i - P_0)_+ - (2 - r)P_0.
\]

Hence, we finally obtain
\[
\sum_i (2P_i - P_0)_+ = \frac{1}{2} \left( \sum_i |2P_i - P_0| + (2 - r)P_0 \right) \leq I,
\]
as we set out to prove.

Next, we compare the optimal dichotomic discrimination error \( P^*_{e,dich} \) to the optimal pairwise discrimination error \( P^*_{e,2} \). It is easy to show that the pairwise error does not exceed one half of the dichotomic error, and we conjecture that it can not be less than the dichotomic error up to another constant factor (depending only on the number of hypotheses). We can prove this conjecture for pure states, whereas for mixed states we are able to prove a weaker inequality.

Our first result is:

**Theorem 4.3.** For all \( A_1, \ldots, A_r \in \mathcal{B}(\mathcal{H})_+ \),
\[
P^*_{e,2} \leq \frac{1}{2} P^*_{e,dich}.
\]
Proof.

\[ P_{e,2}^* = \frac{1}{r-1} \sum_{k,l: k < l} \text{Tr GLB}(A_k, A_l) \]

\[ = \frac{1}{2(r-1)} \sum_{k,l: k \neq l} \text{Tr GLB}(A_k, A_l) \]

\[ = \frac{1}{2} \sum_k \frac{1}{r-1} \sum_{l:l \neq k} \text{Tr GLB}(A_k, A_l) \]

\[ \leq \frac{1}{2} \sum_k \frac{1}{r-1} \sum_{l:l \neq k} \text{Tr GLB}(A_k, \overline{A_k}) \]

\[ = \frac{1}{2} \sum_k \text{Tr GLB}(A_k, \overline{A_k}) \]

\[ = \frac{1}{2} P_{e,dich}^*. \]

The inequality used here is the monotonicity of the GLB together with the fact that \( A_l \leq \overline{A_k} \) for \( l \neq k \), since \( A_l \) is one of the terms in \( \overline{A_k} \).

\[ \square \]

Remark 4.4. Note that Theorem 4.3 combined with the lower bound of Theorem 4.1 yields an alternative proof for Theorem 2.2.

Based on extensive numerical simulations we have been led to believe that the inequality in Theorem 4.3 can be reversed in the following sense:

Conjecture 4.5. There exists a constant \( c \), at most depending on the number of hypotheses \( r \), such that for all \( A_1, \ldots, A_r \in B(\mathcal{H})_+ \),

\[ P_{e,dich}^* \leq c P_{e,2}^*. \]

Explicitly,

\[ P_{e,dich}^* = \sum_{i=1}^r \text{Tr GLB}(A_i, \overline{A_i}) \leq c(r) \frac{1}{r-1} \sum_{(i,j): i \neq j} \text{Tr GLB}(A_i, A_j) \]

\[ = \tilde{c}(r) \sum_{(i,j): i \neq j} P_e^*(A_i, A_j). \] (41)

Numerical simulations suggest that \( c(r) = 4(r-1) \) is best possible. Clearly, validity of this conjecture would prove validity of Conjecture 2.3.

We can prove the following weaker versions of Conjectures 4.5 and 2.3:

Theorem 4.6. Let \( A_1, \ldots, A_r \in B(\mathcal{H})_+ \). Then

\[ P_e^*(A_1, \ldots, A_r) \leq P_{e,dich}^*(A_1, \ldots, A_r) \leq \sqrt{\text{Tr} A_0} \sum_{(i,j): i \neq j} \sqrt{P_e^*(A_i, A_j)}. \]
If $A_i$ is rank one for all $i$ then

$$P_e^*(A_1,\ldots,A_r) \leq P_{e,dich}^*(A_1,\ldots,A_r) \leq \frac{\text{Tr} A_0}{\min_i \text{Tr} A_i} \sum_{i,j:i\neq j} P_e^*(A_i,A_j). \quad (42)$$

**Proof.** The inequality $P_e^*(A_1,\ldots,A_r) \leq P_{e,dich}^*(A_1,\ldots,A_r)$ is due to Theorem 4.1, and the rest is immediate from the definition of $P_{e,dich}^*$ and Theorem 3.3.

**Remark 4.7.** Note that using the second line in (30), we get the bound

$$P_{e,dich}^*(A_1,\ldots,A_r) \leq (\text{Tr} A_0) \sum_{i,j:i\neq j} P_e^* \left( \frac{A_i}{\text{Tr} A_i}, \frac{A_j}{\text{Tr} A_j} \right)$$

instead of (42).

We have seen in the previous section that no bound of the form $\text{Tr} \text{GLB}(A_1,A_1) \leq c \sum_{l=2}^r \text{Tr} \text{GLB}(A_1,A_l)$ may hold in general, but amending the RHS with cross terms, i.e., error probabilities between $A_k,A_l, k,l \neq 1$ may yield a valid upper bound. Although such a bound would not have been useful for the purposes of Section 3, it would be sufficient for Conjecture 4.5 and numerical simulations suggest that it is indeed true. Hence, we have the following

**Conjecture 4.8.** There exist constants $c_1$ and $c_2$, at most depending on the number of hypotheses $r$, such that for all $A_i \geq 0$

$$\text{Tr} \text{GLB}(A_1,A_1) \leq c_1 \sum_{l=2}^r \text{Tr} \text{GLB}(A_1,A_l) + c_2 \sum_{k,l=2, k \neq l}^r \text{Tr} \text{GLB}(A_k,A_l). \quad (43)$$

An equivalent conjecture in terms of POVM elements (using the primal SDP characterisation of error probabilities) is:

**Conjecture 4.9.** There exist constants $c_1$ and $c_2$, at most depending on the number of hypotheses $r$, such that for any $0 \leq F_i \leq I$ (for $2 \leq i \leq r$) and $0 \leq G_{j,k} \leq I$ (for $2 \leq j < k \leq r$) there exists an $E$ in the intersection of operator intervals

$$I - c_1 \sum_{i=2}^r (I - F_i) \leq E \leq \begin{cases} 1 & \\ c_1 F_j + c_2 \left( \sum_{k=j+1}^r G_{j,k} + \sum_{k=2}^{j-1} (I - G_{k,j}) \right), & j = 2,\ldots,r. \end{cases} \quad (44)$$

Note, however, that operator intervals behave very differently than ordinary intervals of real numbers and are not very well understood. See for example the papers by Ando on this subject (e.g. [2]).

**Proof of equivalence of Claims 4.8 and 4.9** The correspondence between the two claims is based on the following equivalent characterisations of the error probabilities:

$$\begin{align*}
\text{Tr} \text{GLB}(A_1,A_1) &= \min_E \text{Tr}((I-E)A_1 + E \sum_{j=2}^r A_j) \\
\text{Tr} \text{GLB}(A_1,A_i) &= \min_{F_i} \text{Tr}((I-F_i)A_1 + F_i A_i) \\
\text{Tr} \text{GLB}(A_j,A_k) &= \min_{G_{j,k}} \text{Tr}(G_{j,k} A_j + (I-G_{j,k}) A_k),
\end{align*}$$

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where $E, F_i, G_{j,k}$ are POVM elements and satisfy $0 \leq E, F_i, G_{j,k} \leq I$. Hence (43) holds if and only if

$$0 \leq c_1 \sum_{i=2}^r \min_{F_i} \text{Tr}((I-F_i)A_1 + F_i A_i)$$
$$+ c_2 \sum_{j=2}^r \sum_{k=2}^r \min_{G_{j,k}} \text{Tr}(G_{j,k} A_j + (I-G_{j,k}) A_k)$$
$$- \min_{E} \text{Tr}((I-E)A_1 + E \sum_{j=2}^r A_j)$$

$$= \min c_1 \sum_{i=2}^r \text{Tr}((I-F_i)A_1 + F_i A_i)$$
$$+ \min_{G_{j,k}} c_2 \sum_{j=2}^r \sum_{k=2}^r \text{Tr}(G_{j,k} A_j + (I-G_{j,k}) A_k)$$
$$+ \max_{E} - \text{Tr}((I-E)A_1 + E \sum_{j=2}^r A_j)$$

$$= \min \min_{F_i} \min_{G_{j,k}} \max_{E} \text{Tr} A_1 \left(E - I + c_1 \sum_{i=2}^r (I-F_i)\right)$$
$$+ \sum_{j=2}^r \text{Tr} A_j \left(-E + c_1 F_j + c_2 \left(\sum_{k=j+1}^r G_{j,k} + \sum_{k=2}^{j-1} (I-G_{k,j})\right)\right)$$

holds for all $A_i \geq 0$. This quantification can be rephrased as the requirement that the minimisation of the RHS over all $A_i \geq 0$ is non-negative. By von Neumann’s minimax theorem, the order between this minimisation and the minimisation over $E$ can be interchanged:

$$0 \leq \min \min_{F_i} \min_{G_{j,k}} \max_{E} \text{Tr} A_1 \left(E - I + c_1 \sum_{i=2}^r (I-F_i)\right)$$
$$+ \sum_{j=2}^r \min_{A_j \geq 0} \text{Tr} A_j \left(-E + c_1 F_j + c_2 \left(\sum_{k=j+1}^r G_{j,k} + \sum_{k=2}^{j-1} (I-G_{k,j})\right)\right).$$

The minimisations over $F_i$ and $G_{j,k}$ and the maximisation over $E$ can now be replaced by quantifications: for all POVM elements $F_i$ and $G_{j,k}$ there should exist a POVM element $E$ such that

$$0 \leq \min_{A_i \geq 0} \text{Tr} A_1 \left(E - I + c_1 \sum_{i=2}^r (I-F_i)\right)$$
$$+ \sum_{j=2}^r \min_{A_j \geq 0} \text{Tr} A_j \left(-E + c_1 F_j + c_2 \left(\sum_{k=j+1}^r G_{j,k} + \sum_{k=2}^{j-1} (I-G_{k,j})\right)\right).$$

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Since $\text{Tr} \ AB \geq 0$ for all $A \geq 0$ if and only if $B \geq 0$, this is so if and only if
\[
E - I + c_1 \sum_{i=2}^r (I - F_i) \geq 0
\]
and, for all $j \geq 2$,
\[
-E + c_1 F_j + c_2 \left( \sum_{k=j+1}^r G_{j,k} + \sum_{k=2}^{j-1} (I - G_{k,j}) \right) \geq 0.
\]
Combining this with the requirement $0 \leq E \leq I$ yields the inequalities of Claim 4.9.

5 Nussbaum’s mixed exponents approach

In [42] Nussbaum presented a different approach towards splitting up the multi-hypothesis testing problem into pairwise tests, in which one pair of hypotheses is treated in a preferential way. This leads to an upper bound on the total error probability in which different pairwise error probabilities appear with different exponents. Here we generalise his approach and by combining it with our results we improve his bounds on the total error probability.

First we need a lemma about POVM elements, the content of which is implicit in [42]:

Lemma 5.1. For any $E$ and $Q$ satisfying $0 \leq E, Q \leq I$,
\[
\frac{1}{2} Q^{1/2} E Q^{1/2} \leq I - Q + E.
\] (45)

Proof. For any operator $X$, we have $0 \leq (X - 2)^*(X - 2)$, which can be rewritten as $X^*X/2 \leq (I - X)^*(I - X) + I$. In particular, let $E$ be positive definite and $Q$ positive semidefinite and let $X = E^{1/2} Q^{1/2} E^{-1/2}$. Then we obtain
\[
\frac{1}{2} E^{-1/2} Q^{1/2} E Q^{1/2} E^{-1/2} \leq E^{-1/2} (I - Q^{1/2}) E (I - Q^{1/2}) E^{-1/2} + I,
\]
which yields, after multiplying with $E^{1/2}$ on the left and on the right,
\[
\frac{1}{2} Q^{1/2} E Q^{1/2} \leq (I - Q^{1/2}) E (I - Q^{1/2}) + E.
\]
By continuity, this inequality also holds for positive semidefinite $E$. If we now impose $E, Q \leq I$ then the RHS can be bounded above by a simplified expression:
\[
(I - Q^{1/2}) E (I - Q^{1/2}) + E \leq (I - Q^{1/2})^2 + E \leq I - Q + E.
\]

Nussbaum’s result relies on the following decomposition lemma, proven by him for the case of uniform priors and for $K = 2$. We provide the lemma in full generality, and with a somewhat shorter proof, but still based on Nussbaum’s main idea to decompose the POVM in a clever way into two parts.
Lemma 5.2. Let $A_1, \ldots, A_r \in \mathcal{B}(\mathcal{H})_+$. For all $1 \leq K \leq r$,
\[ P_e^*(A_1, \ldots, A_r) \leq 2P_e^*(A_1, \ldots, A_K) + P_e^*(3A^{(K)}, A_{K+1}, \ldots, A_r), \tag{46} \]
where $A^{(K)} := \sum_{i=1}^K A_i$.

Proof. Let $\mathcal{F} = \{F_1, \ldots, F_K\}$ be the optimal POVM for discriminating between $A_1, \ldots, A_K$, and let $\mathcal{E}^{(K)} = \{E, E_{K+1}, \ldots, E_r\}$ be the optimal POVM for discriminating between $3A^{(K)}$, $A_{K+1}, \ldots, A_r$. Define $E_i := Q^{1/2}F_iQ^{1/2}$ for $i = 1, \ldots, K$. Then $\mathcal{E} = \{E_1, \ldots, E_r\}$ is a POVM.

In terms of the POVM $\mathcal{E}$ we have, for $i = 1, \ldots, K$,
\[ \text{Tr} A_i E_i = \text{Tr} A_i (Q - (Q - E_i)) = \text{Tr} A_i Q - \text{Tr} A_i Q^{1/2}(I - F_i)Q^{1/2}. \]
The total error probability for this POVM (an upper bound on $P_e^*$) is given by
\[ P_e(\mathcal{E}) = \sum_i \text{Tr} A_i (I - E_i) \]
\[ = \text{Tr} A^{(K)}(I - Q) + \sum_{i=1}^K \text{Tr} A_i Q^{1/2}(I - F_i)Q^{1/2} + \sum_{i=K+1}^r \text{Tr} A_i (I - E_i). \]

Using (45) of Lemma 5.1, the second sum can be bounded above by
\[ 2 \left( \text{Tr} \sum_{i=1}^K A_i (I - F_i) + \text{Tr} A^{(K)}(I - Q) \right) = 2P_e^*(A_1, \ldots, A_K) + 2 \text{Tr} A^{(K)}(I - Q). \]

Then
\[ P_e^* \leq P_e(\mathcal{E}) \leq 2P_e^*(A_1, \ldots, A_K) + 3 \text{Tr} A^{(K)}(I - Q) + \sum_{i=K+1}^r \text{Tr} A_i (I - E_i) \]
\[ = 2P_e^*(A_1, \ldots, A_K) + P_e^*(3A^{(K)}, A_{K+1}, \ldots, A_r), \]
proving (46). \hfill \square

Because we now have Theorem 3.3 to our disposal, we can obtain a stronger bound on the total error probability from Nussbaum’s decomposition lemma:

Theorem 5.3. Let $A_1, \ldots, A_r \in \mathcal{B}(\mathcal{H})_+$ and $\kappa := 3 \max_{1 \leq i < j \leq r} \sqrt{\text{Tr} A_i + \text{Tr} A_j}$. Then
\[ P_e^*(A_1, \ldots, A_r) \leq 2^{r-2}P_e^*(A_1, A_2) + \kappa \sum_{k=2}^{r-1} 2^{r-1-k} \sum_{l=1}^k \sqrt{P_e^*(A_l, A_{k+1})}. \tag{47} \]

If $A_k$ is of rank one for $k = 3, \ldots, r$ then
\[ P_e^*(A_1, \ldots, A_r) \leq 2^{r-2}P_e^*(A_1, A_2) + \kappa' \sum_{k=2}^{r-1} 2^{r-1-k} \sum_{l=1}^k P_e^*(A_l, A_{k+1}), \tag{48} \]
where $\kappa' := 3 \text{Tr} A_0 / (\min_{3 \leq i \leq r} \text{Tr} A_i)$.  

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Proof. Using Lemma 5.2 recursively with $K$ going down from $r - 1$ to 2:

$$P_e^s(A_1, \ldots, A_r) \leq 2P_e^s(A_1, \ldots, A_{r-1}) + P_e^s(3A^{(r-1)}, A_r)$$
$$\leq 4P_e^s(A_1, \ldots, A_{r-2}) + 2P_e^s(3A^{(r-2)}, A_{r-1}) + P_e^s(3A^{(r-1)}, A_r)$$
$$\leq \ldots$$
$$\leq 2^{r-2}P_e^s(A_1, A_2) + \sum_{k=2}^{r-1} 2^{r-1-k}P_e^s(3A^{(k)}, A_{k+1}).$$

Note that $P_e^s(3A^{(k)}, A_{k+1}) \leq 3P_e^s(A^{(k)}, A_{k+1})$, and applying Theorem 3.3 to each term in the summand yields the inequalities of the theorem. \hfill \square

6 Upper bounds from suboptimal measurements

When the number of hypotheses $r$ is larger than 2, there is no explicit expression known for the optimal error probability $P_e^s(A_1, \ldots, A_r)$ in general. Obviously, any measurement yields an upper bound on the optimal success probability, some of which are known to have the same asymptotics in the limit of infinitely many copies as the optimal error probability. Here we briefly review the pretty good measurement and Tyson’s square measurement, and show upper decoupling bounds on the optimal error based on the latter.

Let $A_1, \ldots, A_r \in \mathcal{B}(\mathcal{H})_+$ represent the hypotheses as usual, and for every $\alpha \in \mathbb{R}$, define the $\alpha$-weighted POVM $\mathcal{E}^{(\alpha)}$ by

$$E_k^{(\alpha)} := S^{-1/2}_\alpha A_k^\alpha S^{-1/2}_\alpha, \quad S_\alpha := \sum_k A_k^\alpha.$$

Note that if $A_k = |\psi_k\rangle \langle \psi_k|$ for some vectors $\psi_k$ then $E_k^{(\alpha)} = |\psi_k^{(\alpha)}\rangle \langle \psi_k^{(\alpha)}|$ with $\psi_k^{(\alpha)} := S^{-1/2}_\alpha \|\psi_k\|^{1-\alpha} \psi_k$, and $\sum_k |\psi_k^{(\alpha)}\rangle \langle \psi_k^{(\alpha)}| = (\sum_k A_k)^0$. In particular, if $\psi_1, \ldots, \psi_r$ are linearly independent then $\psi_1^{(\alpha)}, \ldots, \psi_r^{(\alpha)}$ is an orthonormal system, spanning the same subspace as the original $\psi$ vectors. That is, the above procedure yields an orthogonalization of the original set of vectors, which is different from the Gram-Schmidt orthogonalization in general.

The case $\alpha = 1$ yields the so-called pretty good measurement (PG) [15]. Barnum and Knill [8] have shown that in the case of weighted states, the success probability of the PG measurement is bounded below by the square of the optimal success probability: $(P_e^s)^2 \leq P_e^{PG} \leq P_e^s$, which in turn yields that $\frac{1}{2}P_e^{PG} \leq P_e^s \leq P_e^{PG}$. In particular, $P_e^s$ and $P_e^{PG}$ have the same exponential decay rate in the asymptotic setting.

The error probability for the PG measurement is easily calculated. Since the success probability is given by

$$P_s^{PG} = \sum_k \text{Tr} A_k E_k = \sum_k \text{Tr} A_k A_0^{-1/2} A_k A_0^{-1/2},$$
the error probability is
\[
P_e^{PG} = \sum_k \text{Tr} \, A_k (I - A_0^{-1/2} A_k A_0^{-1/2})
\]
\[
= \sum_k \text{Tr} \, A_k A_0^{-1/2} A_k A_0^{-1/2}
\]
\[
= \sum_{k \neq l} \text{Tr} \, A_k A_0^{-1/2} A_l A_0^{-1/2}.
\]

While this bound seems promising, as it easily decomposes in pairwise error terms, it is actually useless for our purposes. Indeed, suppose we have a set of states \( A_k \) such that \( A_0 = I / \text{Tr} \, I = I / d \), then \( \text{Tr} \, A_k A_0^{-1/2} A_l A_0^{-1/2} = d \, \text{Tr} \, A_k A_l \). The presence of the dimension \( d \) as a factor renders this approach useless for obtaining good bounds on asymptotic error rates. In the \( n \)-copy case, this factor will become \( d^n \), giving rise to an offset \( \log d \) in the formula for the bound on the asymptotic rate. Hence, despite its early promises, the pretty good measurement is not good enough for us.

The case \( \alpha = 2 \) yields the square measurement (SQ), with POVM elements
\[
E_{SQ;k} = X_{SQ;k}^* X_{SQ;k}, \quad X_{SQ;k} = A_k \left( \sum_k A_k^2 \right)^{-1/2}.
\]

This type of measurement has been used by various authors \cite{9,11,26,24}, and it features in Tyson’s bounds on the error probability \cite{50}, which we briefly review below. For a comprehensive overview of the pretty good and the square measurements, see \cite{51}.

For any set \( \{X_k\} \) of measurement operators (i.e., \( \sum_k X_k^* X_k \leq I \)), let
\[
\Gamma(\{X_k\}) := \text{Tr} \, A_0 - \sum_{k=1}^{r} ||X_k A_k||_1. \tag{49}
\]

Minimising over all possible choices of \( \{X_k\} \) yields the optimal value \( \Gamma^* \):
\[
\Gamma^* := \inf_{\{X_k\}: \sum_k X_k^* X_k = I} \Gamma(\{X_k\}). \tag{50}
\]

The importance of this quantity \( \Gamma \) comes from a combination of two facts. First, it differs from the error probability \( P_e \) only by a factor between 1 and at most 2. Hence, \( \Gamma^* \) is a good approximation of \( P_e^* \), especially in the asymptotic regime. Moreover, unlike the optimal error probability, \( \Gamma^* \) can be calculated explicitly by a closed-form expression. This is the content of the following two theorems, first proven by Tyson \cite{50}. For completeness, we provide short proofs in Appendix B.

**Theorem 6.1** (Tyson). Let \( A_1, \ldots, A_r \in B(\mathcal{H})_+ \) and \( \{E_k = X_k^* X_k\} \) be a POVM. Then
\[
\Gamma(\{X_k\}) \leq P_e(\{E_k\}) \leq 2 \Gamma(\{X_k\}).
\]

In particular, for the optimal POVM and optimal \( X_k \) that achieve the minimum:
\[
\Gamma^* \leq P_e^* \leq 2 \Gamma^*. \tag{51}
\]

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Theorem 6.2 (Tyson). Let $A_1, \ldots, A_r \in B(\mathcal{H})_+$ and $A_0 := \sum_i A_i$. Then
\[
\Gamma^* = \text{Tr} A_0 - \text{Tr} \left( \sum_{i=1}^r A_i^2 \right)^{1/2},
\] (52)
with the optimal measurement operators being those of the SQ measurement.

From (52) it follows that $\Gamma^*$ can take values between 0 (when all $A_i$ are mutually orthogonal) and $(\text{Tr} A_0)(1 - 1/\sqrt{r})$ (when all $A_i$ are equal), whereas $P_e^*$ lies between 0 and $(\text{Tr} A_0)(1 - 1/r)$.

We now relate Tyson’s $\Gamma^*$ to the pairwise Chernoff divergences, in a similar spirit as we have done before with the dichotomic error. These bounds are based on the following proposition:

Proposition 6.3. Let $A_1, \ldots, A_r \in B(\mathcal{H})_+$. Then
\[
\text{Tr} \left( \sum_j A_j^2 \right)^{1/2} \geq (\text{Tr} A_0)^{3/2} \left( (\text{Tr} A_0) + 2 \sum_{j<k} \text{Tr} A_j^{1/2} A_k^{1/2} \right)^{-1/2}
\]

\[
\geq (\text{Tr} A_0) - (\text{Tr} A_0)^{3/2} \sum_{j<k} \text{Tr} A_j^{1/2} A_k^{1/2}.
\]

Proof. According to Lieb’s theorem, the functional $(B, C) \mapsto \text{Tr}(B^t C^{1-t})$ is jointly concave for $0 < t \leq 1$. That is, for $n$ PSD operators $B_j$ and $C_j$,
\[
\text{Tr} \sum_j B_j^t C_j^{1-t} \leq \text{Tr}(\sum_j B_j)^t(\sum_j C_j)^{1-t}.
\]
Then, using the fact $|\text{Tr} X| \leq ||X||_1$ and Hölder’s inequality,
\[
\text{Tr} \sum_j B_j^t C_j^{1-t} \leq ||(\sum_j B_j)^t(\sum_j C_j)^{1-t}||_1
\]
\[
\leq ||(\sum_j B_j)^t||_1/s \ ||(\sum_j C_j)^{1-t}||_1/(1-s).
\]
Now take $t = 2/3$, $s = 1/3$, $B_j = A_j^{1/2}$ and $C_j = A_j^{2/3}$, then
\[
\text{Tr} \sum_j A_j^{1/3} A_j^{2/3} \leq ||(\sum_j A_j^{1/2})^{2/3} ||_3 \ ||(\sum_j A_j^{2/3})^{1/3}||_3^{2/3}
\]
\[
= \left( \text{Tr} \left( \sum_j A_j^{1/2} \right)^2 \right)^{1/3} \ \left( \text{Tr} \left( \sum_j A_j^{2/3} \right)^{1/2} \right)^{2/3}.
\]
Obviously, the LHS equals $\text{Tr} A_0$. Taking the $3/2$ power and rearranging then yields

$$\text{Tr} \left( \sum_j A_j^2 \right)^{1/2} \geq (\text{Tr} A_0)^{3/2} \left( \text{Tr} \left( \sum_j A_j^{1/2} \right)^2 \right)^{-1/2} = (\text{Tr} A_0)^{3/2} \left( \sum_{j,k} \text{Tr} A_j^{1/2} A_k^{1/2} \right)^{-1/2}$$

$$= (\text{Tr} A_0)^{3/2} \left( \text{Tr} A_0 + 2 \sum_{j<k} \text{Tr} A_j^{1/2} A_k^{1/2} \right)^{-1/2}$$

$$\geq \text{Tr} A_0 - (\text{Tr} A_0)^{3/2} \sum_{j<k} \text{Tr} A_j^{1/2} A_k^{1/2},$$

where in the last line we exploited the inequality $\left( a + x \right)^{-1/2} \geq a^{-1/2} - x/2$. \hfill \qed

**Theorem 6.4.** Let $A_1, \ldots, A_r \in \mathcal{B}(\mathcal{H})_+$ and let $p_k := \text{Tr} A_k$, $\sigma_k := A_k/\text{Tr} A_k$. Then

$$\frac{1}{2} P_e^* \leq \Gamma^* \leq \left( \sum_k p_k \right)^{3/2} \sum_{j<k} \sqrt{p_j p_k} \ Q_{\text{min}}(\sigma_j, \sigma_k)^{1/2}. \tag{53}$$

In the special case that all states $\sigma_k$ are pure, we have the improved bound

$$\frac{1}{2} P_e^* \leq \Gamma^* \leq \left( \sum_k p_k \right)^{3/2} \sum_{j<k} \sqrt{p_j p_k} \ Q_{\text{min}}(\sigma_j, \sigma_k). \tag{54}$$

**Proof.** The first inequalities in (53) and (54) are due to (51). It is shown in [6] that any pair of states $\sigma_j$ and $\sigma_k$ satisfies the inequality

$$\text{Tr} \sigma_j^{1/2} \sigma_k^{1/2} \leq Q_{\text{min}}(\sigma_j, \sigma_k)^{1/2},$$

As this inequality is achievable, the square root can not be removed in general. Thus, with $A_j = p_j \sigma_j$,

$$\text{Tr} A_j^{1/2} A_k^{1/2} \leq \sqrt{p_j p_k} Q_{\text{min}}(\sigma_j, \sigma_k)^{1/2}.$$

Applying Proposition 6.3 and recalling that $\Gamma^* = \text{Tr} A_0 - \text{Tr}(\sum_j A_j^2)^{1/2}$, we immediately get (53).

For pure states we have $\sigma_j^s = \sigma_j$ for any $s$, hence $Q_{\text{min}}(\sigma_j, \sigma_k) = \text{Tr} \sigma_j \sigma_k$ and also

$$\text{Tr} A_j^{1/2} A_k^{1/2} = \sqrt{p_j p_k} \ \text{Tr} \sigma_j \sigma_k.$$

Therefore, for pure states,

$$\text{Tr} A_j^{1/2} A_k^{1/2} = \sqrt{p_j p_k} \ Q_{\text{min}}(\sigma_j, \sigma_k),$$

so that (54) follows. \hfill \qed

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When all states are pure and the prior is uniform (i.e., \( p_k = \frac{1}{r} \forall k \)), we can use another argument. By the inequality \( \text{Tr} \rho \sigma \leq 1 - \frac{1}{2} \| \rho - \sigma \|_1 \), we get
\[
\text{Tr} \sigma_j \sigma_k \leq 1 - \frac{1}{2} \| \sigma_j - \sigma_k \|_1.
\]
Hence,
\[
\text{Tr} A_{j}^{1/2} A_{k}^{1/2} = \frac{1}{r} \text{Tr} \sigma_j \sigma_k \leq \frac{1}{r} \left( 2 - \| \sigma_j - \sigma_k \|_1 \right),
\]
so that
\[
1 - \Gamma^* \geq \left( 1 + \frac{2}{r} \sum_{j < k} (2 - \| \sigma_j - \sigma_k \|_1) \right)^{-1/2}.
\] (55)

Based on extensive numerical simulations, we conjecture that the latter bound also holds for mixed states and for non-uniform priors:

**Conjecture 6.5.** For any \( A_i \geq 0 \) with \( \sum_i \text{Tr} A_i = 1 \),
\[
\Gamma^* \leq 1 - \left( 1 + 4(r - 1)P_{e,2}^* \right)^{-1/2} \leq 2(r - 1)P_{e,2}^*.
\] (56)

By Theorem 6.1, this would imply the inequality of Conjecture 2.3 for weighted states:
\[
P_e^* \leq 4(r - 1)P_{e,2}^*.
\]

**7 Asymptotics: the Chernoff bound**

Armed with a number of upper bounds on the multiple-hypothesis discrimination error probability, let us now turn to the study of its asymptotic behaviour. Let our hypotheses be represented by the sequences \( \tilde{A}_i := \{ A_{i,n} \}_{n \in \mathbb{N}}, \ i = 1, \ldots, r \), and define \( A_{0,n} := \sum_{i=1}^{r} A_{i,n} \). Recall the definitions of \( p_e(\tilde{A}_1, \ldots, \tilde{A}_r) \) and \( \overline{p}_e(\tilde{A}_1, \ldots, \tilde{A}_r) \) from (2)–(3). Due to Theorem 22, we have
\[
p_e(\tilde{A}_1, \ldots, \tilde{A}_r) \geq \max_{(i,j): i \neq j} p_e(\tilde{A}_i, \tilde{A}_j)
\] (57)

Our aim here is to complement the above inequality by giving upper bounds on \( \overline{p}_e(\tilde{A}_1, \ldots, \tilde{A}_r) \) in terms of the pairwise exponents. Recall the definition of the asymptotic Chernoff divergence from (25)
\[
C(\tilde{A}_1, \tilde{A}_2) = \lim_{n \to \infty} \frac{1}{n} C(A_{1,n}, A_{2,n}) = - \lim_{n \to \infty} \frac{1}{n} \log \min_{0 \leq s \leq 1} \text{Tr} A_{1,n}^s A_{2,n}^{1-s}.
\]

We conjecture that the following converse to (57) holds under very mild conditions:
\[
\overline{p}_e(\tilde{A}_1, \ldots, \tilde{A}_r) \leq \max_{(i,j): i \neq j} \overline{p}_e(\tilde{A}_i, \tilde{A}_j) \leq - \min_{(i,j): i \neq j} C(\tilde{A}_1, \tilde{A}_2).
\] (58)

Note that the second inequality is always true, due to (24). Below we show that the weaker inequality
\[
\overline{p}_e(\tilde{A}_1, \ldots, \tilde{A}_r) \leq \frac{1}{2} \max_{(i,j): i \neq j} \overline{p}_e(\tilde{A}_i, \tilde{A}_j) \leq \frac{1}{2} \min_{(i,j): i \neq j} C(\tilde{A}_1, \tilde{A}_2)
\] (59)
is always true as long as \( \limsup_{n \to \infty} \frac{1}{n} \log \text{Tr} A_{0,n} = 0 \), which is trivially satisfied in the case of weighted states. We also show (58) in a number of special cases.

We have the following general result:

**Theorem 7.1.** Assume that \( \limsup_{n \to \infty} \frac{1}{n} \log \text{Tr} A_{0,n} = 0 \). Then

\[
\overline{p}_e (\vec{A}_1, \ldots, \vec{A}_r) \leq \frac{1}{2} \max_{(i,j): i \neq j} \overline{p}_e (\vec{A}_i, \vec{A}_j) \leq - \frac{1}{2} \min_{(i,j): i \neq j} C(\vec{A}_i, \vec{A}_j). \quad (60)
\]

If \( A_{i,n} \) is of rank one for every \( i \) and \( n \), and \( \limsup_{n \to \infty} \frac{1}{n} \log \frac{\text{Tr} A_{0,n}}{\min \text{Tr} A_{i,n}} = 0 \) then we have the stronger inequality

\[
\overline{p}_e (\vec{A}_1, \ldots, \vec{A}_r) \leq \max_{(i,j): i \neq j} \overline{p}_e (\vec{A}_i, \vec{A}_j) \leq - \min_{(i,j): i \neq j} C(\vec{A}_i, \vec{A}_j). \quad (61)
\]

**Proof.** Immediate from Theorem 4.6, Lemma 2.1, and (24). \( \square \)

**Remark 7.2.** Note that the first inequalities in (60) and (61) can also be obtained from Theorem 5.3. The inequalities between the first and the last terms in (60)–(61) can also be obtained from Theorem 6.4.

The second part of Theorem 7.1 can be improved in various ways by using Theorem 5.3.

**Theorem 7.3.** Assume that \( A_{i,n} \) is rank one for every \( n \in \mathbb{N} \) for at least \( r-2 \) of the hypotheses. If we also have \( \limsup_{n \to \infty} \frac{1}{n} \log \frac{\text{Tr} A_{0,n}}{\min \text{Tr} A_{i,n}} = 0 \) then

\[
\overline{p}_e (\vec{A}_1, \ldots, \vec{A}_r) \leq \max_{(i,j): i \neq j} \overline{p}_e (\vec{A}_i, \vec{A}_j) \leq - \min_{(i,j): i \neq j} C(\vec{A}_i, \vec{A}_j).
\]

**Proof.** We can assume without loss of generality that at most hypotheses 1 and 2 are not represented by rank one operators. Then the assertion follows immediately from (48). \( \square \)

**Theorem 7.4.** Assume that (58) holds for hypotheses \( \vec{A}_i, i = 1, \ldots, r \), and that \( A_{r+1,n} \) is rank one for every \( n \). If \( \limsup_{n \to \infty} \frac{1}{n} \log \frac{\text{Tr}\sum_{i=1}^{r} A_i}{\text{Tr} A_{r+1,n}} = 0 \) then

\[
\overline{p}_e (\vec{A}_1, \ldots, \vec{A}_r, \vec{A}_{r+1}) \leq \max \left\{ \overline{p}_e (\vec{A}_i, \vec{A}_j) : 1 \leq i < j \leq r+1 \right\}
\leq - \min \left\{ C(\vec{A}_i, \vec{A}_j) : 1 \leq i < j \leq r+1 \right\}.
\]

**Proof.** By (46),

\[
P^* (A_1, \ldots, A_{r,n}) \leq 2P^* (A_1, \ldots, A_r) + P^* (3^r, A_{r+1}).
\]

Applying then (30) to the second term yields the assertion. \( \square \)

Inequality (58) has been proved in [42] for the i.i.d. case under the assumption that there exists a pair of states \( \sigma_k, \sigma_l, k \neq l \), such that \( C(\sigma_k, \sigma_l) \leq \frac{1}{6} C(\sigma_i, \sigma_j) \) for every \( (i, j) \neq (k, l), i \neq j \). Theorem 7.5 below shows that the constant 1/6 can be improved to 1/2.
Theorem 7.5. Assume that \( \lim \sup_{n \to \infty} \frac{1}{n} \log \text{Tr} A_{0,n} = 0 \). For any pair \((k, l)\), \(k \neq l\),
\[
\overline{p}_e \left( \vec{A}_1, \ldots, \vec{A}_r \right) \leq \max \left\{ \overline{p}_e \left( \vec{A}_i, \vec{A}_k \right), \frac{1}{2} \overline{p}_e \left( \vec{A}_i, \vec{A}_j \right), i \neq j, (i, j) \neq (k, l) \right\}
\leq - \min \left\{ C \left( \vec{A}_k, \vec{A}_l \right), \frac{1}{2} C \left( \vec{A}_i, \vec{A}_j \right), i \neq j, (i, j) \neq (k, l) \right\}.
\]
In particular, if there exists a pair \((k, l)\), \(k \neq l\), such that \(\overline{p}_e \left( \vec{A}_k, \vec{A}_l \right) \geq \frac{1}{2} \overline{p}_e \left( \vec{A}_i, \vec{A}_j \right), i \neq j, (i, j) \neq (k, l)\), then
\[
\overline{p}_e \left( \vec{A}_1, \ldots, \vec{A}_r \right) \leq \max_{(i, j): i \neq j} \overline{p}_e \left( \vec{A}_i, \vec{A}_j \right) \leq - \min_{(i, j): i \neq j} C \left( \vec{A}_i, \vec{A}_j \right).
\]
Proof. Immediate from Theorem 5.3.

Finally, we note that in many important cases, we have the optimality relation
\[
P_e \left( \vec{A}_i, \vec{A}_j \right) \geq - C \left( \vec{A}_i, \vec{A}_j \right). \tag{62}
\]
For instance, this happens in the standard state discrimination problem if the hypotheses \(i, j\) are i.i.d. \[38\], or Gibbs states of a finite-range, translation-invariant Hamiltonian on a spin chain \[21\], or Gibbs states of interaction-free fermionic or bosonic chains \[30\] \[31\]. In these cases, if \[59\] is satisfied then we have
\[
- \min_{(i, j): i \neq j} C \left( \vec{A}_i, \vec{A}_j \right) \leq P_e \left( \vec{A}_1, \ldots, \vec{A}_r \right) \leq \overline{p}_e \left( \vec{A}_1, \ldots, \vec{A}_r \right) \leq - \frac{1}{2} \min_{(i, j): i \neq j} C \left( \vec{A}_i, \vec{A}_j \right).
\]
If, moreover, \[58\] is satisfied then we get the stronger statement
\[
\lim_{n \to +\infty} \frac{1}{n} \log P_e^* \left( A_1,n, \ldots, A_r,n \right) = - \min_{(i, j): i \neq j} C \left( \vec{A}_i, \vec{A}_j \right).
\]

Appendix

A The classical case

In the classical case the hypotheses (in the single-shot setting) are represented by non-negative functions \(A_i : \mathcal{X} \to \mathbb{R}_+\), where \(\mathcal{X}\) is some finite set, and POVM elements are replaced by non-negative functions \(E_i : \mathcal{X} \to \mathbb{R}_+\), satisfying \(\sum_i E_i(x) \leq 1, \forall x \in \mathcal{X}\), which we may call a classical POVM. The success probability corresponding to a classical POVM \(\{E_i\}\) is \(P_e \left( \{E_i\} \right) = \sum_{i=1}^r \sum_{x \in \mathcal{X}} A_i(x) E_i(x)\). Obviously, we can assign to each non-negative function \(F : \mathcal{X} \to \mathbb{R}_+\) a diagonal operator \(\hat{F}\) on \(\mathcal{C}\mathcal{X}\) in an obvious way, and under this identification we get \(\sum_{i=1}^r \sum_{x \in \mathcal{X}} A_i(x) E_i(x) = \sum_{i=1}^r \text{Tr} \hat{A}_i \hat{E}_i\), which is the success probability corresponding to hypotheses \(\hat{A}_i\) and POVM elements \(\hat{E}_i\). On the other hand, if \(A_1, \ldots, A_r \in \mathcal{B}(\mathcal{H})_+\) are mutually commuting then there exists a basis in \(\mathcal{H}\), labelled by the elements of some
Indeed, the classical case can be represented both by functions and diagonal operators, and we will assume that the hypotheses are diagonal in a given basis then it is enough to consider POVM elements 

\[ \tilde{A}, \tilde{B}, \ldots, \tilde{E} \]

where for \( \tilde{A}, \tilde{B}, \ldots, \tilde{E} \) are POVM, and \( \sum_{i=1}^{r} \sum_{x \in \mathcal{X}} \tilde{A}(x)\tilde{E}(x) = \sum_{i=1}^{r} \text{Tr} \{ A_i E_i \} \). Hence, if the operators representing the hypotheses are diagonal in a given basis then it is enough to consider POVM elements that are also diagonal in the same basis, which reduces the problem into a classical one. Thus, the classical case can be represented both by functions and diagonal operators, and we will not make a difference in the notation between the two representations in what follows.

Consider first the classical binary state discrimination problem with hypotheses \( A_1 = A \) and \( A_2 = \sum_{i=1}^{r} B_i \). Then we have the following strengthening of Theorem 3.3:

\[
P_e^* \left( A, \sum_{i} B_i \right) \leq \sum_i P_e^* (A, B_i). \tag{63}
\]

Indeed,

\[
P_e^* \left( A, \sum_{i} B_i \right) = \frac{1}{2} \text{Tr} \left( A + \sum_{i} B_i \right) - \frac{1}{2} \left\| A - \sum_{i} B_i \right\|_1
\]

\[
= \frac{1}{2} \sum_{x} \left[ A(x) + \sum_{i} B_i(x) - \left| A(x) + \sum_{i} B_i(x) \right| \right]
\]

\[
= \frac{1}{2} \sum_{x} f_x \left( \sum_{i} B_i(x) \right),
\]

where \( f_x(t) := t + x - |t - x| = 2 \min \{t, x\} \). It is easy to see that \( f_x \) is subadditive for every \( x \), and hence the above can be continued as

\[
P_e^* \left( A, \sum_{i} B_i \right) = \frac{1}{2} \sum_{x} f_x \left( \sum_{i} B_i(x) \right) \leq \frac{1}{2} \sum_{x} \sum_{i} f_x(B_i(x)) = \sum_i \frac{1}{2} \sum_{x} f_x(B_i(x))
\]

\[
= \sum_i \left( \frac{1}{2} \text{Tr} (A + B_i) - \frac{1}{2} \left\| A - B_i \right\|_1 \right) = \sum_i P_e^* (A, B_i).
\]

Combining this with Theorem 4.1, we get

\[
P_e^* (A_1, \ldots, A_r) \leq P_e^* = \sum_{k=1}^{r} P_e^* \left( A_k, \sum_{l \neq k} A_l \right) \leq \sum_{(k,l): k \neq l} P_e^* (A_k, A_l), \tag{64}
\]

proving Conjecture 2.3 with \( c = 2(r - 1) \). Below we give a more direct proof of this, without using Theorem 4.1.

Consider now the asymptotic problem i.i.d. vs. averaged i.i.d. problem with hypotheses \( A_{1,n} = p \rho \sigma_i \) and \( B_{i,n} = (1 - p) q_i \sigma_i \), where \( p \in (0,1) \) and \( q \) is a probability distribution. Then we have

\[
\sum_i q_i P_e^* \left( p \rho \sigma_i, (1 - p) q_i \sigma_i \right) \leq P_e^* \left( p \rho \sigma_i, (1 - p) \sum_i q_i \sigma_i \right)
\]

\[
\leq \sum_i P_e^* \left( p \rho \sigma_i, (1 - p) q_i \sigma_i \right) \leq \sum_i P_e^* \left( \rho \sigma_i, (1 - p) q_i \sigma_i \right),
\]

33
Thus, any POVM $\{E_k\}$ if
\[
\text{max}_k P_{\text{e}}(E_k) \leq \text{max}_k m(x) E_k(x) \leq \sum_k m(x) E_k(x) = \text{Tr} \max \{A_1, \ldots, A_r\},
\]
where the first inequality is due to the convexity of the trace-norm, the second is due to the subadditivity relation (63), and the last inequality is obvious from the definition of the error probability. This yields immediately Conjecture 3.2 in the classical case, i.e.,
\[
\lim_{n \to \infty} \frac{1}{n} \log P_{e}^n \left( p \sigma^n + (1 - p) \sum_i q_i \sigma_i^{\otimes n} \right) = - \min \{\rho, \sigma_i\}.
\]

Consider now the classical single-shot state discrimination problem with hypotheses $A_1, \ldots, A_r : \mathcal{X} \to \mathbb{R}_+$ and let $m(x) := \max_k A_k(x)$. We say that a POVM $\{E_k\}_{k=1}^r$ is a maximum likelihood POVM if $E_k(x) = 0$ when $A_k(x) < m(x)$, and for every $x \in \mathcal{X}$, $\sum_k E_k(x) = 1$. For any POVM $\{E_k\}_{k=1}^r$, we have
\[
P_e(E_1, \ldots, E_r) = \sum_k \sum_x A_k(x) E_k(x) \leq \sum_k \sum_x m(x) E_k(x) \leq \sum_x m(x) = \text{Tr} \max \{A_1, \ldots, A_r\},
\]
where $\max \{A_1, \ldots, A_r\} := \sum_x m(x)|x\rangle\langle x|$. The above inequality holds with equality if and only if $\{E_k\}_{k=1}^r$ is a maximum likelihood POVM, and hence we have
\[
P^*_e(A_1, \ldots, A_r) = \text{Tr} \max \{A_1, \ldots, A_r\}.
\]

Now let $E_1, \ldots, E_r$ be a maximum likelihood measurement. Then the individual error probabilities are, for each $k$,
\[
P_{e,k} = \sum_x A_k(x) (1 - E_k(x)) = \sum_{x: A_k(x) < m(x)} A_k(x) + \sum_{x: A_k(x) = m(x)} A_k(x) (1 - E_k(x)).
\]
Obviously, if $A_k(x) < m(x)$ then there exists an $l \neq k$ such that $A_k(x) < A_l(x)$, and if $A_k(x) = m(x)$ and $A_k(x) (1 - E_k(x)) > 0$ then there exists and $l \neq k$ such that $A_k(x) = A_l(x)$. Hence,
\[
P_{e,k} \leq \sum_{l \neq k: A_k(x) < A_l(x)} A_k(x) + \sum_{l \neq k: A_k(x) = A_l(x)} A_k(x) = \sum_{l \neq k: A_k(x) \leq A_l(x)} A_k(x)
\]
Thus,
\[
P^*_e(A_1, \ldots, A_r) = \sum_{k=1}^r P_{e,k} \leq \sum_{k=1}^r \sum_{l \neq k: A_k(x) \leq A_l(x)} A_k(x)
\]
\[
\leq \sum_{k=1}^r \sum_{l \neq k: x: A_k(x) \leq A_l(x)} A_k(x) + \sum_{x: A_k(x) > A_l(x)} A_l(x)
\]
\[
= \sum_{k=1}^r \sum_{l \neq k: x: A_k(x) \leq A_l(x)} \left[ \frac{1}{2} \text{Tr}(A_k + A_l) - \frac{1}{2} \|A_k - A_l\|_1 \right]
\]
\[
= \sum_{(k,l): k \neq l} P^*_e(A_k, A_l),
\]
thus recovering (64).
B The pure state case

Let $A_1, A_2 \in \mathcal{B}(\mathcal{H})_+$ be rank one operators; then we can write them as $A_i = |x_i\rangle\langle x_i| = p_i|\psi_i\rangle\langle\psi_i| = p_i\sigma_i$, where $p_i := \text{Tr} A_i$. Many of the divergence measures coincide in this case; indeed, it is easy to see that

$$|\langle \psi_1, \psi_2 \rangle|^2 = F(\sigma_1, \sigma_2)^2 = Q_s(\sigma_1\|\sigma_2) = Q_{\min}(\sigma_1, \sigma_2) = \exp(-C(\sigma_1, \sigma_2)), \quad s \in [0, 1].$$

A straightforward computation gives that $\|A_1 - A_2\|_1 = \sqrt{(p_1 + p_2)^2 - 4p_1p_2|\langle \psi_1, \psi_2 \rangle|^2}$, and hence

$$P_e^*(A_1, A_2) = \frac{1}{2} \text{Tr}(A_1 + A_2) - \frac{1}{2} \|A_1 - A_2\|_1 = \frac{2p_1p_2|\langle \psi_1, \psi_2 \rangle|^2}{p_1 + p_2 + \|A_1 - A_2\|_1}.$$ 

Noting that $0 \leq \|A_1 - A_2\|_1 \leq p_1 + p_2$, we get

$$\frac{p_1p_2}{p_1 + p_2} |\langle \psi_1, \psi_2 \rangle|^2 \leq P_e^*(A_1, A_2) \leq \frac{2p_1p_2}{p_1 + p_2} |\langle \psi_1, \psi_2 \rangle|^2 \quad (65)$$

Consider now two sequences of rank one operators $\tilde{A}_i = \{A_{i,n}\}_{n \in \mathbb{N}}$, $i = 1, 2$, and let $p_{i,n} := \text{Tr} A_{i,n}$, and $A_{i,n} = p_{i,n}|\psi_{i,n}\rangle\langle\psi_{i,n}| = p_{i,n}\sigma_{i,n}$. Applying (65) to each $n$, we get

$$\frac{p_{1,n}p_{2,n}}{p_{1,n} + p_{2,n}} \exp(-C(\sigma_{1,n}, \sigma_{2,n})) \leq P_e^*(A_{1,n}, A_{2,n}) \leq \frac{2p_{1,n}p_{2,n}}{p_{1,n} + p_{2,n}} \exp(-C(\sigma_{1,n}, \sigma_{2,n})).$$

If we assume now that $0 < \liminf_n p_{i,n} \leq \limsup_n p_{i,n} < +\infty$, $i = 1, 2$, then taking the limit $n \to \infty$ in the above formula yields

$$\lim_{n \to \infty} \frac{1}{n} \log P_e^*(A_{1,n}, A_{2,n}) = -C(\sigma_1, \sigma_2) = -C(\tilde{A}_1, \tilde{A}_2),$$

where the last identity is straightforward to verify. Thus in the pure state case we can get the Chernoff bound theorem from the above elementary argument, without using the trace inequality of [4] or the reduction to classical states from [38].

Consider now the case $r > 2$, and let $A_1, \ldots, A_r \in \mathcal{B}(\mathcal{H})_+$ be rank one operators. Let $E_i := A_i^{-1/2}A_iA_i^{-1/2}$ be the POVM elements of the pretty good measurement, where $A_0 := \sum_{i=1}^r A_i$. It was shown in Appendix A of [38] that for every $i$,

$$\text{Tr} A_i(I - E_i) \leq \frac{1}{p_i} \sum_{j: j \neq i} |\langle x_i, x_j \rangle|^2.$$ 

Summing it over $i$, we get

$$P_e^*(A_1, \ldots, A_r) \leq P_e(\{E_1, \ldots, E_r\}) \leq \sum_{i=1}^r \frac{1}{p_i} \sum_{j: j \neq i} |\langle x_i, x_j \rangle|^2 \leq \frac{1}{\min_i p_i} \sum_{(i,j): i \neq j} \exp(-C(A_i, A_j)),$$ 

while Theorem 2.22 yields

$$P_e^*(A_1, \ldots, A_r) \geq \frac{1}{r-1} \sum_{k, l: k \neq l} P_e^*(A_k, A_l) \geq \frac{1}{r-1} \sum_{k, l: k \neq l} \frac{1}{p_k + p_l} \exp(-C(A_i, A_j)),$$ 

(67)
where the last inequality is due to (65). Note that (66) also yields a decoupling bound for the error probabilities, as \( |\langle x_i, x_j \rangle|^2 / p_i \leq (1 + p_j / p_i) P_e^\alpha(A_i, A_j) \) by (65), and hence

\[
P_e^\alpha(A_1, \ldots, A_r) \leq \sum_{i=1}^r \frac{1}{p_i} \sum_{j, j \neq i} |\langle x_i, x_j \rangle|^2 \leq \frac{\text{Tr} A_0}{\min_i p_i} \sum_{(i, j) : i \neq j} P_e^\alpha(A_i, A_j).
\]

Consider now the asymptotic case, with hypotheses \( \bar{A}_i, i = 1, \ldots, r \), and assume as before that \( 0 < \lim \inf_n p_{i,n} \leq \lim \sup_n p_{i,n} < +\infty, \forall i \). Applying (66) and (67) to every \( n \), and taking the limit \( n \to \infty \), we get

\[
\lim_{n \to \infty} \frac{1}{n} \log P_e^\alpha(A_{1,n}, \ldots, A_{r,n}) = - \max_{(i, j) : i \neq j} C \left( \bar{A}_i, \bar{A}_j \right).
\]

\[\text{C Least upper bound and greatest lower bound for operators}\]

As mentioned already in Section 2\textsuperscript{sf 3} for a set \( A_1, \ldots, A_r \) of self-adjoint operators on the same Hilbert space, the set of upper bounds \( \mathcal{A} := \{ Y : Y \geq A_k, k = 1, \ldots, r \} \) has no minimal element in general. The following example shows that a minimal element may not exist even if all the \( A_k \) commute with each other.

\[\text{Example C.1. Let } \mathcal{H} = \mathbb{C}^2, \text{ and let the operators } A_1, A_2, Y_{\alpha,\beta,\delta} \text{ be given by their matrices in the standard basis of } \mathbb{C}^2 \text{ as}
\]

\[
A_1 := \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix}, \quad A_2 := \begin{bmatrix} 2 & 0 \\ 0 & 1 \end{bmatrix}, \quad Y_{\alpha,\beta,\delta} := \begin{bmatrix} 2 + \alpha & \delta \\ \frac{\delta}{\bar{\delta}} & 2 + \beta \end{bmatrix}.
\]

Let \( \mathcal{I} := \{ (\alpha, \beta, \delta) \in \mathbb{R}^3 : \alpha, \beta \geq 0, \min\{\alpha, \beta\} + \alpha \beta \geq |\delta|^2 \} \). It is easy to see that \( \mathcal{U}(A_1, A_2) = \{ Y : Y \geq A_1, A_2 \} = \{ Y_{\alpha,\beta,\delta} : (\alpha, \beta, \delta) \in \mathcal{I} \} \). Assume that \( \mathcal{U}(A_1, A_2) \) has a minimal element \( Y \). The assumption \( Y \geq A_1, A_2 \) yields that \( Y_{11} \geq 2 \) and \( Y_{22} \geq 2 \), while the assumption that \( Y \leq Y_{\alpha,\beta,\delta} \) for all \( (\alpha, \beta, \delta) \in \mathcal{I} \) yields that \( Y_{11} \leq 2 \) and \( Y_{22} \leq 2 \). Hence, \( 0 \leq Y - A_1 = \begin{bmatrix} 1 & Y_{12} \\ Y_{12} & 0 \end{bmatrix} \), which yields \( Y_{12} = 0 \), i.e., \( Y = 2I \). Now, \( Y_{\alpha,\beta,\delta} - Y \geq 0 \) if and only if \( \alpha, \beta \geq 0 \) and \( \alpha \beta \geq |\delta|^2 \), which defines a strictly smaller set than \( \mathcal{I} \), contradicting our initial assumption that \( Y \) is a lower bound to \( \mathcal{U}(A_1, A_2) \).

In general, the set \( \mathcal{A} := \{ Y : Y \geq A_k, k = 1, \ldots, r \} \) is the intersection of \( r \) cones, and the intersection of two cones is not itself a cone, unless one is completely contained in the other. Thus, \( \mathcal{A} \) has no unique minimal element in general, in the sense that there would be an element \( Y_0 \) such that \( Y_0 \leq Y \) for all \( Y \in \mathcal{A} \). Rather, there is an infinity of minimal elements, in the sense that there is an infinity of operators \( Y \in \mathcal{A} \) for which no other \( Y' \in \mathcal{A} \) exists such that \( Y' \leq Y \), and these minima constitute the boundary of \( \mathcal{A} \). The upshot is that one can not define a least upper bound on the basis of the PSD ordering alone.

However, there is a unique minimal element within \( \mathcal{A} \) in terms of the trace ordering. We can therefore define a least upper bound in this more restrictive sense as

\[
\text{LUB}(A_1, \ldots, A_r) := \arg \min_Y \{ \text{Tr} Y : Y \geq A_k, k = 1, \ldots, r \}.
\]
To make sense of the definition, we have to prove the uniqueness of the minimizer. For the proof, we will need the following simple fact, which has been stated, e.g., in [2] without a proof. Here we provide a proof for readers’ convenience.

**Lemma C.2.** Let \( D, T \in \mathcal{B}(\mathcal{H}) \) be self-adjoint operators such that \( D \geq \pm T \). Then \( D \) is positive semidefinite, and its support dominates the support of \( T \).

**Proof.** First, \( D \geq \pm T \) implies \( D \geq (T + (-T))/2 = 0 \), proving that \( D \) is PSD. Let \( \mathcal{H}_1 \) denote the support of \( D \), and decompose \( \mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2 \). Then \( D \) and \( T \) can be written in the corresponding block forms as \( D = \begin{bmatrix} D_{11} & 0 \\ 0 & 0 \end{bmatrix} \) and \( T = \begin{bmatrix} T_{11} & T_{12} \\ T_{12}^* & T_{22} \end{bmatrix} \), and positive semidefiniteness of \( D \pm T \) implies \( 0 \geq T_{22} \geq 0 \). Using again that \( D + T \geq 0 \), we finally obtain that \( T_{12} = 0 \), too, from which the assertion follows. \( \square \)

**Theorem C.3.** Let \( A_1, \ldots, A_r \in \mathcal{B}(\mathcal{H})_{sa} \) be a finite number of self-adjoint operators. Then in the set \( \mathcal{A} := \{ Y : Y \geq A_1, \ldots, A_r \} \) there is a unique element with minimal trace.

**Proof.** Let us assume that there are two distinct elements \( Y_1 \) and \( Y_2 \) in \( \mathcal{A} \) with minimal trace \( \text{Tr} Y_1 = \text{Tr} Y_2 \). Let \( Y_m = (Y_1 + Y_2)/2 \) and \( \Delta = (Y_1 - Y_2)/2 \). Then \( Y_1 = Y_m + \Delta \) and \( Y_2 = Y_m - \Delta \), and \( Y_1, Y_2 \geq A_i \) implies \( Y_m - A_i \geq \pm \Delta \). Hence, by Lemma C.2, there exists a constant \( c_i > 0 \) such that \( Y_m - A_i \geq c_i |\Delta| \) for every \( i = 1, \ldots, r \). Taking \( c := \min_i c_i \), we have \( Y_m - c |\Delta| \geq A_i, i = 1, \ldots, r \). Thus, \( Y_m - c |\Delta| \in \mathcal{A} \), but \( \text{Tr}(Y_m - c |\Delta|) = \text{Tr} Y_m - c \text{Tr} |\Delta| < \text{Tr} Y_m = \text{Tr} Y_i, i = 1, 2 \), contradicting our original assumption. \( \square \)

Next, we explore some properties of the LUB. It is easy to see from (68) that the LUB satisfies the **translation property**:

\[
\text{LUB}(A_1 + B, \ldots, A_r + B) = \text{LUB}(A_1, \ldots, A_r) + B.
\]  
(69)

This is because the addition \( X \mapsto X + B \), with a fixed self-adjoint operator \( B \), is an order-preserving operation. Furthermore, the LUB is jointly homogeneous: for any \( c \geq 0 \),

\[
\text{LUB}(cA_1, \ldots, cA_r) = c \text{LUB}(A_1, \ldots, A_r).
\]  
(70)

The positive part and modulus can be expressed in terms of the LUB.

**Lemma C.4.** For all Hermitian operators \( A \),

\[
A^+ = \text{LUB}(A, 0), \quad \text{and} \quad |A| = \text{LUB}(A, -A).
\]  
(71)

**Proof.** Consider the set \( \mathcal{A} = \{ Y : Y \geq A, Y \geq 0 \} \). Clearly, \( A^+ \in \mathcal{A} \). By Weyl’s monotonicity principle, the eigenvalues of any \( Y \in \mathcal{A} \) are non-negative and not smaller than those of \( A \): that is, \( \lambda_j(Y) \geq \lambda_j(A) \), where \( \lambda_j \) denotes the \( j \)th largest eigenvalue. Hence, \( \lambda_j(Y) \geq \lambda_j(A^+) \), since the spectrum of \( A^+ \) consists of the positive eigenvalues of \( A \) and zero. As the sum of all eigenvalues is the trace, \( A^+ \) is an element (and therefore the element) in \( \mathcal{A} \) with minimal trace.

Using (69) and (70), the modulus \( |A| = 2A^+ - A \) can be similarly expressed as \( |A| = 2 \text{LUB}(A, 0) - A = \text{LUB}(A, -A) \). \( \square \)

Hence, by (69), \( (A - B)^+ = \text{LUB}(A, B) - B \). This immediately leads to a closed form expression for the LUB of two Hermitian operators:
Lemma C.5. For all Hermitian operators $A, B$,

$$
LUB(A, B) = B + (A - B)_+ = \frac{1}{2}(A + B + |A - B|) = A + (A - B)_-.
$$

(72)

From these expressions it is clear that for $A, B \geq 0$, the LUB is PSD as well.

In a similar vein we can define the *greatest lower bound* (GLB) as

$$
GLB(A_1, \ldots, A_r) := \arg \max_Y \{\text{Tr } Y : Y \leq A_k, k = 1, \ldots, r\}.
$$

(73)

Clearly, we have

$$
GLB(A_1, \ldots, A_r) = -LUB(-A_1, \ldots, -A_r).
$$

(74)

Hence, for two operators, we get

Lemma C.6. For all Hermitian operators $A, B$,

$$
GLB(A, B) = \frac{1}{2}(A + B - |A - B|) = A - (A - B)_+ = B - (A - B)_-.
$$

(75)

A warning is in order about the sign of the GLB. When $A$ and $B$ commute, their GLB is given by the entrywise minimum in the joint eigenbasis. If $A$ and $B$ are also PSD, then clearly their GLB will be PSD. When $A$ and $B$ are PSD but do not commute, however, their GLB need not be PSD; only the trace of their GLB will be guaranteed to be non-negative. The reason is that while the function $x \mapsto x_+ = \max(0, x)$ is monotone increasing, it is also convex and therefore not operator monotone. Thus, for $A, B \geq 0$, $(A - B)_+ \leq A$ need not be true. For a concrete counterexample, take $A = |x\rangle\langle x|$, $B = |y\rangle\langle y|$ with $x = (1, 1)$, $y = (1, i)$; then it is easy to check that $0 \not\geq LUB(A, B)$. Similarly, the LUB of two negative semidefinite operators need not be negative semidefinite.

Both LUB and GLB are monotonous in their arguments with respect to the PSD ordering.

Lemma C.7. For all Hermitian operators $\{A_i\}$ and $\{B_i\}$, if $A_i \leq B_i$ then

$$
\text{Tr } LUB(A_1, \ldots, A_r) \leq \text{Tr } LUB(B_1, \ldots, B_r),
$$

$$
\text{Tr } GLB(A_1, \ldots, A_r) \leq \text{Tr } GLB(B_1, \ldots, B_r).
$$

(76) \hspace{1cm} (77)

Proof. By definition, $LUB(B_1, \ldots, B_r) \geq B_i \geq A_i$, for all $i$, so that $LUB(B_1, \ldots, B_r)$ is an upper bound on all $A_i$. In general it is not the minimal one, hence $\text{Tr } LUB(B_1, \ldots, B_r) \geq \text{Tr } LUB(A_1, \ldots, A_r)$. Monotonicity for the GLB follows from this and the correspondence [16].

The LUB and GLB (and their trace) behave in the expected way with respect to the direct sum:

Lemma C.8. For any pair of sets of $A_i \in \mathcal{B}(\mathcal{H}_1)_{sa}$ and $B_i \in \mathcal{B}(\mathcal{H}_2)_{sa}, i = 1, \ldots, r$,

$$
LUB(\{A_i \oplus B_i\}) = LUB(\{A_i\}) \oplus LUB(\{B_i\})
$$

$$
GLB(\{A_i \oplus B_i\}) = GLB(\{A_i\}) \oplus GLB(\{B_i\})
$$

(78) \hspace{1cm} (79)

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Proof. Consider first the LUB. For \( r = 2 \) the assertion follows trivially from the explicit expression \((72)\). For \( r > 2 \), it suffices to show that the LUB of \( \{A_i \oplus B_i\} \) is a direct sum as well, since among all upper bounds that decompose as direct sums, \( \text{LUB}\{A_i\} \oplus \text{LUB}\{B_i\} \) is the one with minimal trace. Let \( X := \text{LUB}\{A_i \oplus B_i\} \), and let \( P_i \) denote the projection onto \( \mathcal{H}_i \) in the direct sum \( \mathcal{H}_1 \oplus \mathcal{H}_2 \). Then \( P_i X P_i \oplus P_2 X P_2 \geq A_i \oplus B_i \) for all \( i \), and \( \text{Tr} \, X = \text{Tr} \, P_i X P_i \oplus P_2 X P_2 \). The uniqueness of the LUB then yields \( X = P_i X P_i \oplus P_2 X P_2 \).

The proof for the GLB goes exactly the same way.

This lemma has an important consequence. For every set of non-normalised states \( \{A_i\} \) there is a set of normalised states \( \{\sigma_i\} \) such that \( \text{Tr} \, \text{GLB}\{A_i\} = \text{Tr} \, \text{GLB}\{\sigma_i\} \), namely \( \sigma_i = A_i \oplus (1 - \text{Tr} \, A_i)\langle i|i \rangle \). This is because the ‘appended’ states \( B_i = (1 - \text{Tr} \, A_i)\langle i|i \rangle \) are mutually orthogonal so that \( \text{Tr} \, \text{GLB}\{B_i\} = 0 \). Similar statements can be made when the arguments of \( \text{Tr} \, \text{GLB} \) are linear combinations of states. The upshot of this is two-fold. First, for a large class of statements it allows one to restrict to normalised states to prove them. Secondly, it aids the heuristic processes of coming up with reasonable conjectures and finding counterexamples (see, e.g., at the end of Section 3).

Finally, we give another representation of the least upper bound as the max-relative entropy center in the case where all the operators are positive semidefinite. For PSD operators \( A, B \in \mathcal{B}(\mathcal{H})_+ \), their max-relative entropy \( D_{\max}(A \parallel B) \) is defined as \([12, 47]\)

\[
D_{\max}(A \parallel B) := \inf \{ \gamma : A \leq 2^\gamma B \}.
\]

For a set of states \( A \subset \mathcal{S}(\mathcal{H}) \), its max-relative entropy radius \( R_{\max}(A) \) is defined as \( R_{\max}(A) := \inf_{\omega \in \mathcal{S}(\mathcal{H})} \sup_{\sigma \in A} D_{\max}(\sigma \parallel \omega) \). For the interpretation of this quantity in quantum information theory, see, e.g. \([27, 32, 33]\) and references therein. We extend this definition to general positive semidefinite operators by keeping the reference \( \omega \) varying only over the set of states. That is, for a set of PSD operators \( A \subset \mathcal{B}(\mathcal{H})_+ \), its max-relative entropy radius \( R_{\max}(A) \) is defined as

\[
R_{\max}(A) := \inf_{\omega \in \mathcal{S}(\mathcal{H})} \sup_{A \in A} D_{\max}(A \parallel \omega).
\]

Any state \( \omega \) where the infimum above is attained is called a \( D_{\max} \)-divergence center of \( A \).

If \( A = \{0\} \) then \( R_{\max}(A) = -\infty \), and any state is a divergence center. Assume for the rest that \( A = \{A_1, \ldots, A_r\} \) is finite, and it contains a non-zero element, and hence \( R := R_{\max}(A) \) is a finite number. By definition, for every \( n \in \mathbb{N} \), there exists an \( \omega_n \in \mathcal{S}(\mathcal{H}) \) such that \( A \leq 2^{R+1/n} \omega_n \) for every \( A \in A \). Since \( \mathcal{S}(\mathcal{H}) \) is compact, there exists a subsequence \( n_k, k \in \mathbb{N} \), such that \( \omega_{n_k}, k \in \mathbb{N} \), is convergent. Let \( \omega^* := \lim_{k \to \infty} \omega_{n_k} \); then \( A \leq 2^R \omega^* \) for every \( A \in A \), and hence \( \omega^* \) is a divergence center. Thus, the set of divergence centers is non-empty. Obviously, if \( \omega \) is a divergence center then \( 2^R \omega \) is an upper bound to \( A \), and hence \( 2^R \omega \geq \text{LUB}(A) \) = \( L \). Let \( \bar{R} := \log \text{Tr} \, L \) and \( \bar{\omega} := L/\text{Tr} \, L \). Then \( 2^\bar{R} \omega \geq L \) yields \( R \geq \bar{R} \), while \( A \leq 2^{\bar{R}} \bar{\omega} \) due to the definition of \( \text{LUB}(A) \), and hence \( R \leq \bar{R} \). Thus, \( R = \bar{R} \), i.e., \( \text{Tr}(2^R \omega) = \text{Tr} \, \text{LUB}(A) \). Taking into account that \( 2^R \omega \geq L \), this implies that \( 2^\bar{R} \omega = \text{LUB}(A) \). Thus, the \( D_{\max} \)-divergence center is unique, and is equal to \( \text{LUB}(A)/\text{Tr} \, \text{LUB}(A) \), while \( R_{\max}(A) = \log \text{Tr} \, \text{LUB}(A) \).

According to \([33]\) (see also Appendix \([12]\)), this can be rewritten as \( \log P_e(A_1, \ldots, A_r) = R_{\max}(A) \). A similar expression for the optimal error probability in terms of the max-relative entropy has been given in \([27]\).
D Semidefinite program representations of success and error probabilities

The average success probability of a POVM \(\{E_k\}\) for discriminating between \(r\) PSD operators \(\{A_k\}_{k=1}^r\) is given by
\[
P_s(\{E_k\}) = \sum_{k=1}^r \text{Tr}(A_k E_k),
\]
(80)
and the optimal success probability \(P^*_s\) is the maximum over all POVMs:
\[
P^*_s = \max \{P_s(\{E_k\}) : \{E_k\}_{k=1}^r \text{ POVM}\}.
\]
(81)

In this section we consider the consequences of the following simple observation \cite{53}: in (81) the maximum of a linear functional is taken over the set of POVMs, which is a convex set. This optimisation problem is therefore a so-called semidefinite program (SDP) \cite{52}. One consequence is that \(P^*_s\) can be efficiently calculated numerically by SDP solvers even when no closed form analytical solution exists. Another, theoretically important consequence is that the duality theory of SDPs allows to express the value of \(P^*_s\) in a dual way as a minimisation problem \cite{13,26}.

The Lagrangian of problem (81) is
\[
\mathcal{L} = \sum_k \text{Tr}(A_k E_k) + \sum_k \text{Tr}(Z_k E_k) + \text{Tr} Y \left( I - \sum_k E_k \right)
\]
\[
= \text{Tr} Y + \sum_k \text{Tr} E_k (A_k + Z_k - Y),
\]
where the operators \(Z_k\) and \(Y\) are the Lagrange multipliers of the problem. If the \(Z_k\) are taken to be PSD, we see that always \(P_s(\{E_k\}) \leq \mathcal{L}\). This does not change when maximising over all POVMs, and certainly not when in the maximisation of \(\mathcal{L}\) over the \(E_k\) the POVM constraints are dropped. Hence \(P^*_s \leq \max_{E_k} \mathcal{L}\). This unconstrained maximisation is easy to do; when \(Y = A_k + Z_k\) for all \(k\), \(\max_{E_k} \mathcal{L} = \text{Tr} Y\), otherwise it is positive infinity. Minimising this upper bound over all PSD \(Z_k\) and all \(Y\) yields the best upper bound on \(P^*_s\). The positivity condition on the \(Z_k\) can be replaced by requiring that for all \(k\), \(Y \geq A_k\). Minimising over such \(Y\) then gives
\[
P^*_s \leq \min_Y \{\text{Tr} Y : Y \geq A_k, k = 1 \ldots r\},
\]
which is again an SDP, called the dual of the original (primal) SDP (a result first derived in \cite{13} equations (15) and (16)).

Therefore, the optimal success probability is bounded above by the trace of the LUB of all weighted density operators:
\[
P^*_s \leq \text{Tr LUB}(A_1, \ldots, A_r).
\]
(82)
Note that in the classical case (all \(A_k\) are diagonal, with diagonal elements \(A_k(j) = p_i q_i(j)\)) the LUB is the entrywise maximum, so that the dual SDP reproduces the maximum-likelihood formula \(P^*_s = \sum_j \max_i(A_i(j))\).
The difference between the maximum of the primal SDP \( P^*_s \) and the minimum of the dual SDP is called the duality gap. One can show that the duality gap is zero, provided some mild technical conditions are satisfied (e.g. Slater’s conditions), in which case equality holds:

\[
P^*_s = \text{Tr} \text{LUB}(A_1, \ldots, A_r).
\]  

(83)

If the duality gap is zero, then the optimal \( Z_k \) and the optimal POVM \( \{ E_k \} \) must necessarily satisfy a simple relation, called the complementary slackness condition. Indeed, as \( \text{Tr} Y^* = \text{Tr}(Y \sum_k E_k^*) \) and \( Y - A_k = Z_k \), the equality \( \sum_k \text{Tr} A_k E_k^* = \text{Tr} Y^* \) implies \( \sum_k \text{Tr}(Z_k^* E_k^*) = 0 \). Since all \( Z_k^* \) and \( E_k^* \) are required to be PSD, this actually means that

\[
Z_k^* E_k^* = 0, \forall k.
\]  

(84)

A simple consequence of these complementary slackness conditions is obtained by summing over \( k \):

\[
\sum_k Z_k^* E_k^* = 0.
\]

(85)

Combined with the conditions \( Y^* \geq A_k \) for all \( k \), these are the optimality conditions first obtained by Yuen, Kennedy and Lax [53].

## E Proof of Tyson’s theorems

(Theorem 6.1). Let \( A_1, \ldots, A_r \in \mathcal{B}(\mathcal{H})_+ \) and \( \{ E_k = X_k^* X_k \} \) be a POVM. Then

\[
\Gamma(\{X_k\}) \leq P_e(\{E_k\}) \leq 2 \Gamma(\{X_k\}).
\]

In particular, for the optimal POVM and optimal \( X_k \) that achieve the minimum:

\[
\Gamma^* \leq P^*_e \leq 2 \Gamma^*.
\]

Proof. For any operator \( X \) with \( \|X\| \leq 1 \) and any quantum state \( \sigma \) we have

\[
1 - \|X\sigma\|_1 \leq 1 - \text{Tr}(X^* X \sigma) \leq 1 - \|X\sigma\|_1^2 \leq 2(1 - \|X\sigma\|_1).
\]  

(86)

The first two inequalities both follow from Hőlder’s inequality ([10], Cor IV.2.6):

\[
\text{Tr}(X^* X \sigma) \leq \|X^* X \sigma\|_1 \leq \|X\sigma\|_1 \|X\| \leq \|X\sigma\|_1,
\]

and

\[
\|X\sigma\|_1^2 = \left\| (X\sigma^{1/2}) \sigma^{1/2} \right\|_1^2 \leq \left\| X \sigma^{1/2} \right\|_2 \left\| \sigma^{1/2} \right\|_2^2 = \text{Tr} X^* X \sigma
\]

and the last inequality follows from \( 1 - x^2 \leq 2(1 - x) \) for all \( x \). Applying (86) for \( \sigma_k := A_k / \text{Tr} A_k \) and \( X_k \) and summing over \( k \) yields

\[
\sum_{k=1}^r (\text{Tr} A_k) (1 - \|X_k \sigma_k\|_1) \leq \sum_{k=1}^r (\text{Tr} A_k) (1 - \text{Tr}(X_k^* X_k \sigma_k)) \leq 2 \sum_{k=1}^r (\text{Tr} A_k) (1 - \|X_k \sigma_k\|_1).
\]

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Taking the minimum over all \( X_k \) then yields the inequalities of the theorem.

**Theorem 6.2.** Let \( A_1, \ldots, A_r \in \mathcal{B}(\mathcal{H})_+ \) and \( A_0 := \sum_i A_i \). Then

\[
\Gamma^* = \text{Tr} A_0 - \text{Tr} \left( \sum_{i=1}^r A_i^2 \right)^{1/2},
\]

with the optimal measurement operators being those of the SQ measurement.

**Proof.** In the following we will abbreviate the expression \( \sum_{k=1}^r A_k^2 \) by \( S \).

First note that the operator \( \bigoplus_k X_k A_k \) is a pinching of the block operator \( (X_j A_k)_{j,k} \). This operator is the product of the column block operator \( \mathcal{X} := (X_j)_{j,1} \) and the row block operator \( \mathcal{A} := (A_k)_{1,k} \). Because unitarily invariant norms do not increase under pinchings, we get

\[
\sum_k \| X_k A_k \|_1 = \left\| \bigoplus_k X_k A_k \right\|_1 \leq \|(X_j A_k)_{j,k}\|_1 = \|\mathcal{X} \mathcal{A}\|_1 = \text{Tr} (\mathcal{A}^* \mathcal{X}^* \mathcal{X} \mathcal{A})^{1/2}.
\]

Noting that \( \mathcal{X}^* \mathcal{X} = \sum_k X_k^* X_k = I \) yields

\[
\text{Tr} (\mathcal{A}^* \mathcal{X}^* \mathcal{X} \mathcal{A})^{1/2} = \text{Tr} (\mathcal{A}^* \mathcal{A})^{1/2} = \|\mathcal{A}\|_1 = \|\mathcal{A}^*\|_1 = \text{Tr} S^{1/2}.
\]

Hence,

\[
\sum_k \| X_k A_k \|_1 \leq \text{Tr} S^{1/2}.
\]

Equality can be achieved by taking the SQ measurement, \( X_k = A_k S^{-1/2} \). Indeed, from \( X_k A_k = A_k S^{-1/2} A_k \geq 0 \), we get

\[
\sum_k \| X_k A_k \|_1 = \sum_k \text{Tr}(X_k A_k) = \text{Tr} \left( S^{-1/2} \sum_k A_k^2 \right) = \text{Tr} S^{1/2}.
\]

This shows that the maximum of \( \sum_k \| X_k A_k \|_1 \) over any complete set of \( r \) measurement operators \( \{X_k\} \) is achieved for \( X_k = A_k S^{-1/2} \) and is given by \( \text{Tr} S^{1/2} \). Hence, \( \Gamma^* = \text{Tr} A_0 - \text{Tr} S^{1/2} \), which is (87).

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