Distinguishability and Accessible Information in Quantum Theory

Dissertation
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To

my mother Geraldine, who has been with me every day of my life

and to

my brother Mike, who gave me a frontier to look toward
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Distinguishability and Accessible Information in Quantum Theory

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ABSTRACT

Quantum theory forbids physical measurements from giving observers enough evidence to distinguish nonorthogonal quantum states—this is an expression of the indeterminism inherent in all quantum phenomena. As a consequence, operational measures of how distinct one quantum state is from another must depend exclusively on the statistics of measurements and nothing else. This compels the use of various information-theoretic measures of distinguishability for probability distributions as the starting point for quantifying the distinguishability of quantum states. The process of translating these classical distinguishability measures into quantum mechanical ones is the focus of this dissertation. The measures so derived have important applications in the young fields of quantum cryptography and quantum computation and, also, in the more established field of quantum communication theory.

Three measures of distinguishability are studied in detail. The first—*the statistical overlap* or *fidelity*—upper bounds the decrease (with the number of measurements on identical copies) of the probability of error in guessing a quantum state’s identity. The second—*the Kullback-Leibler relative information*—quantifies the distinction between the frequencies of measurement outcomes when the true quantum state is one or the other of two fixed possibilities. The third—*the mutual information*—is the amount of information that can be recovered about a state’s identity from a measurement; this quantity dictates the amount of redundancy required to reconstruct reliably a message whose bits are encoded by quantum systems prepared in the specified states. For each of these measures, an optimal quantum measurement is one for which the measure is as large or as small (whichever is appropriate) as it can possibly be. The “quantum distinguishability” for each of the three measures is its value when an optimal measurement is used for defining it. Generally all these quantum distinguishability measures correspond to different optimal measurements.

The results reported in this dissertation include the following. An exact expression for the quantum fidelity is derived, and the optimal measurement that gives rise to it is studied in detail. The techniques required for proving this result are very useful and may be applied to other, quite different problems. Several upper and lower bounds on the quantum mutual information are derived via similar techniques and compared to each other. Of particular note is a simplified derivation for the important upper bound first proved by Holevo in 1973. An explicit expression is given for another (tighter) upper bound that appears implicitly in the same derivation. Several upper and lower bounds to the quantum Kullback information are also derived. Particular attention is paid to a technique for generating successively tighter lower bounds, contingent only upon one’s ability to solve successively higher order nonlinear matrix equations.

In the final Chapter, the distinguishability measures developed here are applied to a question at the foundation of quantum theory: to what extent must quantum systems be disturbed by
information gathering measurements? This is tackled in two ways. The first is in setting up a general formalism for ferreting out the tradeoff between inference and disturbance. The main breakthrough in this is that it gives a way of expressing the problem so that it appears as algebraic as that of the problem of finding quantum distinguishability measures. The second result on this theme is the proof of a theorem that prohibits “broadcasting” an unknown quantum state. That is to say, it is proved that there is no way to replicate an unknown quantum state onto two separate quantum systems when each system is considered without regard to the other (though there may well be correlation or quantum entanglement between the systems). This result is a significant extension and generalization of the standard “no-cloning” theorem for pure states.
## Contents

1 Prolegomenon
   1.1 Introduction ........................................... 1
   1.2 Summary of Results ................................... 3
   1.3 Essentials ............................................. 8
      1.3.1 What Is a Probability? ........................... 8
      1.3.2 What Is a Quantum State? ......................... 9
      1.3.3 What Is a Quantum Measurement? ................. 10

2 The Distinguishability of Probability Distributions ........ 12
   2.1 Introduction ........................................... 12
   2.2 Distinguishability via Error Probability and the Chernoff Bound ... 13
      2.2.1 Probability of Error ............................. 13
      2.2.2 The Chernoff Bound ................................ 16
   2.3 Distinguishability via “Keeping the Expert Honest” .............. 20
      2.3.1 Derivation of the Kullback-Leibler Information ... 21
      2.3.2 Properties of the Relative Information .......... 25
   2.4 Distinguishability via Mutual Information .................... 29
      2.4.1 Derivation of Shannon’s Information Function .... 30
      2.4.2 An Interpretation of the Shannon Information .... 35
      2.4.3 The Mutual Information ............................ 41

3 The Distinguishability of Quantum States ..................... 42
   3.1 Introduction ........................................... 42
   3.2 The Quantum Error Probability .......................... 44
      3.2.1 Single Sample Case ............................... 44
      3.2.2 Many Sample Case ................................ 46
   3.3 The Quantum Fidelity ................................... 47
      3.3.1 The General Derivation ............................ 50
      3.3.2 Properties ....................................... 55
      3.3.3 The Two-Dimensional Case ....................... 59
   3.4 The Quantum Rényi Overlaps ............................. 60
   3.5 The Accessible Information ............................... 64
      3.5.1 The Holevo Bound .................................. 65
      3.5.2 The Lower Bound $L(t)$ ............................ 72
      3.5.3 The Upper Bound $L(t)$ ............................. 74
      3.5.4 The Two-Dimensional Case ....................... 79
      3.5.5 Other Bounds ..................................... 82
<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.5.6 Photo Gallery</td>
<td>88</td>
</tr>
<tr>
<td>3.6 The Quantum Kullback Information</td>
<td>89</td>
</tr>
<tr>
<td>3.6.1 The Umegaki Relative Information</td>
<td>96</td>
</tr>
<tr>
<td>3.6.2 One Million One Lower Bounds</td>
<td>98</td>
</tr>
<tr>
<td>3.6.3 Upper Bound Based on Ando’s Inequality and Other Bounds from the Literature</td>
<td>100</td>
</tr>
<tr>
<td>4 Distinguishability in Action</td>
<td>102</td>
</tr>
<tr>
<td>4.1 Introduction</td>
<td>102</td>
</tr>
<tr>
<td>4.2 Inference vs. Disturbance of Quantum States: Extended Abstract</td>
<td>102</td>
</tr>
<tr>
<td>4.2.1 The Model</td>
<td>103</td>
</tr>
<tr>
<td>4.2.2 The Formalism</td>
<td>105</td>
</tr>
<tr>
<td>4.2.3 Tradeoff Relations</td>
<td>108</td>
</tr>
<tr>
<td>4.3 Noncommuting Quantum States Cannot Be Broadcast</td>
<td>113</td>
</tr>
<tr>
<td>5 References for Research in Quantum Distinguishability and State Disturbance</td>
<td>122</td>
</tr>
<tr>
<td>5.1 Progress Toward the Quantum Problem</td>
<td>122</td>
</tr>
<tr>
<td>5.2 Classical Distinguishability Measures and Information Theory</td>
<td>135</td>
</tr>
<tr>
<td>5.3 Matrix Inequalities, Operator Relations, and Mathematical Techniques</td>
<td>145</td>
</tr>
<tr>
<td>Bibliography</td>
<td>155</td>
</tr>
</tbody>
</table>
List of Figures

2.1 Binary Question Schemes ................................................. 36
2.2 Coding Tree Imbedded in a Full Tree ................................. 38

3.1 Probability of error in guessing a photon’s polarization that is either horizontal or 45° from the horizontal. Error probability is plotted here as a function of measurement (i.e., radians from the horizontal) and number of measurement repetitions $M$ before the guess is made. .................................................. 48
3.2 The Holevo upper bound $S(t)$, the upper bound $L(t)$, the information $I(t)$ extractable by optimal orthogonal projection-valued measurement (found numerically), the lower bound $M(t)$, and the Jozsa-Robb-Wootters lower bound $Q(t)$, all for the case that $\hat{\rho}_0$ is pure ($a = 1$), $\hat{\rho}_1$ is mixed with $b = 2/3$, and the angle between the two Bloch vectors is $\pi/3$. ............................................................... 83
3.3 All the bounds to accessible information studied here, for the case that $\hat{\rho}_0$ is pure ($a = 1$), $\hat{\rho}_1$ is mixed with $b = 2/3$, and the angle between the two Bloch vectors is $\pi/4$. ............................................................. 90
3.4 All the bounds to accessible information studied here, for the case that $\hat{\rho}_0$ and $\hat{\rho}_1$ are pure states ($a = b = 1$) and the angle between the two Bloch vectors is $\pi/4$. For this case, $M(t) = P(t) = I(t)$. ................................................. 91
3.5 All the bounds to accessible information studied here, for the case that $\hat{\rho}_0$ and $\hat{\rho}_1$ are mixed states with $a = \frac{4}{5}$ and $b = \frac{3}{5}$ and the angle between the two Bloch vectors is $\pi/3$. ................................................................. 92
3.6 All the bounds to accessible information studied here, for the case that $\hat{\rho}_0$ and $\hat{\rho}_1$ are pure states ($a = b = 1$) and the angle between the two Bloch vectors is $\pi/3$. For this case, $M(t) = P(t) = I(t)$. ................................................. 93
3.7 The bounds $S(t)$, $L(t)$, $M(t)$, and $P(t)$ for the case that $\hat{\rho}_0$ and $\hat{\rho}_1$ are mixed states with $a = \frac{4}{5}$ and $b = \frac{3}{5}$ and the angle between the two Bloch vectors is $\pi/5$. ...................................................... 94
3.8 The bounds $S(t)$, $L(t)$, $M(t)$, and $P(t)$ for the case that $\hat{\rho}_0$ and $\hat{\rho}_1$ are mixed states with $a = b = \frac{4}{5}$ and the angle between the two Bloch vectors is $\pi/4$. ...................................................... 95

4.1 Set-up for Inference–Disturbance Tradeoff .............................. 104
Chapter 1

Prolegomenon

“The information’s unavailable to the mortal man.”
—Paul Simon
Slip Slidin’ Away

1.1 Introduction

Suppose a single photon is secretly prepared in one of two known but nonorthogonal linear polarization states $\vec{e}_0$ and $\vec{e}_1$. A fundamental consequence of the indeterminism inherent in all quantum phenomena is that there is no measurement whatsoever that can discriminate which of the two states was actually prepared. For instance, imagine an attempt to ascertain the polarization value by sending the photon through a beam splitter; the photon will either pass straight through or be deflected in a direction dependent upon the crystal’s orientation $\vec{n}$. In this example, the only means available for the photon to “express” the value of its polarization is through the quantum mechanical probability law for it to go straight

$$p_i = |\vec{e}_i \cdot \vec{n}|^2, \quad i = 0, 1.$$  \hspace{1cm} (1.1)

Since the polarization vectors $\vec{e}_i$ are nonorthogonal, there is no orientation $\vec{n}$ that can assure that only one preparation will pass straight through while the other is deflected. To the extent that one can gain information by sampling a probability distribution, one can also gain information about the preparation, but indeed only to that extent. If the photon goes straight through, one might conjecture that $p_i$ is closer to 1 than not, and thus that the actual polarization is the particular $\vec{e}_i$ most closely aligned with the crystal orientation $\vec{n}$, but there is no clean-cut certainty here. Ultimately one must make do with a guess. The necessity of this guess is the unimpeachable signature of quantum indeterminism.

Fortunately, quantum phenomena are manageable enough that we are allowed at least the handle of a probability assignment in predicting their behavior. The world is certainly not the higgledy-piggledy place it would be if we were given absolutely no predictive power over the phenomena we encounter. This fact is the foundation for this dissertation. It provides a starting point for building several notions of how distinct one quantum state is from another.

Since there is no completely reliable way to identify a quantum state by measurement, one cannot simply reach into the space of quantum states, place a yardstick next to the line connecting two of them, and read off a distance. Similarly one cannot reach into the ethereal space of probability assignments. Nevertheless classical information theory does give several ways to gauge the
distinction between two probability distributions. The idea of the game of determining a quantum distinguishability measure is to start with one of the ones specified by classical information theory. The probabilities appearing in it are assumed to be generated by a measurement on a system described by the quantum states that one wants to distinguish. The quantum distinguishability is defined by varying over all possible measurements to find the one that makes the classical distinguishability the best it can possibly be. The best classical distinguishability found in this search is dubbed the quantum measure of distinguishability.

Once reasonable measures of quantum distinguishability are in hand, there are a great number of applications in which they can be used. To give an example—one to which we will return in the final chapter—step back to 1927, the year quantum mechanics became a relatively stable theory. The question that was the rage was why an electron could not be ascribed a classical state of motion. The answer—so the standard story of that year and thereafter goes—is that whenever one tries to discern the position of an electron, one necessarily disturbs its momentum in an uncontrollable way. Similarly, whenever one tries to discern the momentum, the position is necessarily disturbed. One can never get at both quantities simultaneously. Thus there are no means to specify operationally a phase space trajectory for the electron.

Yet if one looks carefully at the standard textbook Heisenberg relation of Robertson [1], the first one derived without recourse to semiclassical thought experiments, one finds nothing even remotely resembling this picture. What is found instead is that when many copies of a system are all prepared in the same quantum state $\psi(x)$, if one makes enough position measurements on the copies to get an estimate of $\Delta x$, and similarly makes enough momentum measurements on (different!) copies to get $\Delta p$, then one can be assured that the product of the numbers so found will be no smaller than $\hbar/2$. Any attempt to extend the meaning of this relation beyond this is dangerous and unwarranted.

Nevertheless there is most certainly truth to the idea that information gathering measurements in quantum theory necessarily cause disturbances. This is one of the greatest distinctions between classical physics and quantum physics, and is—after all—the ultimate reason that quantum systems cannot be ascribed classical states of motion. It is just that this is not captured properly by the Heisenberg relation. What is needed, among other things, are two ingredients considered in detail in this dissertation. The first is a notion of the information that can be gained about the identity of quantum state from a given measurement model. The second is a way of comparing the quantum state that describes a system before measurement to the quantum state that describes it after measurement—in short, one of the quantum distinguishability measures described above.

This gives some hint of the wealth that may lie at the end of the rainbow of quantum distinguishability and accessible information. First, however, there are many rainbows to be made [See Fig. 3.2], and this is the focus of the work reported here. In the remainder of this Chapter, we summarize the main results of our research and describe the salient features of probabilities, quantum states, and quantum measurements that will be the starting point for the later chapters. In Chapter 2, we describe in great detail the motivations for and derivations of several classical measures of distinguishability for probability distributions. Many of the things presented there are not well known to the average physicist, but little of the work represents original research. In Chapter 3—the main chapter of new results—we report everything we know about the quantum mechanical versions of the classical distinguishability measures introduced in Chapter 2. Chapter 4 applies the methods and measures developed in Chapter 3 to the deeper question of the tradeoff between information gathering and disturbance in quantum theory. The first section of Chapter 4 is devoted to developing a general formalism for tackling questions of this ilk. The second section (which represents a collaboration with H. Barnum, C. M. Caves, R. Jozsa, and B. Schumacher) proves that there is a very general sense in which it is impossible to make a copy of an unknown
quantum state. This is a result that extends the now-standard “no-cloning” theorem for pure quantum states \[2, 3\]. Chapter 5 caps off the dissertation with a comprehensive bibliography of 527 books and articles relevant to quantum distinguishability and quantum state disturbance.

1.2 Summary of Results

Mutual Information

As stated already, the main focus of this work is in deriving distinguishability measures for quantum mechanical states. First and foremost in importance among these is the one defined by the question of accessible information. In this problem’s simplest form, one considers a binary communication channel—i.e., a channel in which the alternative transmissions are 0 and 1. The twist in the quantum mechanical case is that the 0 and 1 are encoded physically as distinct states \( \hat{\rho}_0 \) and \( \hat{\rho}_1 \) of some quantum system (described on a \( D \)-dimensional Hilbert space, \( D \) being finite); the states \( \hat{\rho}_0 \) and \( \hat{\rho}_1 \) need not be orthogonal nor pure states for that matter. The idea here is to think of the transmissions more literally as “letters” that are mere components in much longer words and sentences, i.e., the meaningful messages to be sent down the channel. When the quantum states occur with frequencies \( \pi_0 \) and \( \pi_1 \), the channel encodes, according to standard information theory,

\[
H(\pi) = -(\pi_0 \log_2 \pi_0 + \pi_1 \log_2 \pi_1)
\]

(1.2)

bits of information per transmission. This scenario is of interest precisely because of the way in which quantum indeterminism bars any receiver from retrieving the full information encoded in the individual transmissions: there is generally no measurement with outcomes uniquely corresponding to whether 0 or 1 was transmitted.

The amount of information that is recoverable in this scheme is quantified by an expression called the mutual information. This quantity can be understood as follows. When the receiver performs a measurement to recover the message, he initially sees the quantum system neither in state \( \hat{\rho}_0 \) nor in state \( \hat{\rho}_1 \) but rather in the mean quantum state

\[
\hat{\rho} = \pi_0 \hat{\rho}_0 + \pi_1 \hat{\rho}_1 ;
\]

(1.3)

this is an expression of the fact that he does not know which message was sent. Therefore the raw information he gains upon measuring some nondegenerate Hermitian operator \( \hat{M} \), say,

\[
\hat{M} = \sum_b m_b |b\rangle\langle b|
\]

(1.4)

is the Shannon information

\[
H(p) = -\sum_b \langle b|\hat{\rho}|b\rangle \log_2 \langle b|\hat{\rho}|b\rangle
\]

(1.5)

of the distribution \( p(b) = \langle b|\hat{\rho}|b\rangle \) for the outcomes \( b \). This raw information, however, is not solely about the transmission; for, even if the receiver knew the system to be in one state over the other, measuring \( \hat{M} \) would still give him a residual information gain quantified by the Shannon formula for the appropriate distribution,

\[
p_0(b) = \langle b|\hat{\rho}_0|b\rangle \quad \text{or} \quad p_1(b) = \langle b|\hat{\rho}_1|b\rangle
\]

(1.6)

The residual information gain is due to the fact that the measurement outcome \( b \) is not deterministically predictable even with the transmission, 0 or 1, known. Given this, the mutual information
The uniquely quantum mechanical question that arises in this context is which measurement maximizes the mutual information for this channel and what is that maximal amount; this is the question of accessible information in quantum theory. The value of the maximal information, $I$, is called the accessible information.

Until recently, little has been known about the accessible information of a general quantum communication channel. The trouble is in not having sufficiently powerful techniques for searching over all possible quantum measurements, i.e., not only those measurements corresponding to Hermitian operators, but also the more general positive-operator-valued measures (POVMs) with any number of outcomes. Aside from a few contrived examples in which the accessible information can be calculated explicitly, the most notable results have been in the form of bounds—bounds on the number of outcomes in an optimal measurement \[4\] and bounds on the accessible information itself \[5, 6\].

Along these lines, several new tighter ensemble-dependent bounds are reported. Two of these—an upper and a lower bound—are found in the process of simplifying the derivation of the Holevo upper bound (an exercise useful in and of itself). The lower bound of this pair takes on a particularly pleasing form when $\hat{\rho}_0$ and $\hat{\rho}_1$ have a common null subspace:

$$
\pi_0 \text{tr} \left( \hat{\rho}_0 \log_2 \mathcal{L}_{\hat{\rho}}(\hat{\rho}_0) \right) + \pi_1 \text{tr} \left( \hat{\rho}_1 \log_2 \mathcal{L}_{\hat{\rho}}(\hat{\rho}_1) \right) \leq I ,
$$

where $\mathcal{L}_{\hat{\rho}}(\hat{\rho}_i)$, $i = 0, 1$, are operators that satisfy the anti-commutator equation

$$
\hat{\rho} \mathcal{L}_{\hat{\rho}}(\hat{\rho}_i) + \mathcal{L}_{\hat{\rho}}(\hat{\rho}_i) \hat{\rho} = 2 \hat{\rho}_i ,
$$

which has a solution in this case. It turns out that there is actually a measurement that generates this bound and—at least for two-dimensional Hilbert spaces—it is often very close to being optimal. When $\hat{\rho}_0$ and $\hat{\rho}_1$ are pure states this lower bound actually equals the accessible information.

Another significant bound on the accessible information comes about by thinking of the states $\hat{\rho}_0$ and $\hat{\rho}_1$ as arising from a partial trace over some larger Hilbert space with two possible pure states $|\psi_0\rangle$ and $|\psi_1\rangle$ on it. For any two such purifications the corresponding accessible information
will be larger than that for the original mixed states; this is because by expanding a Hilbert space one can only add distinguishability. However, the accessible information for two pure states can be calculated exactly; it is given by the appropriate analog to Eq. (1.10). Using a result for the maximal possible overlap between two purifications due to Uhlmann [7], one arrives at the tightest possible upper bound of this form.

**Statistical Overlap**

The second most important way of defining a notion of statistical distinguishability (see Section 3.3) concerns the following scenario. One imagines a finite number of copies, \( N \), of a quantum system secretly prepared in the same quantum state—either the state \( \hat{\rho}_0 \) or the state \( \hat{\rho}_1 \). It is the task of an observer to perform the same measurement on each of these copies and then, based on the collected data, to make a guess as to the identity of the quantum state. Intuitively, the more “distinguishable” the quantum states, the easier the observer’s task, but how does one go about quantifying such a notion? The idea is to rely on the probability of error \( P_e(N) \) in this inference problem to point the way. For instance, one might take the probability of error itself as a measure of statistical distinguishability and define the quantum distinguishability to be that quantity minimized over all possible quantum measurements. Appealing as this may be, a difficulty crops up in that the optimal quantum measurement in this case explicitly depends on the number of measurement repetitions, \( N \).

To get past this blemish, one can ask instead which measurement will cause the error probability to decrease exponentially as fast as possible in \( N \); that is to say, what is the smallest \( \lambda \) for which

\[
P_e(N) \leq \lambda^N.
\]

Classically, the best bound of this form is called the Chernoff bound, and is given by

\[
\lambda = \min_{0 \leq a \leq 1} \sum_b p_0(b)^a p_1(b)^{1-a},
\]

where \( p_0(b) \) and \( p_1(b) \) are the probability distributions for the measurement outcomes. The exponential rate of decrease in error probability, \( \lambda \), optimized over all measurements must be, by definition, independent of the number of measurement repetitions, and thus makes a natural (operationally defined) candidate for a measure of quantum distinguishability. Unfortunately the search for an explicit expression for this quantity remains a subject for future research. On the brighter side, however, there is a closely related upper bound on the Chernoff bound that is of interest in its own right—the **statistical overlap**.

If a measurement generates probabilities \( p_0(b) \) and \( p_1(b) \) for its outcomes, then the statistical overlap between these distributions is defined to be

\[
F(p_0, p_1) = \sum_b \sqrt{p_0(b) p_1(b)}.
\]

This quantity, as stated, gives a more simply expressed upper bound on \( \lambda \). This is quite important because this expression is manageable enough that it actually can be optimized to give a useful quantum distinguishability measure (even though it may not be as well-founded conceptually as \( \lambda \) itself). The optimal statistical overlap is given by

\[
F(\hat{\rho}_0, \hat{\rho}_1) = \text{tr} \sqrt{\hat{\rho}_1^{1/2} \hat{\rho}_0 \hat{\rho}_1^{1/2}} = \text{tr} \sqrt{\hat{\rho}_0^{1/2} \hat{\rho}_1 \hat{\rho}_0^{1/2}},
\]

which is explicitly independent of the number of measurement repetitions, \( N \).
a quantity known as the *fidelity for quantum states*, which has appeared in other mathematical physics contexts \[7, 9\]. (Here we start the trend in notation that the same function is used to denote both the classical distinguishability and its quantum version; notice that the former has the probability distributions as its argument and the latter has the density operators themselves.) This measure of distinguishability has many useful properties and is crucial to the proof of “no-broadcasting” in Chapter 4.

Of particular note is the way the technique used in finding the quantum fidelity reveals the actual measurement by which Eq. (1.14) is minimized. This measurement (i.e., orthonormal basis) is the one specified by the Hermitian operator

\[
\hat{M} = \hat{\rho}_1^{-1/2} \sqrt{\hat{\rho}_1^{1/2} \hat{\rho}_0 \hat{\rho}_1^{-1/2} \hat{\rho}_1^{1/2}},
\]

when \(\hat{\rho}_1\) is invertible. This technique comes in very handy for the problems considered in Chapter 4.

**Kullback-Leibler Relative Information**

The final information theoretic measure of distinguishability we consider can be specified by the following problem (see Section 3.6). Suppose \(N \gg 1\) copies of a quantum system are all prepared in the same state \(\hat{\rho}_1\). If some observable is measured on each of these, the most likely frequencies for its various outcomes \(b\) will be those given by the probabilities \(p_1(b)\) assigned by quantum theory. All other frequencies beside this “natural” set will become less and less likely for large \(N\) as statistical fluctuations in the frequencies eventually damp away. In fact, any set of outcome frequencies \(\{f(b)\}\)—distinct from the “natural” ones \(\{p_1(b)\}\)—will become exponentially less likely with the number of measurements according to \[10\]

\[
\text{PROB}\left(\text{freq }= \{f(b)\} \mid \text{prob }= \{p_1(b)\}\right) \approx e^{-NK(f/p_1)},
\]

where

\[
K(f/p_1) = \sum_b f(b) \ln \left( \frac{f(b)}{p_1(b)} \right)
\]

is the Kullback-Leibler relative information \[11\] between the frequency distribution \(f(b)\) and the probability distribution \(p_1(b)\). Therefore the quantity \(K(f/p_1)\), which controls the behavior of this exponential decline, says something about how dissimilar the frequencies \(\{f(b)\}\) are from the “natural” ones \(\{p_1(b)\}\). This gives an easy way to gauge the distinguishability of two probability distributions, as will be seen presently.

Suppose now that the same measurements as above are performed on quantum systems all prepared in the state \(\hat{\rho}_0\). The outcome frequencies most likely to appear in this scenario are again those specified by the probability distribution given by quantum theory—in this case \(p_0(b)\). This simple fact points to a natural way to define an optimal measurement for this problem. An optimal measurement is one for which the natural frequencies of outcomes for state \(\hat{\rho}_0\) are maximally improbable, given that \(\hat{\rho}_1\) is actually controlling the statistics. That is to say, an optimal measurement is one for which

\[
K(p_0/p_1) = \sum_b p_0(b) \ln \left( \frac{p_0(b)}{p_1(b)} \right)
\]

is as large as it can be. The associated quantum measure of distinguishability, called the *quantum Kullback information*, is just that maximal value \[12\].
The quantum Kullback information is much like the accessible information in that it contains a nasty logarithm in its definition. As such we have only been able to find bounds on this quantity. Two of the lower bounds take on particularly pretty forms:

\[
K_F(\hat{\rho}_0/\hat{\rho}_1) \equiv \text{tr} \left( \hat{\rho}_0 \ln \left( \mathcal{L}_{\hat{\rho}_1}(\hat{\rho}_0) \right) \right),
\]

and

\[
K_B(\hat{\rho}_0/\hat{\rho}_1) \equiv 2 \text{tr} \left( \hat{\rho}_0 \ln \left( \hat{\rho}_1^{-1/2} \sqrt{\hat{\rho}_1^{1/2} \hat{\rho}_0} \hat{\rho}_1^{1/2} \hat{\rho}_0^{-1/2} \hat{\rho}_1^{-1/2} \right) \right).\]

A very general procedure has also been found for generating successively tighter lower bounds than these. This procedure is, however, contingent upon one’s ability to solve higher and higher order nonlinear matrix equations. Several upper bounds to the quantum Kullback information are also reported.

**Inference–Disturbance Tradeoff for Quantum States**

With some results on the quantum distinguishability measures in hand, we turn our attention to the sorts of problems in which they may be used. A typical one is that already described in the Introduction: how might one gauge the necessary tradeoff between information gain and disturbance in quantum measurement? Not many results have yet poured from this direction, but we are able to go a long way toward defining the problem in its most general setting. The main breakthrough is in realizing a way to express the problem so that it becomes as algebraic as that of finding explicit formulae for the quantum distinguishability measures.

**The No-Broadcasting Theorem**

Suppose a quantum system, secretly prepared in one state from the set \( \mathcal{A} = \{\hat{\rho}_0, \hat{\rho}_1\} \), is dropped into a “black box” whose purpose is to broadcast or replicate that quantum state onto two separate quantum systems. That is to say, a state identical to the original should appear in each system when it is considered without regard to the other (though there may be correlation or quantum entanglement between the systems). Can such a black box be built?

The “no-cloning theorem” \[4, 3\] insures that the answer to this question is no when the states in \( \mathcal{A} \) are pure and nonorthogonal; for the only way to have each of the broadcast systems described separately by a pure state \( |\psi\rangle \) is for their joint state to be \( |\psi\rangle \otimes |\psi\rangle \). When the states are mixed, however, things are not so clear. There are many ways each broadcast system can be described by \( \hat{\rho} \) without the joint state being \( \hat{\rho} \otimes \hat{\rho} \), the mixed state analog of cloning. The systems may also be entangled or correlated in such a way as to give the correct marginal density operators.

For instance, consider the limiting case in which \( \hat{\rho}_0 \) and \( \hat{\rho}_1 \) commute and so may be thought of as probability distributions \( p_0(b) \) and \( p_1(b) \) for their eigenvectors. In this case, one easily sees that the states can be broadcast; the broadcasting device need merely perform a measurement of the eigenbasis and prepare two systems, each in the state corresponding to the outcome it finds. The resulting joint state is not of the form \( \hat{\rho} \otimes \hat{\rho} \) but still reproduces the correct marginal probability distributions and thus, in this case, the correct marginal density operators.

It turns out that two states \( \hat{\rho}_0 \) and \( \hat{\rho}_1 \) can be broadcast if and only if they commute.\[1\] The way this is demonstrated is via a use of the quantum fidelity derived in Chapter 3. One can show that the most general process or “black box” allowed by quantum mechanics can never increase

\[1\]This finding represents a collaboration with H. Barnum, C. M. Caves, R. Jozsa, and B. Schumacher.
the distinguishability of quantum states (as measured by fidelity); yet broadcasting requires that
distinguishability actually increase unless the quantum states commute.

This theorem is important because it draws a communication theoretic distinction between
commuting and noncommuting density operators. This is a distinction that has only shown up
before in the Holevo bound to accessible information: the bound is achieved by the accessible infor-
mation if and only if the signal states commute. The no-broadcasting result also has implications
for quantum cryptography.

1.3 Essentials

What are probability distributions? What are quantum systems? What are quantum states?
What are quantum measurements? We certainly cannot answer these questions in full in this short
treatise. However we need at least working definitions for these concepts to make any progress
at all in our endeavors. This Section details some basic ideas and formalism used throughout the
remainder of the dissertation. Also it lays the groundwork for some of the ideas presented in the
Postscript.

1.3.1 What Is a Probability?

In this document, we hold fast to the Bayesian view of probability [13, 14]. This is that a prob-
ability assignment summarizes what one does and does not know about a particular situation. A
probability represents a state of knowledge; its numerical value quantifies the plausibility one is
willing to give a hypothesis given some background information.

This point of view should be contrasted with the idea that probability must be identified
with the relative frequency of the various outcomes in an infinite repetition of a given experiment. The
difficulties with the frequency theory of probabilities are numerous [15] and need not be repeated
here. Suffice it to point out that if one takes the frequency idea seriously then one may never apply
the probability calculus to situations where an experiment cannot—by definition—be repeated more
than once. For instance, I say that the probability that my heart will stop beating at 10:29 this
evening is about one in a million. There can be no real infinite ensemble of repetitions for this
experiment. Alternatively, if I must construct an “imaginary” conceptual ensemble to understand
the probability statement, then why bother? Why not call it a degree of belief to begin with?

The Bayesian point of view should also be contrasted with the propensity theory of probability
[10]. This is the idea that a probability expresses an objective tendency on the part of the experi-
mental situation to produce one outcome over the other. If this were the case, then one could
hardly apply the probability calculus to situations where the experimental outcome already exists
at the time the experiment is performed. For instance, I give it an 98% chance there will be a
typographical error in this manuscript the night I defend it. But surely there either will or will not
be such an error on the appropriate night, independently of the probability I have assigned.

One might argue that probabilities in quantum mechanics are something different from the
Bayesian sort [17, 18, 19], perhaps more aligned with the propensity idea [20, 21]. This idea is
taken to task in Ref. [22]. The argument in a nutshell is that if it looks like a Bayesian probability
and smells like a Bayesian probability, then why draw a distinction where none is to be found.

With all that said and done, what is a probability? Formally, it is the plausibility \( P(H|S) \) of a
hypothesis \( H \) given some background information \( S \) and satisfies the probability calculus:

\[
\begin{align*}
& P(H|S) \geq 0, \\
& P(H|S) + P(\neg H|S) = 1, \text{ where } \neg H \text{ signifies the negation of } H,
\end{align*}
\]

8
plausibilities are updated according to Bayes’ rule upon the acquisition of new evidence $E$, i.e.

$$P(H|E,S) = \frac{P(H|S) \times P(E|H,S)}{P(E|S)}, \quad (1.22)$$

when it is clear that the background information is not changed by the process of acquiring the evidence.

These properties are essential for the work presented here and will be used over and over again.

### 1.3.2 What Is a Quantum State?

We take a very pragmatic approach to the meaning of a quantum state in this dissertation. Quantum states are the formal devices we use to describe what we do and do not know about a given quantum system—nothing more, nothing less [23, 24, 25, 22]. In this sense, quantum states are quite analogous to the Bayesian concept of probability outlined above. (Though more strictly speaking, they form the background information $S$ that may be used in a Bayesian probability assignment.)

What is a quantum system? To say it once evocatively, a line drawn in the sand. A quantum system is any part of the physical world that we may wish to conceptually set aside for consideration. It need not be microscopic and it certainly need not be considered in complete isolation from the remainder of our conceptual world—it may interact with an environment.

Mathematically speaking, in this dissertation what we call a quantum state is any density operator $\hat{\rho}$ over a $D$-dimensional Hilbert space, where $D$ is finite. The properties of a density operator are that it be Hermitian with nonnegative eigenvalues and that its trace be equal to unity. A very special class of density operators are the one-dimensional projectors $\hat{\rho} = |\psi\rangle\langle\psi|$. These are called pure states as opposed to density operators of higher rank, which are often called mixed states.

Pure states correspond to states of maximal knowledge in quantum mechanics [22]. Mixed states, on the other hand, correspond to less than maximal knowledge. This can come about in at least two ways. The first is simply by not knowing—to the extent that one could in principle—the precise preparation of a quantum system. The second is in having maximal knowledge about a composite quantum system, i.e., describing it via a pure state $|\psi\rangle\langle\psi|$ on some tensor-product Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2$, but restricting one’s attention completely to a subsystem of the larger system: quantum theory generally requires that one’s knowledge of a subsystem be less than maximal even though maximal knowledge has been attained concerning the composite system. Formally, the states corresponding to the subsystems are given by tracing out the irrelevant Hilbert space. That is to, if $|1_i\rangle|2_\alpha\rangle$ is a basis for $\mathcal{H}_1 \otimes \mathcal{H}_2$, and

$$|\psi\rangle = \sum_{i\alpha} c_{i\alpha} |1_i\rangle|2_\alpha\rangle \quad (1.23)$$

then the state on subsystem 1 is

$$\hat{\rho}_1 = \text{tr}_2(|\psi\rangle\langle\psi|)$$

$$= \sum_\beta \langle 2_\beta|\psi\rangle\langle\psi|2_\beta\rangle$$

$$= \sum_{i\alpha} c_{i\alpha} c^*_{i\alpha} |1_i\rangle\langle 1_i| \quad (1.24)$$
A similar mixed state comes about when attention is restricted to subsystem 2. Calling the reduced density operator the quantum state of the subsystem ensures that the form of the probability formula for measurement outcomes will remain the same in going from composite system to subsystem.

1.3.3 What Is a Quantum Measurement?

We shall be concerned with a very general notion of quantum measurement throughout this dissertation, and it will serve us well to make the ideas plain at the outset. We take as a quantum measurement any physical process that can be used on a quantum system to generate a probability distribution for some “outcomes.”

To make this idea rigorous, we recall two standard axioms for quantum theory. The first is that when the conditions and environment of a quantum system are completely specified and no measurements are being made, then the system’s state evolves according to the action of a unitary operator $\hat{U}$,

$$\hat{\rho} \rightarrow \hat{U}\hat{\rho}\hat{U}^\dagger.$$  \hspace{1cm} (1.25)

The second is that a repeatable measurement corresponds to some complete set of projectors $\hat{\Pi}_b$ (not necessarily one-dimensional) onto orthogonal subspaces of the quantum system’s Hilbert space. The probabilities of the outcomes for such a measurement are given according to the von Neumann formula,

$$p(b) = \text{tr}(\hat{\rho}\hat{\Pi}_b).$$  \hspace{1cm} (1.26)

With these two basic facts, we can lay out the structure of a general quantum measurement.

The most general action that can be performed on a quantum system to generate a set of “outcomes” is

1. to allow the system to be placed in contact with an auxiliary system or ancilla prepared in a standard state,

2. to have the two evolve unitarily so as to become correlated or entangled, and then

3. to perform a repeatable measurement on the ancilla.

One might have thought that a measurement on the composite system as a whole—in the last stage of this—could lead to a more general set of measurements, but, in fact, it cannot. For this can always be accomplished in this scheme by a unitary operation that first swaps the system’s state into a subspace of the ancilla’s Hilbert space and then proceeds as above.

More formally, these steps give rise to a probability distribution in the following way. Suppose the system and ancilla are initially described by the density operators $\hat{\rho}_s$ and $\hat{\rho}_a$ respectively. The conjunction of the two systems is then described by the initial quantum state

$$\hat{\rho}_{sa} = \hat{\rho}_s \otimes \hat{\rho}_a.$$  \hspace{1cm} (1.27)

Then the unitary time evolution leads to a new state,

$$\hat{\rho}_{sa} \rightarrow \hat{U}\hat{\rho}_{sa}\hat{U}^\dagger.$$  \hspace{1cm} (1.28)

Finally, a reproducible measurement on the ancilla is described via a set of orthogonal projection operators $\{\hat{1} \otimes \hat{\Pi}_b\}$ acting on the ancilla’s Hilbert space, where $\hat{1}$ is the identity operator. Any particular outcome $b$ is found with probability

$$p(b) = \text{tr}\left(\hat{U}(\hat{\rho}_s \otimes \hat{\rho}_a)\hat{U}^\dagger(\hat{1} \otimes \hat{\Pi}_b)\right).$$  \hspace{1cm} (1.29)
The number of outcomes in this generalized notion of measurement is limited only by the dimensionality of the ancilla’s Hilbert space—in principle, there can be arbitrarily many. There are no limitations on the number of outcomes due to the dimensionality of the system’s Hilbert space.

It turns out that this formula for the probabilities can be re-expressed in terms of operators on the system’s Hilbert space alone. This is easy to see. If we let $|s_\alpha\rangle$ and $|a_c\rangle$ be an orthonormal basis for the system and ancilla respectively, $|s_\alpha\rangle|a_c\rangle$ will be a basis for the composite system. Then using the cyclic property of the trace in Eq. (1.29), we get

$$
p(b) = \sum_{ac} \langle s_\alpha|a_c\rangle \left( (\hat{\rho}_s \otimes \hat{\rho}_a) \hat{U}^\dagger (\hat{1} \otimes \hat{\Pi}_b) \hat{U} \right) |s_\alpha\rangle |a_c\rangle 
$$

It follows that we may write

$$
p(b) = \text{tr}_s(\hat{\rho}_s \hat{E}_b) ,
$$

where

$$
\hat{E}_b = \text{tr}_s\left( (\hat{1} \otimes \hat{\rho}_a) \hat{U} (\hat{1} \otimes \hat{\Pi}_b) \hat{U}^\dagger \right)
$$

is an operator that acts on the Hilbert space of the original system only. Here $\text{tr}_a$ and $\text{tr}_s$ denote partial traces over the system and ancilla Hilbert spaces, respectively.

Note that the $\hat{E}_b$ are positive operators, i.e., Hermitian operators with nonnegative eigenvalues, usually denoted

$$
\hat{E}_b \geq 0 ,
$$

because they are formed from the partial trace of the product of two positive operators. Moreover, these automatically satisfy a completeness relation of a sort,

$$
\sum_b \hat{E}_b = \hat{1} .
$$

These two properties taken together are the defining properties of something called a **Positive Operator-Valued Measure or POVM**. Sets of operators $\{\hat{E}_b\}$ satisfying this are so called because they give an obvious (mathematical) generalization of the probability concept. As opposed to a complete set of orthogonal projectors, the POVM elements $\hat{E}_b$ need not commute with each other.

A theorem, originally due to Neumark [28], that is very useful for our purposes is that any POVM can be realized in the fashion of Eq. (1.32). This allows us to make full use of the defining properties of POVMs in setting up the optimization problems considered here. Namely, whenever we wish to optimize something like the mutual information, say, over all possible quantum measurements, we just need write the expression in terms of a POVM $\{\hat{E}_b\}$ and optimize over all operator sets satisfying Eqs. (1.33) and (1.34).

Why need we go to such lengths to describe a more general notion of measurement than the standard textbook one? The answer is simple: because there are situations in which the repeatable measurements, i.e., the orthogonal projection-valued measurements $\{\hat{\Pi}_b\}$, are just not general enough to give the optimal measurement. The paradigmatic example of such a thing [29] is that of a quantum system with a 2-dimensional Hilbert space—a spin-$\frac{1}{2}$ particle say—that can be prepared in one of three pure states, all with equal prior probabilities. If the possible states are each 120° apart on the Bloch sphere, then the measurement that optimizes the information recoverable about the quantum state’s identity is one with three outcomes. Each outcome excludes one of the possibilities, narrowing down the state’s identity to one of the other two. Therefore this measurement cannot be described by a standard two-outcome orthogonal projection-valued measurement.
Chapter 2

The Distinguishability of Probability Distributions

“... and as these are the only ties of our thoughts, they are really to us the cement of the universe, and all the operations of the mind must, in a great measure, depend on them.”

—David Hume
An Abstract of a Treatise of Human Nature

2.1 Introduction

The idea of distinguishing probability distributions is slippery business. What one means in saying “two probability distributions are distinguishable” depends crucially upon one’s prior state of knowledge and the context in which the probabilities are applied. This chapter is devoted to developing three quantitative measures of distinguishability, each tailor-made to a distinct problem.

To make firm what we strive for in developing these measures, one should keep at least one or the other of two models in mind. The first, very concrete, one is the model of a noisy communication channel. In this model, things are very simple. A sender prepares a simple message, 0 or 1, encoded in distinct preparations of a physical system, with probability $\pi_0$ and $\pi_1$. A receiver performs some measurement on the system he receives for which the measurement outcomes $b$ have conditional probability $p_0(b)$ or $p_1(b)$, depending upon the preparation of the system. The idea is that a notion of distinguishability of probability distributions should tell us something about what options are available to the receiver once he collects his data—what sort of inferences or estimates the receiver may make about the sender’s actual preparation. The more distinguishable the probability distributions, the more the receiver’s data should give him some insight (in senses to be defined) about the actual preparation.

The second, more abstract, model is that of the “quantum-information channel” [30, 31]—though at this level applied within a purely classical context. Here we start with a physical system that we describe via some probability distribution $p_0(b)$, and we wish to transpose that state of knowledge onto another physical system in the possession of someone with which we may later communicate. This transposition process must by necessity be carried out by some physical means, even if only by actually transporting our system to the other person. The only difference between this and a standard communication transaction is that no mention will be made as to what the
receiver of the “signal” will actually find if he makes an observation on it. Rather we shall be concerned with what we, the senders, can predict about what he would find in an observational situation. This distinction is crucial, for it leads to the following point.

If the state of knowledge is left truly intact during the transposition process, then the system possessed by the receiver will be described by the sender via the initial probability distribution \( p_0(b) \). If on the other hand—through lack of absolute control of the physical systems concerned or through the intervention of a third party—the state of knowledge changes during the transposition attempt, the receiver’s system will have to be described by some different distribution \( p_1(b) \). We might even imagine a certain probability \( \pi_0 \) that the transposition will be faithful and a probability \( \pi_1 \) that it will be imperfect. The question we should like to address is to what extent the states of knowledge \( p_0(b) \) and \( p_1(b) \) can be distinguished one from the other given these circumstances. In what quantifiable and operational sense can one state be said to be distinct from the other?

This language, it should be noted, makes no mention of probability distributions being either true or false. Neither \( p_0(b) \) nor \( p_1(b) \) need have anything to do with the receiver’s subjective expectation for his observational outcomes; the focus here is completely upon the distinction in predictions the sender may make under the opposing circumstances and how well he himself might be able to check that something did or did not go amiss during the transposition process.

In the following chapters these measures will be applied to the quantum mechanical context, where states of knowledge are more completely represented by density operators \( \hat{\rho}_0 \) and \( \hat{\rho}_1 \). For the time being, however, it may be useful—though not necessary—to think of the distributions as arising from some fixed measurement POVM \( \hat{E}_b \) via

\[
p_0(b) = \text{tr}(\hat{\rho}_0 \hat{E}_b) \quad \text{and} \quad p_1(b) = \text{tr}(\hat{\rho}_1 \hat{E}_b).
\]

This representation, of course, will be the starting point for the quantum mechanical considerations of the next chapter.

### 2.2 Distinguishability via Error Probability and the Chernoff Bound

Perhaps the simplest way to build a notion of distinguishability for probability distributions is through a simple decision problem. In this problem, an observer blindly samples once from either the distribution \( p_0(b) \) or the distribution \( p_1(b) \), \( b = 1, \ldots, n \); at most he might know prior probabilities \( \pi_0 \) and \( \pi_1 \) for which distribution he samples. If the distributions are distinct, the outcome of the sampling will reveal something about the identity of the distribution from which it was drawn. An easy way to quantify how distinct the distributions are comes from imagining that the observer must make a guess or inference about the identity after drawing his sample. The observer’s best-possible probability of error in this game says something about the distinguishability of the distributions \( p_0(b) \) and \( p_1(b) \) with respect to his prior state of knowledge (as encapsulated in the distribution \( \{\pi_0, \pi_1\} \)). This idea we develop as our first quantitative measure of distinguishability. Afterward we generalize it to the possibility of many samplings from the same distribution. This gives rise to a measure of distinguishability associated with the exponential decrease of error probability with the number of samplings, the Chernoff bound.

#### 2.2.1 Probability of Error

What is the best possible probability of error for the decision problem? This can be answered easily enough by manipulating the formal definition of error probability. Let us work at this immediately.
A decision function is any function
\[ \delta : \{1, \ldots, n\} \to \{0, 1\} \]  
representing the method of guess an observer might use in this problem. The probability that such a guess will be in error is
\[ P_e(\delta) = \pi_0 P(\delta = 1 \mid 0) + \pi_1 P(\delta = 0 \mid 1), \]  
(2.2)
where \( P(\delta = 1 \mid 0) \) denotes the probability that the guess is \( p_1(b) \) when, in fact, the distribution drawn from is really \( p_0(b) \). Similarly \( P(\delta = 0 \mid 1) \) denotes the probability that the guess is \( p_0(b) \) when, in fact, the distribution drawn from is really \( p_1(b) \).

A natural decision function is the one such that 0 or 1 is chosen according to which has the highest posterior probability, given the sampling’s outcome \( b \). Since the posterior probabilities are given by Bayes’ Rule,
\[ p(i \mid b) = \frac{\pi_i p_i(b)}{p(b)} = \frac{\pi_i p_i(b)}{\pi_0 p_0(b) + \pi_1 p_1(b)}, \]  
(2.3)
where \( i = 0, 1 \) and
\[ p(b) = \pi_0 p_0(b) + \pi_1 p_1(b) \]  
(2.4)
is the total probability for outcome \( b \), this decision function is called Bayes’ decision function. Symbolically, Bayes’ decision function translates into
\[ \delta_B(b) = \begin{cases} 
0 & \text{if } \pi_0 p_0(b) < \pi_1 p_1(b) \\
1 & \text{if } \pi_1 p_1(b) < \pi_0 p_0(b) \\
\text{anything} & \text{if } \pi_0 p_0(b) = \pi_1 p_1(b) 
\end{cases} \]  
(2.5)
(When the posterior probabilities are equal, it makes no difference which guessing method is used.) It turns out, not unexpectedly, that this decision method is optimal as far as error probability is concerned [32]. This is seen easily. (In this Chapter, we denote the beginning and ending of proofs by \( \triangle \) and \( \Box \), respectively.)

\( \triangle \) Note that for any decision procedure \( \delta \), Eq. (2.3) can be rewritten as
\[ P_e(\delta) = \pi_0 \sum_{b=1}^{n} \delta(b) p_0(b) + \pi_1 \sum_{b=1}^{n} [1 - \delta(b)] p_1(b), \]  
(2.6)
because \( \sum_b \delta(b) p_0(b) \) is the total probability of guessing 0 when the answer is 0 and \( \sum_b [1 - \delta(b)] p_1(b) \) is the total probability of guessing 0 when the answer is 1. Then it follows that
\[ P_e(\delta) - P_e(\delta_B) = \sum_{b=1}^{n} (\delta(b) - \delta_B(b))(\pi_0 p_0(b) - \pi_1 p_1(b)). \]  
(2.7)
Suppose \( \delta \neq \delta_B \). Then the only nonzero terms in this sum occur when \( \delta(b) \neq \delta_B(b) \) and \( \pi_0 p_0(b) \neq \pi_1 p_1(b) \). Let us consider these terms. When \( \delta(b) = 0 \) and \( \delta_B(b) = 1 \), \( \pi_0 p_0(b) - \pi_1 p_1(b) < 0 \); thus the term in the sum is positive. When \( \delta(b) = 1 \) and \( \delta_B(b) = 0 \), we have \( \pi_0 p_0(b) - \pi_1 p_1(b) > 0 \), and again the term in the sum is positive. Therefore it follows that
\[ P_e(\delta) > P_e(\delta_B), \]  
(2.8)
for any decision function \( \delta \) other than Bayes’. This proves Bayes’ decision function to be optimal. \( \Box \)
We shall hereafter denote the probability of error with respect to Bayes’ decision method simply by $P_e$. This quantity is expressed more directly by noticing that, when the outcome $b$ is found, the probability of a correct decision is just $\max\{p(0|b), p(1|b)\}$. Therefore

$$
P_e = \sum_{b=1}^{n} p(b) \left(1 - \max\{p(0|b), p(1|b)\}\right)
$$

$$
= \sum_{b=1}^{n} p(b) \min\{p(0|b), p(1|b)\} 
= \sum_{b=1}^{n} \min\{\pi_0 p_0(b), \pi_1 p_1(b)\} 
$$

(2.10)

Eq. (2.10) follows because, for any $b$, $p(0|b)+p(1|b) = 1$. Equation (2.11) gives a concrete expression for the sought after measure of distinguishability: the smaller this expression is numerically, the more distinguishable the two distributions are.

Notice that Eq. (2.11) depends explicitly on the observer’s subjective prior state of knowledge through $\pi_0$ and $\pi_1$ and is not solely a function of the probability distributions to be distinguished. This dependence is neither a good thing nor a bad thing, for, after all, Bayesian probabilities are subjective notions to begin with: they are always defined with respect to someone’s state of knowledge. One need only be aware of this extra dependence.

The main point of interest for this measure of distinguishability is that it is operationally defined and can be written in terms of a fairly simple expression—one expressed in terms of the first power of the probabilities. However, one should ask a few simple immediate questions to test the robustness of this concept. For instance, why did we not consider two samplings before a decision was made? Indeed, why not three or four or more? If the error probabilities in these scenarios lead to nothing new and interesting, then one’s work is done. On the other hand, if such cases lead to seemingly different measures of distinguishability, then the foundation of this approach might require examination.

These questions are settled by an example due to Cover [33]. Consider the following four different probability distributions over two outcomes: $p_0 = \{.96, .04\}$, $p_1 = \{.04, .96\}$, $q_0 = \{.90, .10\}$, and $q_1 = \{0, 1\}$. Let us compare the distinguishability of $p_0$ and $p_1$ via Eq. (2.11) to that of $q_0$ and $q_1$, both under the assumption of equal prior probabilities:

$$
P_e(p_0, p_1) = \frac{1}{2} \min\{.96, .04\} + \frac{1}{2} \min\{.04, .96\} = .04 ,
$$

(2.12)

and

$$
P_e(q_0, q_1) = \frac{1}{2} \min\{.90, 0\} + \frac{1}{2} \min\{.10, 1\} = .05 .
$$

(2.13)

Therefore

$$
P_e(p_0, p_1) < P_e(q_0, q_1) ,
$$

(2.14)

and so, by this measure, the distributions $p_0$ and $p_1$ are more distinguishable from each other than the distributions $q_0$ and $q_1$.

On the other hand, consider modifying the scenario so that two samples are taken before a guess is made about the identity of the distribution. This scenario falls into the same framework as before, only now there are four possible outcomes to the experiment. These must be taken into account in calculating the Bayes’ decision rule probability of error. Namely, in obvious notation,

$$
P_e(p_0^2, p_1^2) = \frac{1}{2} \min\{.96 \times .96, .04 \times .04\} + \frac{1}{2} \min\{.96 \times .04, .04 \times .96\}
$$
\[
+ \frac{1}{2} \min \{.04 \times .96, .96 \times .04\} + \frac{1}{2} \min \{.04 \times .96, .96 \times .96\} \\
= .04,
\]
and
\[
P_e(q_0^2, q_1^2) = \frac{1}{2} \min \{.90 \times .90, 0 \times 0\} + \frac{1}{2} \min \{.90 \times .10, 0 \times 1\} \\
+ \frac{1}{2} \min \{.10 \times .90, 1 \times 0\} + \frac{1}{2} \min \{.10 \times .10, 1 \times 1\} \\
= .005.
\]

Therefore
\[
P_e(q_0^2, q_1^2) < P_e(p_0^2, p_1^2).
\]

The distributions \(q_0\) and \(q_1\) are actually more distinguishable from each other than the distributions \(p_0\) and \(p_1\), when one allows two samplings into the decision problem.

This example suggests that the probability of error, though a perfectly fine measure of distinguishability for the particular problem of decision-making after one sampling, still leaves something to be desired. Even though it is operationally defined, it is not a measure that adapts easily to further data acquisition. For this one needs a measure that is not explicitly tied to the exact number of samplings in the decision problem.

### 2.2.2 The Chernoff Bound

The optimal probability of error in the decision problem—the one given by using Bayes’ decision rule—must decrease toward zero as the number of samplings increases. This is intuitively clear. The exact form of that decrease, however, may not be so obvious. It turns out that the decrease asymptotically approaches an exponential in the number of samples drawn before the decision. The particular value of this exponential is called the Chernoff bound [34, 35, 10] because it is not only achieved asymptotically, but also envelopes the true decrease from above.

The Chernoff bound thus forms an attractive notion of distinguishability for probability distributions: the faster two distributions allow the probability of error to decrease to zero in the number of samples, the more distinguishable the distributions are. It is operationally defined by being intimately tied to the decision problem. Yet it neither depends on the prior probabilities \(\pi_0\) and \(\pi_1\) nor on the number of samples drawn before the decision. The formal statement of the Chernoff bound is given in the following theorem.

**Theorem 2.1 (Chernoff)** Let \(P_e(N)\) be the probability of error for Bayes’ decision rule after sampling \(N\) times one of the two distributions \(p_0(b)\) or \(p_1(b)\). Then
\[
P_e(N) \leq \lambda^N
\]
where
\[
\lambda = \min_{\alpha} F_\alpha(p_0/p_1),
\]
and
\[
F_\alpha(p_0/p_1) = \sum_{b=1}^n p_0(b)^\alpha p_1(b)^{1-\alpha},
\]
for \(\alpha\) restricted to be between 0 and 1. Moreover this bound is approached asymptotically in the limit of large \(N\).
\[ \text{Let us demonstrate the first part of this theorem. Denote the outcome of the } k\text{'th trial by } b_k. \text{ Then the two probability distributions for the outcomes of a string of } N \text{ trials can be written} \]

\[ p_0(b_1b_2 \ldots b_N) = p_0(b_1)p_0(b_2) \cdots p_1(b_N), \]

and

\[ p_1(b_1b_2 \ldots b_N) = p_1(b_1)p_1(b_2) \cdots p_1(b_N). \]

Now note that, for any two positive numbers \( a \) and \( b \) and any \( 0 \leq \alpha \leq 1 \),

\[ \min\{a, b\} \leq a^\alpha b^{1-\alpha}. \]

This follows easily. First suppose \( a \leq b \). Then, because \( 1 - \alpha \geq 0 \), we know

\[ \left( \frac{b}{a} \right)^{1-\alpha} \geq 1. \]

So

\[ \min\{a, b\} = a \leq a \left( \frac{b}{a} \right)^{1-\alpha} = a^\alpha b^{1-\alpha}. \]

Alternatively, suppose \( b \leq a \); then

\[ \left( \frac{a}{b} \right)^\alpha \geq 1, \]

and

\[ \min\{a, b\} = b \leq b \left( \frac{a}{b} \right)^\alpha = a^\alpha b^{1-\alpha}. \]

Putting the notation and the small mathematical fact from the last paragraph together, we obtain that for any \( \alpha \in [0, 1] \),

\[ P_e(N) = \sum_{b_1b_2 \ldots b_N} \min\{\pi_0p_0(b_1b_2 \ldots b_N), \pi_0p_0(b_1b_2 \ldots b_N)\} \]

\[ \leq \pi_0^\alpha \pi_1^{1-\alpha} \sum_{b_1b_2 \ldots b_N} p_0(b_1b_2 \ldots b_N)^\alpha p_0(b_1b_2 \ldots b_N)^{1-\alpha} \]

\[ = \pi_0^\alpha \pi_1^{1-\alpha} \sum_{b_1b_2 \ldots b_N} \left( \prod_{k=1}^{N} p_0(b_k)^\alpha p_1(b_k)^{1-\alpha} \right) \]

\[ = \pi_0^\alpha \pi_1^{1-\alpha} \prod_{k=1}^{N} \left( \sum_{b_k=1}^{n} p_0(b_k)^\alpha p_1(b_k)^{1-\alpha} \right) \]

\[ = \pi_0^\alpha \pi_1^{1-\alpha} \left( \sum_{b=1}^{n} p_0(b)^\alpha p_1(b)^{1-\alpha} \right)^N \]

\[ \leq \left( \sum_{b=1}^{n} p_0(b)^\alpha p_1(b)^{1-\alpha} \right)^N. \]

The tightest bound of this form is found by further minimizing the right hand side of Eq. (2.28) over \( \alpha \). This completes the proof that the Chernoff bound is indeed a bound on \( P_e(N) \). The remaining part of the theorem, that the bound is asymptotically achieved, is more difficult to demonstrate and we shall not consider it here; see instead Ref. [10]. \( \Box \)
The value $\alpha^*$ of $\alpha$ that achieves the minimum in Eq. (2.19) generally cannot be expressed any more explicitly than there. This is because to find it in general one must solve a transcendental equation. A notable exception is when the probability distributions $p_0 \equiv \{q, 1 - q\}$ and $p_1 \equiv \{r, 1 - r\}$ are distributions over two outcomes. Let us write out this special case. Here

$$F_\alpha(p_0, p_1) = q^\alpha r^{1-\alpha} + (1-q)^\alpha (1-r)^{1-\alpha}. \quad (2.29)$$

Setting the derivative of this (with respect to $\alpha$) equal to zero, we find that the optimal $\alpha$ must satisfy

$$q^\alpha r^{1-\alpha} \ln \left( \frac{q}{r} \right) = -(1-q)^\alpha (1-r)^{1-\alpha} \ln \left( \frac{1-q}{1-r} \right); \quad (2.30)$$

hence

$$\alpha^* = \left[ \ln \left( \frac{q(1-r)}{r(1-q)} \right) \right]^{-1} \ln \left( \frac{1-r}{r} \ln(1-q) - \ln(1-r) \right) \quad (2.31)$$

With this and a lot of algebra, one can show

$$\ln F_{\alpha^*}(p_0, p_1) = -x \ln \left( \frac{x}{q} \right) - (1-x) \ln \left( \frac{1-x}{1-q} \right)$$

$$= -x \ln \left( \frac{x}{r} \right) - (1-x) \ln \left( \frac{1-x}{1-r} \right) \quad (2.32)$$

where

$$x = \left[ \ln \left( \frac{q(1-r)}{r(1-q)} \right) \right]^{-1} \ln \left( \frac{1-r}{1-q} \right). \quad (2.33)$$

That is to say, using an expression to be introduced in Section 2.3, the optimal $\ln F_{\alpha}(p_0, p_1)$ is given by the Kullback-Leibler relative information \cite{11} between the distribution $p_0$ (or $p_1$) and the “distribution” $\{x, 1-x\}$.

This property, relating the Chernoff bound to a Kullback-Leibler relative information is more generally true and worth mentioning. The precise statement is the following theorem; details of its proof may be found in Ref. \cite{10}.

**Theorem 2.2 (Chernoff)** The constant $\lambda$ in the Chernoff bound can also be expressed as

$$\lambda = K(p_{\alpha^*}/p_0) = K(p_{\alpha^*}/p_1), \quad (2.34)$$

where $K(p_{\alpha}/p_0)$ is the Kullback-Leibler relative information between the distributions $p_{\alpha}(b)$ and $p_0(b)$,

$$K(p_{\alpha}/p_0) = \sum_{b=1}^{n} p_{\alpha}(b) \ln \left( \frac{p_{\alpha}(b)}{p_0(b)} \right), \quad (2.35)$$

and the distribution $p_{\alpha}(b)$—depending upon the parameter $\alpha$—is defined by

$$p_{\alpha}(b) = \frac{p_0(b)^\alpha p_1(b)^{1-\alpha}}{\sum_{b} p_0(b)^\alpha p_1(b)^{1-\alpha}}. \quad (2.36)$$

The particular value of $\alpha$ used in this, i.e., $\alpha^*$, is the one for which

$$K(p_{\alpha^*}/p_0) = K(p_{\alpha^*}/p_1). \quad (2.37)$$
Statistical Overlap

Because the Chernoff bound is generally hard to get at analytically, it is worthwhile to reconsider the other bounds arising in the derivation of Theorem 2.1. These are all quantities of the form

\[ F_\alpha(p_0/p_1) = \sum_{b=1}^{n} p_0(b)^\alpha p_1(b)^{1-\alpha}, \]

for \( 0 < \alpha < 1 \). We shall call the functions appearing in Eq. (2.38) the \textit{Rényi overlaps} of order \( \alpha \) because of their close connection to the relative information of order \( \alpha \) introduced by Rényi [36, 37].

\[ K_\alpha(p_0/p_1) = \frac{1}{\alpha - 1} \ln \left( \sum_{b=1}^{n} p_0(b)^\alpha p_1(b)^{1-\alpha} \right). \]

Each \( F_\alpha(p_0/p_1) \) forms a notion of distinguishability in its own right, albeit not as operationally defined as the Chernoff bound. All these quantities are bounded between 0 and 1—reaching the minimum of 0 if and only if the distributions do not overlap at all, and reaching 1 if and only if the the distributions are identical. For a fixed \( \alpha \), the smaller \( F_\alpha(p_0/p_1) \) is, the more distinguishable the distributions are. Moreover each of these can be used for generating a valid notion of nearness—more technically, a topology [38]—on the set of probability distributions [39, 40].

A particular Rényi overlap that is quite useful to study because of its many pleasant properties is the one of order \( \alpha = \frac{1}{2} \),

\[ F(p_0, p_1) = \sum_{b=1}^{n} \sqrt{p_0(b)} \sqrt{p_1(b)}. \]

We shall dub this measure of distinguishability the \textit{statistical overlap} or \textit{fidelity}. It has had a long and varied history, being rediscovered in different contexts at different times by Bhattacharyya [41, 42], Jeffreys [43], Rao [44], Rényi [36], Csiszár [39], and Wootters [45, 8, 46]. Perhaps its most compelling foundational significance is that the quantity

\[ D(p_0/p_1) = \cos^{-1} \left( \sum_{b=1}^{n} \sqrt{p_0(b)} \sqrt{p_1(b)} \right) \]

corresponds to the geodesic distance between \( p_0(b) \) and \( p_1(b) \) on the probability simplex when its geometry is specified by the Riemannian metric

\[ ds^2 = \sum_{b=1}^{n} \frac{(\delta p(b))^2}{p(b)}. \]

This metric is known as the Fisher information metric [47, 48, 10] and is useful because it appears in expressions for the decrease (with the number of samplings) of an estimator’s variance in maximum likelihood parameter estimation.

Unfortunately, \( F(p_0/p_1) \) does not appear to be strictly tied to any statistical inference problem or achievable resource bound as are most other measures of distinguishability studied in this Chapter (in particular the probability of error, the Chernoff bound, the Kullback-Leibler relative information, the mutual information, and the Fisher information) [10]. However, it nevertheless remains an extremely useful quantity mathematically as will be seen in the following chapters. Moreover it remains of interest because of its intriguing resemblance to a quantum mechanical inner product [43, 8, 46]: it is equal to the sum of a product of “amplitudes” (square roots of probabilities) just as the quantum mechanical inner product is.

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1Imre Csiszár, private communication.
2.3 Distinguishability via “Keeping the Expert Honest”

We have already agreed that probabilities must be interpreted as subjective states of knowledge. How then can we ever verify whether a probability assignment is “true” or not? Simply put, we cannot. We can never know whether a source of probability assignments, such as a weatherman or economic forecaster, is telling the truth or not. The best we can hope for in a situation where we must rely on someone else’s probability assignment is that there is an effective strategy for inducing him to tell the truth, an effective strategy to steer him to be as true to his state of knowledge as possible when disseminating what he knows. This is the problem of “keeping the expert honest” \[49, 50, 51, 52, 53\]. The resolution of this problem gives rise to another measure of distinguishability for probability distributions, the Kullback-Leibler relative information \[11\].

Let us start this section by giving a precise statement of the honest-expert problem. Suppose an expert’s knowledge of some state of affairs is quantified by a probability distribution \( p_0(b) \), \( b = 1, \ldots, n \), and he is willing to communicate that distribution for a price. If we agree to pay for his services, then, barring the use of lie detector tests and truth serums, we can never know whether we got our money’s worth in the deal. There is no way to tell just by looking at the outcome of an experiment whether the distribution \( p_0(b) \) represents his true state of knowledge or whether some other distribution \( p_1(b) \) does. The only thing we can do to safeguard against dishonesty is to agree exclusively to payment schemes that somehow build in an incentive for the expert to be honest.

Imagine the expert agrees to the following payment scheme. If the expert gives a probability distribution \( p_1(b) \), then after we perform an experiment to elicit the actual state of affairs, he will be paid an amount that depends upon which outcome occurs and the distribution \( p_1(b) \). This particular type of payment is proposed because, though probabilities do not dictate the outcomes of an experiment, the events themselves nevertheless do give us an objective handle on the problem.

Say, for instance, we pay an amount \( F_b(p_1(b)) \) if outcome \( b \) actually occurs, where

\[
F_b : [0, 1] \to \mathbb{R} , \quad b = 1, \ldots, n
\]  

(2.43)

is some fixed set of functions independent of the probabilities under consideration. Depending upon the form of the functions \( F_b \), it may well be in the expert’s best interest to lie in reporting his probabilities. That is to say, if the expert’s true state of knowledge is captured by the distribution \( p_0(b) \), his expected earnings for reporting the distribution \( p_1(b) \) will be

\[
\overline{F} = \sum_{b=1}^{n} p_0(b)F_b(p_1(b)) .
\]  

(2.44)

Unless his expected earnings turn out to be less upon lying than in telling the truth, i.e.,

\[
\sum_{b=1}^{n} p_0(b)F_b(p_1(b)) \leq \sum_{b=1}^{n} p_0(b)F_b(p_0(b)) ,
\]  

(2.45)

there is no incentive for him to be honest (that is, if the expert acts rationally!). In this context, the problem of “keeping the expert honest” is that of trying to find a set of functions \( F_b \) for which Eq. (2.45) remains true for all distributions \( p_0(b) \) and \( p_1(b) \), \( b = 1, \ldots, n \).

If such a program can be carried out, then it will automatically give a measure of distinguishability for probability distributions. Namely, the difference between the maximal expected payoff and the expected payoff for a dishonesty,

\[
K(p_0/p_1) \equiv \sum_{b=1}^{n} p_0(b) \left[ \overline{F}_b(p_0(b)) - \overline{F}_b(p_1(b)) \right] ,
\]  

(2.46)

20
becomes an attractive notion of distinguishability. (The tildes over the \( F \) in this formula signify that they are functions optimal for keeping the expert honest.) This quantity captures the idea that the more distinguishable two probability distributions are, the harder it should be for an expert to pass one off for the other. In this case, the bigger the expert’s lie, the greater the expected loss he will have to take in giving it.

Of course, one could consider using any payoff function whatsoever in Eq. (2.46) and calling the result a measure of distinguishability, but that would be rather useless. Only a payment scheme optimal for this problem is relevant for distilling a probability distribution’s identity. Only this sort of payment scheme has a useful interpretation.

Nevertheless, one would be justified in expecting even more from a measure of distinguishability. For instance, the honest-expert problem does not, at first sight, appear to restrict the class of optimal functions very tightly at all. For instance, one might further want a measure of distinguishability that attains its minimal value of zero \( f \) if and only if \( \mathbf{p}_1(b) = \mathbf{p}_0(b) \). Or one might want it to have certain concavity properties. Interestingly enough, these sorts of things are already assured—though not explicit—in the posing of the honest-expert problem.

### 2.3.1 Derivation of the Kullback-Leibler Information

Let us use the work of Aczél [54] to demonstrate an exact expression for Eq. (2.46). When \( n \geq 3 \) it turns out that, up to various constants, there is a unique function satisfying Eq. (2.45) for all distributions \( \mathbf{p}_0(b) \) and \( \mathbf{p}_1(b) \). We shall consider this case first by proving the following theorem.

**Theorem 2.3 (Aczél)** Let \( n \geq 3 \). Then the inequality

\[
\sum_{k=1}^{n} p_k F_k(q_k) \leq \sum_{k=1}^{n} p_k F_k(p_k) \tag{2.47}
\]

is satisfied for all \( n \)-point probability distributions \( (p_1, \ldots, p_n) \) and \( (q_1, \ldots, q_n) \) if and only if there exist constants \( \alpha \) and \( \gamma_1, \ldots, \gamma_n \) such that

\[
F_k(p) = \alpha \ln p + \gamma_k, \tag{2.48}
\]

for all \( k = 1, 2, \ldots, n \).

\[ \triangle \] The main point of this theorem is that Eq. (2.45), though appearing quite imprecise, is tremendously restrictive. We shall presently establish the “only if” part of the theorem. To do this we assume the inequality to hold and focus on the functions \( F_1 \) and \( F_2 \). This can be carried out by restricting the distributions \( (p_1, \ldots, p_n) \) and \( (q_1, \ldots, q_n) \) to be such that \( q_i = p_i \) for all \( i \geq 3 \) while \( p_1 \equiv p \), \( q_1 \equiv q \), \( p_2 \) and \( q_2 \) otherwise remain free. Then we can define \( r \equiv p + p_2 = q + q_2 \) where also

\[
r = 1 - \sum_{i=3}^{n} p_k = 1 - \sum_{i=3}^{n} q_k. \tag{2.49}
\]

Note that because \( n \geq 3 \), \( r \) is a number strictly less than unity. With these definitions, Eq. (2.43) reduces to

\[
p F_1(q) + (r - p) F_2(r - q) \leq p F_1(p) + (r - p) F_2(r - p), \tag{2.50}
\]

since all the other terms for \( k \geq 3 \) cancel. This new inequality already contains within it enough to show that \( F_1 \) and \( F_2 \) are monotonically nondecreasing and differentiable at every point in their domain. Let us work on showing these properties straight away.
Eq. \((2.50)\) can be rearranged to become

\[ p [F_1(p) - F_1(q)] \geq (r - p) [F_2(r - q) - F_2(r - p)] . \] (2.51)

Upon interchanging the symbols \(p\) and \(q\), the same reasoning also gives rise to the inequality,

\[ q [F_1(q) - F_1(p)] \geq (r - q) [F_2(r - p) - F_2(r - q)] . \] (2.52)

Multiplying Eq. \((2.51)\) by \((r - q)\), Eq. \((2.52)\) by \((r - p)\), and adding the resultants, we get

\[ (r - q) p [F_1(p) - F_1(q)] + (r - p) q [F_1(q) - F_1(p)] \geq 0 , \] (2.53)

which implies

\[ r (p - q) [F_1(p) - F_1(q)] \geq 0 . \] (2.54)

Then if \(p \geq q\), it must be the case that \(F_1(p) \geq F_1(q)\) so that this inequality is maintained. It follows that \(F_1\) is a monotonically nondecreasing function.

Now we must show the same property for \(F_2\). To do this, we instead multiply Eq. \((2.51)\) by \(q\), Eq. \((2.52)\) by \(p\), and add the results of these operations. This gives

\[ 0 \geq q (r - p) [F_2(r - q) - F_2(r - p)] + p (r - q) [F_2(r - p) - F_2(r - q)] , \] (2.55)

or, after rearranging,

\[ 0 \leq r [(r - p) - (r - q)] [F_2(r - p) - F_2(r - q)] . \] (2.56)

So that, if \((r - p) \geq (r - q)\), we must have in like manner \(F_2(r - p) \geq F_2(r - q)\) to maintain the inequality. Therefore, \(F_2\) must also be a monotonically nondecreasing function.

Putting these two facts to the side for the moment, we presently seek a tighter relation between the functions \(F_1\) and \(F_2\). To this end, we multiply Eq. \((2.51)\) by \(q\), Eq. \((2.52)\) by \(-p\). This gives

\[ p q [F_1(p) - F_1(q)] \geq q (r - p) [F_2(r - q) - F_2(r - p)] , \] (2.57)

and

\[ p q [F_1(p) - F_1(q)] \leq p (r - q) [F_2(r - q) - F_2(r - p)] . \] (2.58)

These two inequalities together imply

\[ \frac{r - p}{p} [F_2(r - q) - F_2(r - p)] \leq F_1(p) - F_1(q) , \] (2.59)

and

\[ F_1(p) - F_1(q) \leq \frac{r - q}{q} [F_2(r - q) - F_2(r - p)] . \] (2.60)

Dividing this through by \((p - q)\), we get finally

\[ \frac{r - p}{p} \left( \frac{F_2(r - q) - F_2(r - p)}{(r - q) - (r - p)} \right) \leq \frac{F_1(p) - F_1(q)}{p - q} , \] (2.61)

and

\[ \frac{F_1(p) - F_1(q)}{p - q} \leq \frac{r - q}{q} \left( \frac{F_2(r - q) - F_2(r - p)}{(r - q) - (r - p)} \right) . \] (2.62)
From this expression we know, by the Pinching Theorem of elementary calculus, that if the limits

\[
\lim_{q \to p} \frac{r - p}{p} \left( \frac{F_2(r - q) - F_2(r - p)}{(r - q) - (r - p)} \right) = \frac{r - p}{p} F_2'(r - p)
\]

(2.63)

and

\[
\lim_{q \to p} \frac{r - q}{q} \left( \frac{F_2(r - q) - F_2(r - p)}{(r - q) - (r - p)} \right) = \frac{r - p}{p} F_2'(r - p)
\]

(2.64)

exist, then so does

\[
\lim_{q \to p} \frac{F_1(p) - F_1(q)}{p - q} = F_1'(p)
\]

(2.65)

and the limits must be identical. In other words, if \( F_2 \) is differentiable at \( r - p \), then \( F_1 \) is differentiable at \( p \) and

\[
pF_1'(p) = (r - p)F_2'(r - p).
\]

(2.66)

Recall, however, that \( p_2 \) is not uniquely fixed by \( p \) since \( n \geq 3 \). Thus neither is \( r \); it can range anywhere between \( p \) and 1. This allows us to write the statement preceding Eq. (2.66) in the converse form: if \( F_1 \) is not differentiable at the point \( p \), then \( F_2 \) is not differentiable at any point \( (r - p) \) in the open set \( (0, 1 - p) \). This is the sought after tight relation between \( F_1 \) and \( F_2 \).

This statement can be combined with the fact that \( F_1 \) and \( F_2 \) are monotonic for the final thrust of the proof. For this we will rely on a theorem from elementary real analysis sometimes called Lebesgue’s theorem [55, page 96]:

**Lemma 2.1** Let \( f \) be an increasing real-valued function on the interval \([a, b]\). Then \( f \) is differentiable almost everywhere. The derivative \( f' \) is measurable, and \( \int_a^b f'(x)dx \leq f(b) - f(a) \).

Actually we are only concerned with the first conclusion of this. It can be seen in a qualitative manner as follows. The points where \( f \) is not differentiable can only correspond to kinks or jumps in its graph that are at best never decreasing in height. Thus one can easily imagine that, in travelling from points \( a \) to \( b \), a continuous infinity of such kinks and jumps (as would be required for a measurable set) would cause the graph to blow up to infinity before the end of the interval were ever reached. A more rigorous demonstration of this theorem will not be given here.

From this theorem we immediately have that \( F_1 \) must be differentiable everywhere on the closed interval \([0, 1]\). For suppose there were a point \( p \) at which it were not differentiable. Then \( F_2 \) would not be differentiable anywhere within the measurable set \((0, 1 - p)\), contradicting the fact that it is a monotonically nondecreasing function. Now, using the Pinching Theorem again, we have that \( F_2 \) is differentiable everywhere.

Therefore, let \( s = r - p \). Since \( p \) and \( s \) are independent and Eq. (2.63) must always hold, it follows that there must be a constant \( \alpha \) such that

\[
pF_1'(p) = sF_2'(s) = \alpha.
\]

(2.67)

Because \( F_1 \) and \( F_2 \) are monotonically nondecreasing, \( \alpha \geq 0 \). So

\[
F_1'(p) = \frac{\alpha}{p} \quad \text{and} \quad F_2'(p) = \frac{\alpha}{p};
\]

(2.68)

integrating this we get

\[
F_1(p) = \alpha \ln p + \gamma_1 \quad \text{and} \quad F_2(p) = \alpha \ln p + \gamma_2
\]

(2.69)

where \( \gamma_1 \) and \( \gamma_2 \) are integration constants.
Running through the same argument but assuming $q_i = p_i$ for all $i$ except $i = 1$ and $i = k$, it follows in like manner that $F_k(p) = \alpha \ln p + \gamma_k$ for all $k = 1, \ldots, n$. This concludes the proof of the “only if” side of the theorem.

To establish the “if” part of the theorem, we need only demonstrate the verity of the Shannon inequality,

$$\sum_{k=1}^{n} p_k \ln q_k \leq \sum_{k=1}^{n} p_k \ln p_k ,$$

(2.70)

with equality if and only if $p_k = q_k$ for all $k$. To see this note that the function $f(x) = \ln x$ is convex (since $f'' = -x^{-2} \leq 0$) and consequently always lies below its tangent line at $x = 1$. In other words, $f(x)$ always lies below the line

$$y = f'(1)x + [f(1) - f'(1)]$$

$$= x - 1 .$$

(2.71)

Hence, $\ln x \leq x - 1$ with equality holding if and only if $x = 1$. Therefore it immediately follows that

$$\ln \left( \frac{q_k}{p_k} \right) \leq \frac{q_k}{p_k} - 1 ,$$

(2.72)

with equality if and only if $p_k = q_k$. This, in turn, implies

$$p_k (\ln q_k - \ln p_k) = p_k \ln \left( \frac{q_k}{p_k} \right) \leq q_k - p_k ,$$

(2.73)

so that

$$\sum_{k=1}^{n} p_k (\ln q_k - \ln p_k) \leq 0 ,$$

(2.74)

with equality holding in the last expression if and only if $p_k = q_k$ for all $k$. Rearranging Eq. (2.74) concludes the proof. □

When $n = 2$, the above method of proof for the “only if” side of Theorem (2.3) fails. This follows technically because, in that case, the quantity $r$ must be fixed to the value 1. Moreover, it turns out that Eq. (2.43), independent of proof method, no longer specifies a relatively unique solution. For instance, even if one were to make the restriction $F_1(p) = F_2(p) \equiv f(p)$, a theorem due to Muszely [56, 57] states that any function of the following form will satisfy the honest-expert inequality for all distributions:

$$f(p) = (1 - p) U \left( p - \frac{1}{2} \right) + \int_{0}^{p - \frac{1}{2}} U(t) \, dt + C ,$$

(2.75)

where $C$ is constant and $U(t)$ is any continuous, increasing, odd function defined on the open interval $(-\frac{1}{2}, \frac{1}{2})$. Thus there are many, many ways of keeping the expert honest when talking about probability distributions over two outcomes.

We, however, shall not let a glitch in the two-outcome case deter us in defining a new measure of distinguishability. Namely, using the robust payoff function defined by Theorem (2.3) in conjunction with Eq. (2.40), we obtain

$$K(p_0/p_1) = \sum_{b=1}^{n} p_0(b) \left[ \ln p_0(b) - \ln p_1(b) \right]$$

$$= \sum_{b=1}^{n} p_0(b) \ln \left( \frac{p_0(b)}{p_1(b)} \right) .$$

(2.76)
This measure of distinguishability has appeared in other contexts and is known by various names: the Kullback-Leibler relative information, cross entropy, directed divergence, update information, and information gain.

2.3.2 Properties of the Relative Information

Though a probability assignment can never be confirmed as true or false, one’s trust in a state of knowledge or probability assignment for some phenomenon can be either strengthened or weakened through observation. The simplest context where this can be seen is when the phenomenon in question is repeatable. Consider, as an example, a coin believed to be unusually weighted so that the probability for heads in a toss is 25%. If, upon tossing the coin 10,000 times, one were to find roughly 50% of the actual tosses giving rise to heads, one might indeed be compelled to reevaluate his assessment. The reason for this is that probability assignments can be used to make relatively sharp predictions about the frequencies of outcomes in repeatable experiments; the standard Law of Large Numbers \[58\] specifies that relative frequencies of outcomes in a set of repeated trials approach the pre-assigned probabilities with probability 1.

Not surprisingly, the probability for an “incorrect” frequency in a set of repeated trials has something to do with our distinguishability measure based on keeping the expert honest. This is because all the payment schemes considered in its definition were explicitly tied to the observational context. It turns out that the Kullback-Leibler relative information controls the exponential rate to zero forced upon the probability of an “incorrect” frequency by the Law of Large Numbers \[59, 10\]. This gives us another useful operational meaning for the Kullback-Leibler information and gives more trust that it is a quantity worthy of study. This subsection is devoted to fleshing out this fact in detail.

Let us start by demonstrating that the most probable frequency distribution in many trials is indeed essentially the probability distribution for the outcomes of a single trial. For this we suppose that an experiment of \( B \) outcomes, \( b \in \mathcal{B} = \{1, \ldots, B\} \), will be repeated \( n \) times. The probability distribution for the outcomes of a single trial will be denoted \( p_0(b) \). The \( n \) outcomes of the \( n \) experiments can be denoted by a vector \( \mathbf{b} = (b_1, b_2, \ldots, b_n) \in \mathcal{B}^n \) where \( b_i \in \mathcal{B} \) for each \( i \). The probability of any event \( E \) on the space \( \mathcal{B}^n \)—that is to say, any set \( E \) of outcome strings—will be denoted by \( P(E) \); the probability of the special case in which \( E \) is a single string \( \mathbf{b} \) will be denoted \( P(\mathbf{b}) \).

The empirical frequency distribution of outcomes in \( \mathbf{b} \) will be written as \( F_{\mathbf{b}}(\mathbf{b}) \),

\[
F_{\mathbf{b}}(\mathbf{b}) = \frac{1}{n} \left( \text{# of occurrences of } \mathbf{b} \text{ in } \mathbf{b} \right),
\]

and the set of all possible frequencies will be denoted by \( \mathcal{F} \),

\[
\mathcal{F} = \left\{ (F_{\mathbf{b}}(1), F_{\mathbf{b}}(2), \ldots, F_{\mathbf{b}}(B)) : \mathbf{b} \in \mathcal{B}^n \right\}.
\]

Note that the cardinality of the set \( \mathcal{F} \), which we shall write as \( |\mathcal{F}| \), is bounded above by \((n + 1)^B\). This follows because there are \( B \) components in the vector specifying any particular frequency \( F_{\mathbf{b}} \), i.e.,

\[
F_{\mathbf{b}} = \left( \frac{n_1}{n}, \frac{n_2}{n}, \ldots, \frac{n_B}{n} \right),
\]

and each of the numerators of these components can take on any value between 0 and \( n \) (subject only to the constraint that \( \sum_i n_i = n \)). Thus there are less than \((n + 1)^B\) choices for the vectors.
The fact that $|F|$ grows only polynomially in $n$ turns out to be quite important for these considerations.

Now to get started, we shall also need a notation for the equivalence class of outcome strings with the same empirical frequency distribution $p_1(b)$; for this we adopt

$$T(p_1) = \left\{ \vec{b} \in \mathcal{B}^n : F_{\vec{b}}(b) = p_1(b) \ \forall \ b \in \mathcal{B} \right\}. \quad (2.80)$$

In this notation, we then have the following theorem.

**Theorem 2.4** Suppose the experimental outcomes are described by a probability distribution $p_0(b)$ that is in fact an element of $F$. Let $P(T(p_1))$ denote the probability that an outcome sequence will be in $T(p_1)$. Then

$$P(T(p_0)) \geq P(T(p_1)). \quad (2.81)$$

That is to say, the most likely frequency distribution in $n$ trials is actually the pre-assigned probability distribution.

Note that this theorem is restricted to probability assignments that are numerically equal to frequencies in $n$ trials. We make this restriction to simplify the techniques involved in proving it and because it is all we will really need for the later considerations.

\[\square\]

To see how this theorem comes about, note that

$$P(T(p_0)) = \sum_{\vec{b} \in T(p_0)} P(\vec{b})$$

$$= \sum_{\vec{b} \in T(p_0)} \prod_{i=1}^{B} p_0(b_i)$$

$$= \sum_{\vec{b} \in T(p_0)} \prod_{b=1}^{B} p_0(b)^{n p_0(b)}$$

$$= |T(p_0)| \prod_{b=1}^{B} p_0(b)^{n p_0(b)} \quad (2.82)$$

and similarly

$$P(T(p_1)) = |T(p_1)| \prod_{b=1}^{B} p_0(b)^{n p_1(b)}. \quad (2.83)$$

Expressions (2.82) and (2.83) can be compared if one realizes that $|T(p_0)|$ is—essentially by definition—identically equal to the number of ways of inserting $n p_0(1)$ objects of type 1, $n p_0(2)$ objects of type 2, etc., into a total $n$ slots. That is to say, $|T(p_0)|$ is a multinomial coefficient,

$$|T(p_0)| = \frac{n!}{(n p_0(1))!(n p_0(2))! \cdots (n p_0(B))!}. \quad (2.84)$$

With this, we have

$$\frac{P(T(p_0))}{P(T(p_1))} = \frac{\left( \prod_{b=1}^{B} (n p_1(b))! \right) \left( \prod_{b=1}^{B} p_0(b)^{n p_0(b)} \right)}{\left( \prod_{b=1}^{B} (n p_0(b))! \right) \left( \prod_{b=1}^{B} p_0(b)^{n p_1(b)} \right)}$$

$$= \prod_{b=1}^{B} \frac{(n p_1(b))!}{(n p_0(b))!} p_0(b)^{n p_0(b) - p_1(b)}. \quad (2.85)$$
The desired result comes about through the inequality

$$\frac{m!}{n!} \geq n^{m-n}. \quad (2.86)$$

Let us quickly demonstrate this before moving on. First, suppose \( m \geq n \). Then,

$$\frac{m!}{n!} = m(m-1) \cdots (n+1) \geq n \cdot n \cdot \cdots \cdot n = n^{m-n} \quad (m-n) \text{ times}$$

(2.87)

Now suppose \( m < n \). Then,

$$\frac{m!}{n!} = [n(n-1) \cdots (m+1)]^{-1} \geq [n \cdot n \cdots n]^{-1} = (n^{n-m})^{-1} = n^{m-n} \quad (n-m) \text{ times}$$

(2.88)

With Eq. (2.86) in hand, Eq. (2.85) gives

$$P(T(p_0)) \geq P(T(p_1)) \geq \prod_{b=1}^{B} (np_0(b))^{|np_1(b) - np_0(b)|} p_0(b)^{np_0(b) - p_1(b)}$$

$$= \prod_{b=1}^{B} n^{np_1(b) - p_0(b)}$$

$$= n^{n \sum_b |p_1(b) - p_0(b)|} = n^0 = 1.$$

(2.89)

Therefore,

$$P(T(p_0)) \geq P(T(p_1)) \geq 1,$$

(2.90)

and this completes the proof that the most likely frequency distribution in \( n \) trials is just the pre-assigned probability distribution. \( \Box \)

The next step toward our goal of demonstrating the Kullback-Leibler information in this new context is to work out an expression for the probability of an outcome string \( \vec{b} \) with an “incorrect” frequency distribution.

**Theorem 2.5** Suppose the experimental outcomes are described by a probability distribution \( p_0(b) \). The probability for a particular string of outcomes \( \vec{b} \in T(p_1) \) with the “wrong” frequencies is

$$P(\vec{b}) = e^{-n[H(p_1) + K(p_1/p_0)]}, \quad (2.91)$$

where

$$H(p_1) = - \sum_{b=1}^{B} p_1(b) \ln p_1(b) \quad (2.92)$$

is the Shannon entropy of the distribution \( p_1(b) \).

\( \triangle \) This can be seen with a little algebra:

$$P(\vec{b}) = \prod_{i=1}^{n} p_0(b_i) = \prod_{b=1}^{B} p_0(b)^{np_1(b)} = \prod_{b=1}^{B} e^{np_1(b) \ln p_0(b)}$$
\[
\prod_{b=1}^{B} \exp \left\{ n \left[ p_1(b) \ln p_0(b) + p_1(b) \ln p_1(b) - p_1(b) \ln p_1(b) \right] \right\}
\]  

\[
= \prod_{b=1}^{B} \exp \left\{ n \left[ p_1(b) \ln p_1(b) + p_1(b) \ln \left( \frac{p_0(b)}{p_1(b)} \right) \right] \right\}
\]  

\[
= \exp \left\{ -n \sum_{b=1}^{B} \left[ -p_1(b) \ln p_1(b) + p_1(b) \ln \left( \frac{p_1(b)}{p_0(b)} \right) \right] \right\}
\]  

\[
= \exp \left\{ -n[H(p_1) + K(p_1/p_0)] \right\} \quad \Box
\]  

(2.93)

A simple corollary to this is,

**Corollary 2.1** If the experimental outcomes are described by \( p_0(b) \), the probability for a particular string \( \vec{b} \in T(p_0) \) with the “correct” frequencies is

\[
P(\vec{b}) = e^{-nH(p_0)}. \quad (2.94)
\]

This follows because \( K(p_0/p_0) = 0 \).

Using this corollary, in conjunction with Theorem 2.4, we can derive a relatively good estimate of the number of elements in \( T(p_1) \). This estimate is necessary for connecting the relative information to the probability of an “incorrect” frequency.

**Lemma 2.2** For any \( p_1(b) \in \mathcal{F} \),

\[
(n + 1)^{-B} e^{nH(p_1)} \leq |T(p_1)| \leq e^{nH(p_1)}. \quad (2.95)
\]

This probability, however, must be less than 1. Hence, \(|T(p_1)| \leq e^{nH(p_1)}\)—proving the right-hand side of the lemma. The left-hand side follows similarly by considering the probability of all possible frequencies and using Theorem 2.4,

\[
1 = \sum_{F_{\vec{b}} \in \mathcal{F}} P \left( T(F_{\vec{b}}) \right) \leq \sum_{F_{\vec{b}} \in \mathcal{F}} \max_{F_{\vec{b}} \in \mathcal{F}} P \left( T(F_{\vec{b}}) \right)
\]

\[
= P(T(p_1)) \left( \sum_{F_{\vec{b}} \in \mathcal{F}} 1 \right) = |\mathcal{F}| P(T(p_1))
\]

\[
\leq (n + 1)^{B} P(T(p_1))
\]

\[
= (n + 1)^{B} |T(p_1)| e^{-nH(p_1)}. \quad (2.97)
\]

Thus \((n + 1)^{-B} e^{nH(p_1)} \leq |T(p_1)|\) and this completes the proof of the lemma. \( \Box \)

Let us now move quickly to our sought after theorem and its proof.
Theorem 2.6 Suppose the experimental outcomes are described by the probability distribution $p_0(b)$. The probability that the outcome string will have some “incorrect” frequency distribution $p_1(b)$ is $P(T(p_1))$. This number is bounded in the following way,

$$(n + 1)^{-B} e^{-nK(p_1/p_0)} \leq P(T(p_1)) \leq e^{-nK(p_1/p_0)} .$$

This is now easy to prove. We just need write

$$P(T(p_1)) = \sum_{\bar{b} \in T(p_1)} P(\bar{b}) = \sum_{\bar{b} \in T(p_1)} P(\bar{b}) e^{-n[H(p_1)+K(p_1/p_0)]} = |T(p_1)| e^{-n[H(p_1)+K(p_1/p_0)]},$$

(2.99)

to see that we can use Lemma 2.2 to give the desired result. □

2.4 Distinguishability via Mutual Information

Consider what happens when one samples a known probability distribution $p(b)$, $b = 1, \ldots, n$. The probability quantifies the extent to which the outcome can be predicted, but it generally does not pin down the precise outcome itself. Upon learning the outcome of a sampling, one, in a very intuitive sense, “gains information” that he does not possess beforehand. For instance, if all the outcomes of the sampling are equally probable, then one will generally gain a lot of information from the sampling; there is essentially nothing that can be predicted about the outcome beforehand. On the other hand, if the probability distribution is highly peaked about one particular outcome, then one will generally gain very little information from the sampling; there will be almost no point in carrying out the sampling—its outcome can be predicted at the outset. This simple idea provides the starting point for building our last notion of distinguishability.

Let us sketch the idea briefly before attempting to make it precise. Suppose there is a reasonable way of quantifying the average information gained when one samples a distribution $q(b)$; denote that quantity, whatever it may be, by $H(q)$. Then, if two probability distributions $p_0(b)$ and $p_1(b)$ are distinct in the sense that one has more unpredictable outcomes than the other, the average information gained upon sampling them will also be distinct, i.e., either $H(p_0) \geq H(p_1)$ or vice versa. For, in sampling the distribution with the more unpredictable outcomes, one can expect to gain a larger amount of information. Thus, immediately, the notion of information gain in a sampling provides a means for distinguishing probability distributions. At this level, however, one is no better off than in simply comparing the probabilities themselves. To get somewhere with this idea, a more interesting scenario must be developed.

The problem in comparing distributions through the information one gains upon sampling them is that the information gain has nothing to say about the distribution itself—that quantity is assumed already known. What would happen, however, if one were to randomly choose between sampling the two different distributions, say with probabilities $\pi_0$ and $\pi_1$? We can make a case for two distinct possibilities. First, perhaps trivially, suppose that in spite of choosing the sampling distribution randomly, one still knows which distribution is in front of him at any given moment. Then an average information gain $H(p_0)$ will ensue when the actual distribution is $p_0(b)$ and $H(p_1)$ will ensue when the actual distribution is $p_1(b)$; that is to say, the expected information gain in a sampling a known distribution is just $\pi_0H(p_0) + \pi_1H(p_1)$. Notice that this quantity, being an
average, is greater than the lesser of the two information gains and less than the greater of the two gains, i.e.,
\[
\min\{H(p_0), H(p_1)\} \leq \pi_0 H(p_0) + \pi_1 H(p_1) \leq \max\{H(p_0), H(p_1)\} .
\] (2.100)

Now consider the opposing case where the identity of the distribution to be sampled remains unknown. In this case, the most one can say about which outcome will occur in the sampling is that it is controlled by the probability distribution \(p(b) = \pi_0 p_0(b) + \pi_1 p_1(b)\). In other words, the sampling outcome will be even more unpredictable than it was in either of the two individual cases; some of the unpredictability will be due to the indeterminism \(p_0(b)\) and \(p_1(b)\) describe and some of the unpredictability will be due to the fact that the individual distribution from which the sample is drawn remains unknown. Hence it must be the case that \(H(p) \geq H(p_0)\) and \(H(p) \geq H(p_1)\).

The excess of \(H(p)\) over \(\pi_0 H(p_0) + \pi_1 H(p_1)\) is the average gain of information one can expect about the distribution itself. This quantity, called the mutual information \([61, 62]\),
\[
J(p_0, p_1; \pi_0, \pi_1) = H(\pi_0 p_0 + \pi_1 p_1) - \left(\pi_0 H(p_0) + \pi_1 H(p_1)\right) ,
\] (2.101)
is the natural candidate for distinguishability that we seek in this section. If the two distributions \(p_0(b)\) and \(p_1(b)\) are completely distinguishable, then all the information gained in a sampling should be solely about the identity of the distribution; the quantity \(J(p_0, p_1; \pi_0, \pi_1)\) should reduce to \(H(\pi)\), the information that can be gained by sampling the prior distribution \(\pi = \{\pi_0, \pi_1\}\). If the distributions \(p_0(b)\) and \(p_1(b)\) are completely indistinguishable, then \(J(p_0, p_1; \pi_0, \pi_1)\) should reduce to zero; this signifies that in sampling one learns nothing whatsoever about the distribution from which the sample is drawn.

Notice that this distinguishability measure depends crucially on the observer’s prior state of knowledge, quantified by \(\pi = \{\pi_0, \pi_1\}\), about whether \(p_0(b)\) or \(p_1(b)\) is actually the case. Thus it is a measure of distinguishability relative to a given state of knowledge. There is, of course, nothing wrong with this, just as there was nothing wrong with the error-probability distinguishability measure; one just needs to recognize it as such.

These are the ideas behind taking mutual information as a measure of distinguishability. In the remainder of this section, we work toward justifying a precise expression for Eq. (2.101) and showing in a detailed way how it can be interpreted in an operational context.

### 2.4.1 Derivation of Shannon’s Information Function

The function \(H(p)\) that quantifies the average information gained upon sampling a distribution \(p(b)\) will ultimately turn out to be the famous Shannon information function \([60, 62]\)
\[
H(p) = -\sum_b p(b) \ln p(b) .
\] (2.102)

What we should like to do here is justify this expression from first principles. That is to say, we shall build up a theory of “information gain” based solely on the probabilities in an experiment and find that that theory gives rise to the expression (2.102).

To start with our most basic assumption, we reiterate the idea that the information gained in performing an experiment or observation is a function of how well the outcomes to that experiment or observation can be predicted in the first place. Other characteristics of an outcome that might convey “information” in the common sense of the word, such as shape, color, smell, feel, etc., will be considered irrelevant; indeed, we shall assume any such properties already part of the very definition of the outcome events. Formally this means that if a set of events \(\{x_1, x_2, \ldots, x_n\}\) has a probability distribution \(p(x)\), not only is the expected information gain in a sampling, \(H(p)\),
exclusively a function of the numbers \( p(x_1), p(x_2), \ldots, p(x_n) \), but also it must be independent of the labelling of that set. In other words, \( H(p) \equiv H(p(x_1), p(x_2), \ldots, p(x_n)) \) is required to be invariant under permutations of its arguments. This is called the requirement of “symmetry.”

The most important technical property of \( H(p) \) is that, even though information gain is a subjective concept depending on the observer’s prior state of knowledge, it should at least be objective enough that it not depend on the method by which knowledge of the experimental outcomes is acquired. We can make this idea firm with a simple example. Consider an experiment with three mutually exclusive outcomes \( x, y, \) and \( z \). Note that the probability that \( z \) does not occur is

\[
p(\neg z) = 1 - p(z) = p(x) + p(y) .
\] (2.103)

The probabilities for \( x \) and \( y \) given that \( z \) does not occur are

\[
p(x|\neg z) = \frac{p(x)}{p(x) + p(y)} \quad \text{and} \quad p(y|\neg z) = \frac{p(y)}{p(x) + p(y)} .
\] (2.104)

There are at least two methods by which an observer can gather the result of this experiment. The first method is by the obvious tack of simply finding which outcome of the three possible ones actually occurred. In this case, the expected information gain is, by our convention,

\[
H\left(p(x), p(y), p(z)\right).
\] (2.105)

The second method is more roundabout. One could, for instance, first check whether \( z \) did or did not occur, and then in the event that it did not occur, further check which of \( x \) and \( y \) did occur. In the first phase of this method, the expected information gain is

\[
H\left(p(\neg z), p(z)\right).
\] (2.106)

For those cases in which the second phase of the method must be carried out, a further gain of information can be expected. Namely,

\[
H\left(p(x|\neg z), p(y|\neg z)\right).
\] (2.107)

Note, though, that this last case is only expected to occur a fraction \( p(\neg z) \) of the time. Thus, in total, the expected information gain by this more roundabout method is

\[
H\left(p(\neg z), p(z)\right) + p(\neg z) H\left(p(x|\neg z), p(y|\neg z)\right).
\] (2.108)

The assumption of “objectivity” is that the quantities in Eqs. (2.103) and (2.108) are identical. That is to say, upon changing the notation slightly to \( p_x = p(x), p_y = p(y), p_z = p(z)\)

\[
H(p_x, p_y, p_z) = H(p_x + p_y, p_z) + (p_x + p_y) H\left(\frac{p_x}{p_x + p_y}, \frac{p_y}{p_x + p_y}\right).
\] (2.109)

In the event that we are instead concerned with \( n \) mutually exclusive events, the same assumption of “objectivity” leads to the identification,

\[
H(p_1, \ldots, p_n) = H(p_1 + p_2, p_3, \ldots, p_n) + (p_1 + p_2) H\left(\frac{p_1}{p_1 + p_2}, \frac{p_2}{p_1 + p_2}\right).
\] (2.110)

It turns out that the requirements of symmetry and objectivity (as embodied in Eq. (2.110)) are enough to uniquely determine the form of \( H(p) \) (up to a choice of units) provided we allow
ourselves one extra convenience, namely, that we allow the introduction of an arbitrary positive parameter \( \alpha \neq 1 \) into Eq. (2.110) in the following way,

\[
H_\alpha(p_1, \ldots, p_n) = H_\alpha(p_1 + p_2, p_3, \ldots, p_n) + (p_1 + p_2)^\alpha H_\alpha\left(\frac{p_1}{p_1 + p_2}, \frac{p_2}{p_1 + p_2}\right),
\]

and define \( H(p) \) to be the limiting value of \( H_\alpha(p) \) as \( \alpha \to 1 \). (The introduction of the subscript on \( H_\alpha(p) \) is made simply to remind us that the solutions to Eq. (2.111) depend upon the parameter \( \alpha \).) This idea is encapsulated in the following theorem.

**Theorem 2.7 (Daróczy)** Let

\[
\Gamma_n = \left\{ (p_1, \ldots, p_n) \mid p_k \geq 0, k = 1, \ldots, n, \text{ and } \sum_{i=1}^{n} p_i = 1 \right\}
\]

be the set of all \( n \)-point probability distributions and let \( \Gamma = \bigcup_n \Gamma_n \) be the set of all discrete probability distributions. Suppose the function \( H_\alpha : \Gamma \to \mathbb{R}, \alpha \neq 1, \) is symmetric in all its arguments and satisfies Eq. (2.111) for each \( n \geq 2 \). Then, under the convention that \( 0 \ln 0 = 0 \), the limiting value of \( H_\alpha \) as \( \alpha \to 1 \) is uniquely specified up to a constant \( C \) by

\[
H(p_1, \ldots, p_n) = -\frac{C}{\ln 2} \sum_{i=1}^{n} p_i \ln p_i.
\]

The constant \( C \) in this expression fixes the “units” of information. If \( C = 1 \), information is said to be measured in bits; if \( C = \ln 2 \), information is said to be measured in nats. (A relatively obscure measure of information is the case \( C = \log_{10} 2 \), where the units are called Hartleys [64].) In this document, we will generally take \( C = \ln 2 \). On the occasion, however, that we do consider information in units of bits we shall write \( \log() \) for the base-2 logarithm, rather than the more common \( \log() \).

\( \Delta \) The proof of Theorem 2.7, deserving wider recognition, is due to Daróczy [63] and proceeds as follows. Define \( s_i = p_1 + \cdots + p_i \) and let

\[
f(x) = H_\alpha(x, 1-x) \quad \text{for} \quad 0 \leq x \leq 1.
\]

Then, by repeated application of condition (2.111), it follows immediately that

\[
H_\alpha(p_1, \ldots, p_n) = \sum_{i=2}^{n} s_i^\alpha f\left(\frac{p_i}{s_i}\right).
\]

Thus all we need do is focus on finding an explicit expression for the function \( f \).

We have from the symmetry requirement that \( H_\alpha(x, 1-x) = H_\alpha(1-x, x) \) and hence,

\[
f(x) = f(1-x).
\]

In particular, \( f(0) = f(1) \). Furthermore, if \( x \) and \( y \) are two nonnegative numbers such that \( x+ y \leq 1 \), we must also have

\[
H_\alpha(x, y, 1-x-y) = H_\alpha(y, x, 1-x-y).
\]
However, by Eq. (2.111)

\[ H_\alpha(x, y, 1 - x - y) = H_\alpha(x, 1 - x) + (1 - x)^\alpha H_\alpha\left(\frac{y}{1 - x}, \frac{1 - x - y}{1 - x}\right) \]

\[ = H_\alpha(x, 1 - x) + (1 - x)^\alpha H_\alpha\left(\frac{y}{1 - x}, \frac{1}{1 - x}\right) \]

\[ = f(x) + (1 - x)^\alpha f\left(\frac{y}{1 - x}\right). \]

(2.118)

Thus it follows that \( f \) must satisfy the functional equation

\[ f(x) + (1 - x)^\alpha f\left(\frac{y}{1 - x}\right) = f(y) + (1 - y)^\alpha f\left(\frac{x}{1 - y}\right), \]

(2.119)

for \( x, y \in [0, 1) \) with \( x + y \leq 1 \). (In the case \( \alpha = 1 \), Eq. (2.119) is known commonly as the fundamental equation of information \[\text{[66].}\]

We base the remainder of our conclusions on the study of Eq. (2.119). Note first that if \( x = 0 \), it reduces to,

\[ f(0) + f(y) = f(y) + (1 - y)^\alpha f(0). \]

(2.120)

Since \( y \) is still arbitrary, it follows from this that \( f(0) = 0 \); thus \( f(1) = 0 \), too. Now let \( p = 1 - x \) for \( x \neq 1 \) and let \( q = y/(1 - x) = y/p \). With this, the information equation (2.119) becomes

\[ f(p) + p^\alpha f(q) = f(pq) + (1 - pq)^\alpha f\left(\frac{1 - p}{1 - pq}\right). \]

(2.121)

We can use this equation to show that

\[ F(p, q) \equiv f(p) + [p^\alpha + (1 - p)^\alpha] f(q) \]

(2.122)

is symmetric in \( q \) and \( p \), i.e., \( F(p, q) = F(q, p) \). From that fact, a unique expression for \( f(p) \) follows trivially. Let us just show this before going further:

\[ 0 = F\left(p, \frac{1}{2}\right) - F\left(\frac{1}{2}, p\right) \]

\[ = f(p) + [p^\alpha + (1 - p)^\alpha] f\left(\frac{1}{2}\right) - f\left(\frac{1}{2}\right) - \left[\left(\frac{1}{2}\right)^\alpha + \left(\frac{1}{2}\right)^\alpha\right] f(p) \]

\[ = \left(1 - 2^{1 - \alpha}\right) f(p) + f\left(\frac{1}{2}\right) [p^\alpha + (1 - p)^\alpha - 1], \]

(2.123)

which implies that

\[ f(p) = C \left(2^{1 - \alpha} - 1\right)^{-1} [p^\alpha + (1 - p)^\alpha - 1], \]

(2.124)

where the constant \( C = f\left(\frac{1}{2}\right) \). Because \( f(0) = f(1) = 0 \), Eq. (2.124) also holds for \( p = 0 \) and \( p = 1 \).

To cap off the derivation of Eq. (2.124), let us demonstrate that \( F(p, q) \) is symmetric. Just expanding and regrouping, we have, by Eq. (2.122), that

\[ F(p, q) = [f(p) + p^\alpha f(q)] + (1 - p)^\alpha f(q) \]

\[ = f(pq) + (1 - pq)^\alpha f\left(\frac{1 - p}{1 - pq}\right) + (1 - p)^\alpha f(q) \]

\[ = f(pq) + (1 - pq)^\alpha \left[f\left(\frac{1 - p}{1 - pq}\right) + \left(\frac{1 - p}{1 - pq}\right)^\alpha f(q)\right]. \]

(2.125)
If we can show that the last term in this expression is symmetric in \( q \) and \( p \), then we will have shown that \( F(p, q) \) is symmetric. To this end, let us define

\[
A(p, q) = f\left(\frac{1 - p}{1 - pq}\right) + \left(\frac{1 - p}{1 - pq}\right)^\alpha f(q). \tag{2.126}
\]

Also, to save a little room, let

\[
z = \frac{1 - p}{1 - pq}. \tag{2.127}
\]

Then,

\[
1 - zq = \frac{1 - q}{1 - pq} \quad \text{and} \quad 1 - z = p\left(\frac{1 - q}{1 - pq}\right). \tag{2.128}
\]

So that, upon using Eq. (2.121) again, we get

\[
A(p, q) = f(z) + z^\alpha f(q)
= f(zq) + (1 - zq)^\alpha f\left(\frac{1 - z}{1 - zq}\right)
= f(1 - zq) + (1 - zq)^\alpha f\left(\frac{1 - z}{1 - zq}\right)
= f\left(\frac{1 - q}{1 - pq}\right) + \left(\frac{1 - q}{1 - pq}\right)^\alpha f(p)
= A(q, p). \tag{2.129}
\]

Thus \( F(p, q) \) is symmetric. This completes the demonstration of Eq. (2.124).

We just need plug the expression for \( f(p) \) into Eq. (2.115) to get a nearly final result,

\[
H_\alpha(p_1, \ldots, p_n) = \sum_{i=2}^{n} s_i^\alpha C \left(2^{1-\alpha} - 1\right)^{-1} \left[\left(\frac{p_i}{s_i}\right)^\alpha + \left(1 - \frac{p_i}{s_i}\right)^\alpha - 1\right]
= C \left(2^{1-\alpha} - 1\right)^{-1} \sum_{i=2}^{n} \left[p_i^\alpha + (s_i - p_i)^\alpha - s_i^\alpha\right]
= C \left(2^{1-\alpha} - 1\right)^{-1} \sum_{i=2}^{n} \left[p_i^\alpha + s_{i-1}^\alpha - s_i^\alpha\right]
= C \left(2^{1-\alpha} - 1\right)^{-1} \left(\sum_{i=2}^{n} p_i^\alpha + s_1^\alpha - s_n^\alpha\right)
= C \left(2^{1-\alpha} - 1\right)^{-1} \left(\sum_{i=1}^{n} p_i^\alpha - 1\right). \tag{2.130}
\]

Now in taking the limit \( \alpha \to 1 \), note that both the numerator and denominator of this expression vanishes. Thus we must use l’Hospital’s rule in the calculating limit, i.e., first take the derivative with respect to \( \alpha \) of the numerator and denominator separately and then take the limit:

\[
\lim_{\alpha \to 0} H_\alpha(p_1, \ldots, p_n) = \lim_{\alpha \to 0} C\left(-2^{1-\alpha} \ln 2\right)^{-1} \left(\sum_{i=1}^{n} p_i^\alpha \ln p_i\right)
\]

34
This completes our derivation of the Shannon information formula (2.102). It is to be hoped that this has conveyed something of the austere origin of the information-gain concept. □

We finally mention that the Daróczy informations of type-α, i.e., Eq. (2.130), appearing in this derivation are of interest in their own right. First of all, there is a simple relation between these and the Renyi informations of degree-α introduced in Section 2.2, namely,

\[
H_\alpha(p) = \frac{1}{\alpha - 1} \ln \left( \sum_{i=1}^{n} p_i^\alpha \right) = \frac{1}{\alpha - 1} \ln \left( \frac{1}{C} \left( 2^{1-\alpha} - 1 \right) H_\alpha(p) + 1 \right).
\]  

(2.132)

Secondly, they share many properties with the Shannon information while being slightly more tractable for some applications, there being no logarithm in their expression.

### 2.4.2 An Interpretation of the Shannon Information

The justification of the information-gain concept can be strengthened through an operational approach to the question. To carry this out, let us develop the following example. Suppose we were to perform an experiment with four possible outcomes \(x_1, x_2, x_3, x_4\), the respective probabilities being \(p(x_1) = \frac{1}{20}\), \(p(x_2) = \frac{1}{5}\), \(p(x_3) = \frac{1}{4}\), and \(p(x_4) = \frac{1}{2}\). The expected gain of information in this experiment is given by Eq. (2.102) and is numerically approximately 1.68 bits. By the fundamental postulate of Section 2.4.1, we know that this information gain will be independent of the method of questioning used in discerning the outcome. In particular, we could consider all possible ways of determining the outcome by way of binary yes/no questions. For instance, we could start by asking, “Is the outcome \(x_1\)?” If the answer is yes, then we are done. If the answer is no, then we could further ask, “Is the outcome \(x_2\)?,” and proceed in similar fashion until the identity of the outcome is at hand. This and three other such binary-question methodologies are depicted schematically in Figure 2.1.

The point of interest to us here is that each such questioning scheme generates, by its very nature, a code for the possible outcomes to the experiment. That code can be generated by writing down, in order, the yes’s and no’s encountered in traveling from the root to each leaf of these schematic trees. For instance, by substituting 0 and 1 for yes and no, respectively, the four trees depicted in Figure 2.1 give rise to the codings:

<table>
<thead>
<tr>
<th>Scheme 1</th>
<th>Scheme 2</th>
<th>Scheme 3</th>
<th>Scheme 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>(x_1 \leftrightarrow 0)</td>
<td>(x_1 \leftrightarrow 00)</td>
<td>(x_1 \leftrightarrow 11)</td>
<td>(x_1 \leftrightarrow 011)</td>
</tr>
<tr>
<td>(x_2 \leftrightarrow 10)</td>
<td>(x_2 \leftrightarrow 01)</td>
<td>(x_2 \leftrightarrow 0)</td>
<td>(x_2 \leftrightarrow 010)</td>
</tr>
<tr>
<td>(x_3 \leftrightarrow 110)</td>
<td>(x_1 \leftrightarrow 10)</td>
<td>(x_1 \leftrightarrow 100)</td>
<td>(x_3 \leftrightarrow 00)</td>
</tr>
<tr>
<td>(x_4 \leftrightarrow 111)</td>
<td>(x_1 \leftrightarrow 11)</td>
<td>(x_1 \leftrightarrow 101)</td>
<td>(x_4 \leftrightarrow 1)</td>
</tr>
</tbody>
</table>

Codes that can be generated from trees in this way are called instantaneous or prefix-free and are noteworthy for the property that concatenated strings of their codewords can be uniquely deciphered just by reading from left to right. This follows because no codeword in such a coding...
Figure 2.1: Binary Question Schemes
can be the “prefix” of any other codeword. As a case in point, using the coding generated by Scheme 1, the “message” 1111100010100110 uniquely corresponds to the concatenation \( x_4 x_3 x_1 x_2 x_2 x_1 x_3 \); there are no other possibilities.

From these four examples, one can see that not all such questioning schemes are equally efficient. For Scheme 1 the expected codeword length, i.e.,

\[
I = \sum p(x_i) l(x_i)
\]

(2.133)

where \( l(x_i) \) is the number of digits in the code word for \( x_i \), is 2.70 binary digits. Those for Schemes 2–4 are 2.00, 2.55, and 1.75 binary digits, respectively. To see where this example is going, note that each expectation value is greater than \( H(p) \), the average information gained in sampling the distribution \( p(x_i) \). This inequality is no accident. As we shall see, the Shannon noiseless coding theorem \[60\] specifies that the expected codeword length of any instantaneous code must be greater than \( H(p) \). Moreover, the minimal average codeword length is bounded above by \( H(p) + 1 \).

Reverting back to the language of questioning schemes, we have that the minimum average number of binary questions required to discern the outcome of sampling \( p(x_i) \) is approximately equal to \( H(p) \).

This we take as a new starting point for interpreting the information function: it is approximately the minimal effort (quantified in terms of expected number of binary questions) required to discern the outcome of an experiment. To make this precise, we presently set out to demonstrate how the noiseless coding theorem comes about within this context.

Our first step in doing this is to demonstrate an elementary lemma of information theory, known as the Kraft inequality \[67\], giving a useful analytic characterization of all possible instantaneous codes.

**Lemma 2.3 (Kraft)** The codeword lengths \( l_1 \leq l_2 \leq \cdots \leq l_n \) of any binary instantaneous code for a set of messages \( \{x_1, x_2, \ldots, x_n\} \) must satisfy the inequality

\[
\sum_{k=1}^{n} 2^{-l_k} \leq 1.
\]

(2.134)

Moreover, for any set of integers \( k_1 \leq k_2 \leq \cdots \leq k_n \) satisfying this inequality, there exists a instantaneous code with these as codeword lengths.

\[\triangle\] The derivation of this lemma is really quite simple. Start with the coding tree generating the instantaneous code and imbed it in a full tree of \( 2^n \) leaves. A full tree is a tree for which each direct path leading from the root to a terminal leaf is of the same length; see Figure 2.4.2. With this, one sees easily that the number of terminal leaves in the full tree stemming from the node associated with the codeword of length \( l_i \) is just \( 2^{l_n-l_i} \), \( i = 1, \ldots, n \). Therefore it follows that the total number of terminal leaves in this tree not associated with codewords must be

\[
\sum_{i=1}^{n} 2^{l_n-l_i}.
\]

(2.135)

This number, however, can be no larger than the number of leaves in the full tree. Thus

\[
\sum_{i=1}^{n} 2^{l_n-l_i} \leq 2^{l_n}.
\]

(2.136)

This proves the first statement of the lemma.
Figure 2.2: Coding Tree Imbedded in a Full Tree
For the second statement of the lemma, start with a full tree of \(^{2k_n}\) leaves. First place the symbol \(x_1\) at some node of depth \(k_1\) and delete all further descendents of that node. Then place the symbol \(x_2\) at any remaining node of depth \(k_2\) and remove its descendents. Iterating this procedure will produce the appropriate coding tree and thus a instantaneous code with the specified codeword lengths. □

With the Kraft inequality in hand, it is a simple matter to derive the Shannon noiseless coding theorem.

**Theorem 2.8 (Shannon)** Suppose messages \(x_1, \ldots, x_n\) occur with probabilities \(p(x_1), \ldots, p(x_n)\). Then the minimal average codeword length \(\bar{t}_{\text{min}}\) for a binary instantaneous coding of these messages satisfies

\[
H(p) \leq \bar{t}_{\text{min}} \leq H(p) + 1,
\]

where \(H(p)\) is the Shannon information of the distribution \(p(x_i)\) measured in bits.

△ To show the left-hand inequality, we just need note that for any instantaneous code the Kraft inequality specifies

\[
\bar{t} - H(p) = \sum_i p(x_i)l(x_i) + \sum_i p(x_i) \log p(x_i)
\]

\[
= -\sum_i p(x_i) \log 2^{-l(x_i)} + \sum_i p(x_i) \log p(x_i)
\]

\[
= \sum_i p(x_i) \log \left( \frac{p(x_i)}{q(x_i)} \right) - \log \left( \sum_i 2^{-l(x_i)} \right)
\]

\[
\geq \sum_i p(x_i) \log \left( \frac{p(x_i)}{q(x_i)} \right),
\]

(2.138)

where

\[
q(x_i) = \frac{2^{-l(x_i)}}{\sum_i 2^{-l(x_i)}}
\]

(2.139)

is a probability distribution constructed for the purpose at hand. Namely, the final quantity on the right-hand side of Eq. (2.138) is then positive by the Shannon inequality, Eq. (2.70), already demonstrated. Thus it follows that

\[
\bar{t} - H(p) \geq 0,
\]

(2.140)

and so the minimal average instantaneous codeword length must be at least as large as \(H(p)\).

Now to show the right hand side of Theorem 2.8 we need only note that there is an instantaneous code with codeword lengths given by

\[
l(x_i) = \lceil -\log p(x_i) \rceil,
\]

(2.141)

where \(\lceil x \rceil\) denotes the smallest integer greater than or equal to \(x\), because these integers satisfy the Kraft inequality. Therefore it must hold that

\[
\bar{t}_{\text{min}} \leq \sum_i p(x_i) \lceil -\log p(x_i) \rceil
\]

\[
\leq \sum_i p(x_i) \left( -\log p(x_i) + 1 \right)
\]

\[
= H(p) + 1.
\]

(2.142)
This concludes our proof of the Shannon noiseless coding theorem. □

This is one precise sense in which \( T_{\text{min}} \approx H(p) \). Actually, the exact value of \( T_{\text{min}} \) can be calculated given the message probabilities \( p(x_1), \ldots, p(x_n) \). This comes about by an optimal coding procedure known as Huffman coding [45, 46, 47, 48]. Therefore, one might have wished to choose \( T_{\text{min}} \) as the appropriate measure of information under the present interpretation. This, however, encounters an immediate objection: the Huffman coding algorithm gives no explicit analytical expression for \( T_{\text{min}} \). Thus using \( T_{\text{min}} \) as a measure of information would be operationally difficult at best. Also, though, there are even tighter upper bounds on \( T_{\text{min}} \) than given by the noiseless coding theorem. For instance if \( p(x_1) \geq p(x_2) \geq \cdots \geq p(x_n) \), then [46, 47]

\[
T_{\text{min}} - H(p) \leq \begin{cases} 
p(x_1) + \sigma & \text{if } p(x_1) < \frac{1}{2} \\
2 - h(p(x_1)) - p(x_1) & \text{if } p(x_1) \geq \frac{1}{2} 
\end{cases} \tag{2.143}
\]

where \( \sigma = 1 - \log e + \log e \approx 0.86 \) and

\[
h(x) = -x \log x - (1 - x) \log(1 - x) . \tag{2.144}
\]

Another bound is

\[
T_{\text{min}} - H(p) \leq 1 - h(p(x_n)) \leq 1 - 2p(x_n) . \tag{2.145}
\]

Tighter bounds than this, in terms of \( p(x_1) \) and \( p(x_n) \), are known [47], but are not so easily expressible. The upshot is that these generally force \( T_{\text{min}} \) closer to \( H(p) \) than the noiseless coding theorem and thus strengthen the notion of “approximate” here.

Finally, in this context, we note that a direct consequence of Theorem 2.8 is the following. If we were to repeat the experiment described by \( p(x_k) \), say, \( N \) times before asking a set of yes–no questions to discern all \( N \) outcomes, the minimum expected number of questions will be some \( T_{\text{min}} \) that satisfies

\[
H(P) \leq T_{\text{min}} \leq H(P) + 1 , \tag{2.146}
\]

where \( P(x_{i_1}, x_{i_2}, \ldots, x_{i_N}) = p(x_{i_1})p(x_{i_2})\cdots p(x_{i_N}) \) is the (product) probability distribution describing all \( N \) outcomes. Using the fact that

\[
H(P) = - \sum_{x_{i_1}, \ldots, x_{i_N}} P(x_{i_1}, \ldots, x_{i_N}) \log P(x_{i_1}, \ldots, x_{i_N})
\]

\[
= - \sum_{x_{i_1}, \ldots, x_{i_N}} P(x_{i_1}, \ldots, x_{i_N}) \left( \sum_{k=1}^{n} \log p(x_k) \right)
\]

\[
= -N \sum_{k=1}^{n} p(x_k) \log p(x_k)
\]

\[
= NH(p) , \tag{2.147}
\]

Eq. (2.146) reduces to

\[
H(p) \leq \frac{1}{N} T_{\text{min}} \leq H(p) + \frac{1}{N} . \tag{2.148}
\]

Therefore, if one is willing to collect data on multiple experiments before asking the yes–no questions required to discern the outcomes, then one can make the expected number of questions \( \text{per experiment} \) as close to \( H(p) \) as one wishes—just by choosing \( N \) sufficiently large. This is another, strong sense in which \( H(p) \) quantifies the minimal effort required to discern the outcome of an experiment.
2.4.3 The Mutual Information

The notion of information gain has now been analyzed from two very different perspectives, one axiomatic and one operational. With a firm expression for this notion finally at hand, we may return to the real object of this section, the measure of distinguishability known as *mutual information*. Using Eq. (2.102) in conjunction with Eq. (2.101), we obtain various formulations of this quantity

\[
J(p_0, p_1; \pi_0, \pi_1) = -\sum_b p(b) \ln p(b) + \pi_0 \sum_b p_0(b) \ln p_0(b) + \pi_1 \sum_b p_1(b) \ln p_1(b)
\]

\[
= \pi_0 \sum_b p_0(b) \ln \left( \frac{p_0(b)}{p(b)} \right) + \pi_1 \sum_b p_1(b) \ln \left( \frac{p_1(b)}{p(b)} \right)
\]

\[
= \pi_0 K(p_0/p) + \pi_1 K(p_1/p) ,
\]

(2.149)

where \( p(b) = \pi_0 p_0(b) + \pi_1 p_1(b) \) and \( K(\cdot) \) denotes the Kullback-Leibler relative information of Section 2.3. The last form gives a secondary interpretation to the mutual information: in an honest expert problem, it is the expert’s expected loss for trying to pass off the mean distribution \( p(b) \) in place of either actual distribution \( p_0(b) \) or \( p_1(b) \).
Chapter 3

The Distinguishability of Quantum States

“... a priori one should expect a chaotic world which cannot be grasped by the mind in any way. One could (yes one should) expect the world to be subjected to law only to the extent that we order it through our intelligence.”

—Albert Einstein
Letter to Maurice Solovine
30 March 1952

3.1 Introduction

For any given quantum state, the outcomes of most possible measurements are completely lawless in their determination. Quantum theory, however, provides the means for calculating probabilities for the outcomes. It is by this handle that the measures of distinguishability for probability distributions can be used to say something about quantum mechanical states. In this Chapter, we work toward “quantizing” the classical distinguishability measures introduced in Chapter 2. The problem of statistically distinguishing quantum states $\hat{\rho}_0$ and $\hat{\rho}_1$ on a $D$-dimensional Hilbert space via quantum measurement is that of using some measurement with $n$ outcomes to generate the probability distributions $p_0(b)$ and $p_1(b)$ used in the classical measures. The number $n$ here should be thought of as a free variable that remains to be fixed; certainly it need not equal $D$. An optimal quantum measurement with respect to any of these measures is just a measurement that makes these quantities as large or as small as they can possibly be. The “quantized” measures are simply the numerical values of the classical measures when an optimal measurement is used.

The strategy for making progress toward precise expressions of these quantities is to use the formalism of positive-operator-valued measures or POVMs [73, 74, 26] introduced in Chapter 1. As a quick reminder, a POVM is a set of positive operators $\hat{E}_b$ which is complete, i.e.,

$$\langle \psi | \hat{E}_b | \psi \rangle \geq 0 \quad \text{for all } b \text{ and all vectors } |\psi\rangle ,$$  \hspace{1cm} (3.1)

and

$$\sum_b \hat{E}_b = \hat{1} = \begin{pmatrix} \text{identity operator} \end{pmatrix} .$$ \hspace{1cm} (3.2)
A consequence of this definition is that the $\hat{E}_b$ are Hermitian operators with nonnegative eigenvalues $(3.8)$. The subscript $b$ here, as before, indexes the possible outcomes of the measurement. Again, the conditions on the $\hat{E}_b$ are those necessary and sufficient for the expression $p(b) = \text{tr}(\hat{\rho}\hat{E}_b)$ to be a valid probability distribution for the $b$. As described in Chapter 1, it turns out that a measurement corresponding to a POVM can always be interpreted as an “ordinary” orthogonal projection-valued measurement (i.e., one for which the outcomes correspond to eigenvalues of a Hermitian operator) on an extended system consisting of the given one along with an independently prepared auxiliary system; the labels $b$ in that interpretation stand for the various outcomes to the ordinary measurement on the composite system $(3.8)$.

The quantum measures of distinguishability we shall focus upon in this chapter are, listed in order of increasing unwieldiness:

- the Quantum Error Probability

$$P_e(\hat{\rho}_0|\hat{\rho}_1) \equiv \min_{\{\hat{E}_b\}} \sum_b \min\{\pi_0\text{tr}(\hat{\rho}_0\hat{E}_b), \pi_1\text{tr}(\hat{\rho}_1\hat{E}_b)\}$$  (3.3)

- the Quantum Fidelity

$$F(\hat{\rho}_0, \hat{\rho}_1) \equiv \min_{\{\hat{E}_b\}} \sum_b \sqrt{\text{tr}(\hat{\rho}_0\hat{E}_b)} \sqrt{\text{tr}(\hat{\rho}_1\hat{E}_b)}$$  (3.4)

- the Quantum Rényi Overlaps

$$F_\alpha(\hat{\rho}_0/\hat{\rho}_1) \equiv \min_{\{\hat{E}_b\}} \sum_b \left(\text{tr}(\hat{\rho}_0\hat{E}_b)\right)^{\alpha} \left(\text{tr}(\hat{\rho}_1\hat{E}_b)\right)^{1-\alpha}, \quad 0 < \alpha < 1$$  (3.5)

- the Quantum Kullback Information

$$K(\hat{\rho}_0/\hat{\rho}_1) \equiv \max_{\{\hat{E}_b\}} \sum_b \text{tr}(\hat{\rho}_0\hat{E}_b) \ln \left(\frac{\text{tr}(\hat{\rho}_0\hat{E}_b)}{\text{tr}(\hat{\rho}_1\hat{E}_b)}\right)$$  (3.6)

- the Accessible Information

$$I(\hat{\rho}_0|\hat{\rho}_1) \equiv \max_{\{\hat{E}_b\}} \sum_b \left(\pi_0\text{tr}(\hat{\rho}_0\hat{E}_b) \ln \left(\frac{\text{tr}(\hat{\rho}_0\hat{E}_b)}{\text{tr}(\hat{\rho}\hat{E}_b)}\right) + \pi_1\text{tr}(\hat{\rho}_1\hat{E}_b) \ln \left(\frac{\text{tr}(\hat{\rho}_1\hat{E}_b)}{\text{tr}(\hat{\rho}\hat{E}_b)}\right)\right)$$  (3.7)

where

$$\hat{\rho} = \pi_0\hat{\rho}_0 + \pi_1\hat{\rho}_1.$$  (3.8)

Notice again that the number of measurement outcomes in these definitions has not been fixed at the outset as must be the case in the classical expressions. The notation used here is meant to convey the following. The comma separating $\hat{\rho}_0$ and $\hat{\rho}_1$ in $F(\hat{\rho}_0, \hat{\rho}_1)$ is meant to convey that this function is symmetric upon their interchange. The slash in $F_\alpha(\hat{\rho}_0/\hat{\rho}_1)$ and $K(\hat{\rho}_0/\hat{\rho}_1)$ is signifies that these functions are explicitly asymmetric in the two density operators. The bar in $P_e(\hat{\rho}_0|\hat{\rho}_1)$ and $I(\hat{\rho}_0|\hat{\rho}_1)$ is used to emphasize that these may or may not be symmetric, depending upon the value of the prior probabilities $\pi_0$ and $\pi_1$.

The difficulty that crops up in extremizing quantities like these is that, so far at least, there seems to be no way to make the problem amenable to a variational approach: the problems associated with allowing $n$ to be arbitrary while enforcing the constraints on positivity and completeness for the
\( \hat{E}_b \) appear to be intractable. Moreover variational techniques generally only lead to the assurance of local extrema, perhaps never revealing the one that is globally best. New methods are required.

Fortunately, the error-probability and statistical overlap distinguishability measures appear to be “algebraic” enough that one could well imagine using standard operator inequalities, such as the Schwarz Inequality for operator inner products, to aid in finding explicit expressions for \( P_e(\hat{\rho}_0|\hat{\rho}_1) \) and \( F(\hat{\rho}_0, \hat{\rho}_1) \). That, in fact, is the case. The expression for \( F_o(\hat{\rho}_0/\hat{\rho}_1) \) appears less tractable, but one might still hope that something like a Hölder Inequality can be of use in this context. This remains an open question. On the other hand, when it comes to finding useful expressions for \( K(\hat{\rho}_0/\hat{\rho}_1) \) and \( I(\hat{\rho}_0|\hat{\rho}_1) \), for the same reason, one should be less optimistic. Progress toward explicit expressions for Eqs. (3.6) and (3.7) are necessarily impeded by the “transcendental” character of the logarithm appearing in their definitions. Generally only bounds for these quantities may be found.

This Chapter is devoted to fleshing out what is known about the quantum measures of distinguishability.

### 3.2 The Quantum Error Probability

#### 3.2.1 Single Sample Case

An interesting particular case of the general quantum decision problem \(^{[27]}\) is connected to the one introduced in Section 2.2. A given quantum mechanical system is secretly prepared either in the (pure or mixed) state \( \hat{\rho}_0 \) or in the state \( \hat{\rho}_1 \). These two possibilities are described by the prior probabilities \( \pi_0 \) and \( \pi_1 \) respectively. It is an observer’s task to perform any quantum measurement he pleases on this system and then to make the “best” possible guess as to the state’s true identity. The word “best” is in quotes because there are many things it can mean—for instance, it may depend upon the observer’s various personal costs for being right or wrong. Here we shall specialize the notion of “best” measurement and “best” guess to be those which, when combined, minimize the expected error probability of the decision. The question is this: what quantum measurement should the observer use so that his expected probability of error is indeed as small as it can possibly be? The answer to this gives rise to an explicit expression for the measure of distinguishability called the Quantum Error Probability:

\[
P_e(\hat{\rho}_0|\hat{\rho}_1) = \min_{\{\hat{E}_b\}} \sum_b \min\left\{ \pi_0 \text{tr}(\hat{\rho}_0 \hat{E}_b), \pi_1 \text{tr}(\hat{\rho}_1 \hat{E}_b) \right\}.
\]  

(3.9)

This problem can be much simplified by noticing the following. Any “measurement + guess” the observer can make can be summed up neatly as the measurement of a binary-valued POVM \( \{\hat{E}_0, \hat{E}_1\} \), i.e., two nonnegative definite operators \( \hat{E}_0 \) and \( \hat{E}_1 \) such that \( \hat{E}_0 + \hat{E}_1 = \hat{1} \). When outcome 0 occurs, the observer chooses the state \( \hat{\rho}_0 \); when outcome 1 occurs, he chooses state \( \hat{\rho}_1 \). Therefore the expected probability of error for a decision based on this measurement can be written as

\[
P_e = \pi_0 \text{tr}(\hat{\rho}_0 \hat{E}_1) + \pi_1 \text{tr}(\hat{\rho}_1 \hat{E}_0).
\]  

(3.10)

That is to say, the expected probability of error is just the probability that \( \hat{\rho}_0 \) is the true state times the conditional probability that the decision will be wrong when this is the case plus a similar term for \( \hat{\rho}_1 \). So, it must be the case that

\[
\min_{\{\hat{E}_b\}} \sum_b \min\left\{ \pi_0 \text{tr}(\hat{\rho}_0 \hat{E}_b), \pi_1 \text{tr}(\hat{\rho}_1 \hat{E}_b) \right\} = \min_{\{\hat{E}_0, \hat{E}_1\}} \left( \pi_0 \text{tr}(\hat{\rho}_0 \hat{E}_1) + \pi_1 \text{tr}(\hat{\rho}_1 \hat{E}_0) \right).
\]  

(3.11)

44
Helstrom’s minimal error-probability measurement is just the POVM \( \{ \hat{E}_0^0, \hat{E}_1^0 \} \) that minimizes Eq. (3.10). In Ref. [27], he showed that this POVM possesses the following explicit form. Both \( \hat{E}_0^0 \) and \( \hat{E}_1^0 \) are diagonal in a basis diagonalizing the Hermitian operator

\[
\hat{\Gamma} \equiv \pi_1 \hat{\rho}_1 - \pi_0 \hat{\rho}_0 .
\]

With respect to this basis, the diagonal elements \( \lambda_j^0 \) of \( \hat{E}_0^0 \) are assigned values according to the diagonal elements \( \gamma_j \) of \( \hat{\Gamma} \) via the rule:

\[
\begin{align*}
\lambda_j^0 &= 1 \quad \text{when} \quad \gamma_j < 0 , \\
\lambda_j^0 &= 0 \quad \text{when} \quad \gamma_j > 0 .
\end{align*}
\]

(3.13)

For \( j \) such that \( \gamma_j = 0 \), \( \lambda_j^0 \) may be assigned any value between 0 and 1; we take it to be 0 for definiteness. The operator \( \hat{E}_1^0 \) is formed simply by working out \( \hat{E}_1^0 = \hat{1} - \hat{E}_0^0 \).

One way the observer can implement this POVM is just to perform a standard von Neumann measurement of the Hermitian operator \( \hat{\Gamma} \) and bin the outcomes according to whether they correspond to positive, negative, or zero eigenvalues. If a positive eigenvalue results, outcome 1 of the POVM is said to be found and the observer makes a decision appropriately. If a negative eigenvalue results, outcome 0 of the POVM is said to be found. If a zero eigenvalue results, the posterior information is that either of the density operators is just as likely as the other. So in that case, any strategy for a decision will do.

In the remainder of this Section, we shall rederive the explicit form of Helstrom’s measurement in an elementary way that does not depend upon the variational techniques of Ref. [27]. This derivation is closely connected to the one appearing in Ref. [76].

Let \( \{ \hat{E}_0, \hat{E}_1 \} \) be an arbitrary binary-valued POVM. Using the fact that \( \hat{E}_0 + \hat{E}_1 = \hat{1} \), Eq. (3.10) becomes

\[
P_e = \pi_0 \text{tr}(\hat{\rho}_0 (\hat{1} - \hat{E}_0)) + \pi_1 \text{tr}(\hat{\rho}_1 \hat{E}_0)
= \pi_0 \text{tr}\hat{\rho}_0 - \pi_0 \text{tr}(\hat{\rho}_0 \hat{E}_0) + \pi_1 \text{tr}(\hat{\rho}_1 \hat{E}_0)
= \pi_0 + \text{tr}\left((\pi_1 \hat{\rho}_1 - \pi_0 \hat{\rho}_0) \hat{E}_0\right) .
\]

(3.15)

Therefore finding the minimum of \( P_e \) reduces to finding the minimum of \( \text{tr}(\hat{\Gamma} \hat{E}_0) \) over all operators \( \hat{E}_0 \) such that \( 0 \leq \hat{E}_0 \leq \hat{1} \).

To do this, suppose the operator \( \hat{\Gamma} \) has a spectral decomposition given by

\[
\hat{\Gamma} = \sum_j \gamma_j |j\rangle\langle j| .
\]

(3.16)

Then

\[
\text{tr}(\hat{\Gamma} \hat{E}_0) = \sum_j \gamma_j \langle j| \hat{E}_0 |j\rangle .
\]

(3.17)

Because \( \hat{\Gamma} \) is neither positive- nor negative-definite, this quantity is bounded below by the sum of its negative terms and, moreover,

\[
\text{tr}(\hat{\Gamma} \hat{E}_0) \geq \sum_j \gamma_j ^\prime ,
\]

(3.18)
where the prime on the summation sign signifies that the sum is restricted to those $j$ for which $\gamma_j \leq 0$. This follows because $0 \leq \langle j|\hat{E}_0|j\rangle \leq 1$ for all $j$. Note that the right hand side of Eq. (3.18) is independent of $\hat{E}_0$. Hence, if we can find any $\hat{E}_0$ that satisfies this inequality via a strict equality, that POVM element must be optimal.

To construct such an optimal $\hat{E}_0$, i.e., one that achieves this lower bound $\sum_j' \gamma_j$, we may start by specifying its diagonal elements in this basis:

$$
\langle j|\hat{E}_0|j\rangle = 1 \quad \text{when} \quad \gamma_j < 0
$$

$$
\langle j|\hat{E}_0|j\rangle = 0 \quad \text{when} \quad \gamma_j > 0 .
$$

(3.19)

For $j$ such that $\gamma_j = 0$, we may take $\langle j|\hat{E}_0|j\rangle$ to be any value between 0 and 1; again we take it to be 0 for definiteness.

Now, since no mention has yet been made of the off-diagonal elements, it might at first appear that there are many optimal measurements for this problem. That, however, is incorrect; for it turns out that any measurement operator $\hat{E}_0$ satisfying Eq. (3.19) must also be diagonal in this basis. To see this, suppose the operator $\hat{E}_0$ has the spectral decomposition

$$
\hat{E}_0 = \sum_k e_k |e_k\rangle\langle e_k| .
$$

(3.20)

Then, first consider a $j$ such that $\gamma_j \geq 0$. For that,

$$
0 = \langle j|\hat{E}_0|j\rangle = \sum_k e_k |\langle e_k|j\rangle|^2 .
$$

(3.21)

Hence, because $|\langle e_k|j\rangle|^2 \geq 0$ in general, it must be the case that $\langle e_k|j\rangle = 0$ whenever $e_k \neq 0$. So

$$
\langle k|\hat{E}_0|j\rangle = \sum_l e_l \langle k|e_l\rangle \langle e_l|j\rangle = 0 ,
$$

(3.22)

for any $k \neq j$ such that $\gamma_j \geq 0$ or $\gamma_k \geq 0$. To see that all other off-diagonal terms must vanish, one just need return to Eq. (3.13) and run through exactly the same argument as above to find that $\langle k|\hat{E}_1|j\rangle = 0$ for any $k \neq j$ such that $\gamma_j \leq 0$ or $\gamma_k \leq 0$. Then because $\hat{E}_0 + \hat{E}_1 = \hat{1}$, it follows that $\langle k|\hat{E}_1|j\rangle = 0$ for all $k \neq j$.

This completes the proof. The measurement operator $\hat{E}_0$ we have specified is unique up to the arbitrary choice of the diagonal elements for which $\gamma_j = 0$, though here we have chosen them to vanish for definiteness. It follows that $\hat{E}_1$ is also unique to the same extent, i.e., in the basis diagonalizing $\hat{\Gamma}$, its $(j,j)$ matrix element is 1 whenever $\gamma_j > 0$—all other matrix elements either vanish or are set by the condition $\hat{E}_0 + \hat{E}_1 = \hat{1}$.

Thus we have an explicit form for the quantum error probability:

$$
P_e(\hat{\rho}_0|\hat{\rho}_1) = \pi_0 + \sum_{\gamma_j \leq 0} \gamma_j ,
$$

(3.23)

where $\gamma_j$ are eigenvalues of the operator $\hat{\Gamma}$ defined in Eq. (3.12).

### 3.2.2 Many Sample Case

What happens to this criterion of distinguishability when there are $M > 1$ copies of the quantum state upon which measurements can be performed? There are at least two ways it loses its unique standing in this situation. The first is that one could imagine making a sophisticated measurement on all $M$ quantum systems at once, i.e. on the $N^M$-dimensional Hilbert space describing the
complete ensemble of quantum states. This measurement is very likely to be more useful than any set of measurements on the systems separately. In particular, the optimal error-probability measurement on the big Hilbert space is a Helstrom measurement operator \( \hat{\Gamma} \), except that the density operators of concern now are \( \hat{\Upsilon}_1 = \hat{\rho}_0 \otimes \cdots \otimes \hat{\rho}_0 \) and \( \hat{\Upsilon}_1 = \hat{\rho}_1 \otimes \hat{\rho}_1 \otimes \cdots \otimes \hat{\rho}_1 \), where each expression contains \( M \) terms and \( \otimes \) is the Kronecker product for matrices. 

Thus the optimal measurement on the big Hilbert space can be written explicitly as the Hermitian operator,

\[
\hat{\Gamma}_M = \pi_0 \left( \bigotimes_{k=1}^{M} \hat{\rho}_0 \right) - \pi_1 \left( \bigotimes_{k=1}^{M} \hat{\rho}_1 \right).
\]  

(3.24)

Clearly the distinguishability \( P_c(\hat{\rho}_0|\hat{\rho}_1) \) will be no simple function of \( P_c(\hat{\rho}_0|\hat{\rho}_1) \).

A second way for \( P_c(\hat{\rho}_0|\hat{\rho}_1) \) to lose its unique standing in the decision problem comes about even when all the measurements are restricted to the individual quantum systems. For instance, suppose that \( \hat{\rho}_0 \) and \( \hat{\rho}_1 \) are equally probable pure linear polarization states of a photon, one along the horizontal and the other 45° from the horizontal. The optimal error-probability measurement for the case \( M = 1 \) is given by the Helstrom operator \( \hat{\Gamma} \) just derived, i.e., the measurement of the yes/no question of whether the photon is polarized 67.50° from the horizontal. On the other hand, if \( M = 2 \), the expression that must be optimized over all (Hermitian operator) measurements is no longer Eq. (3.10), but rather

\[
P_c = \frac{1}{2} \min\{p_0(\uparrow)p_0(\uparrow), p_1(\uparrow)p_1(\uparrow)\} + \min\{p_0(\uparrow)p_0(\downarrow), p_1(\uparrow)p_1(\downarrow)\}
\]

\[
+ \frac{1}{2} \min\{p_0(\downarrow)p_0(\downarrow), p_1(\downarrow)p_1(\downarrow)\}.
\]  

(3.25)

This reflects the fact that this experiment has four possible outcomes: \( \uparrow\uparrow, \downarrow\downarrow, \uparrow\downarrow, \downarrow\uparrow \), with \( \uparrow \) and \( \downarrow \) denoting yes and no outcomes, respectively. The measurement that minimizes Eq. (3.25) can be found easily by numerical means; it turns out to be a polarization measurement 54.54° from the horizontal. In similar fashion, if \( M = 3 \), the optimal measurement is along the axis 49.94° from the horizontal. See Fig. 3.1. The lesson to be learned from this is that the optimal error-probability measurement is expressly dependent upon the number of repetitions \( M \) expected. This phenomenon has already been encountered in the classical example of Chapter 2. If \( M \) is to be left undetermined, then something beside the minimal error probability itself is required for an adequate measure of statistical distinguishability within the context of the decision problem.

### 3.3 The Quantum Fidelity

The solution of Section 2.2.2 to remedy this predicament was to shift focus to the optimal exponential decrease in error probability in the number of samples \( M \). Translated into the quantum context, that would mean we should use the Quantum Chernoff Bound

\[
C(\hat{\rho}_0, \hat{\rho}_1) \equiv \min_{0 \leq \alpha \leq 1} \min_{\{E_b\}} \sum_b \left( \text{tr}(\hat{\rho}_0 \hat{E}_b) \right)^{\alpha} \left( \text{tr}(\hat{\rho}_1 \hat{E}_b) \right)^{1-\alpha}
\]  

(3.26)

as the appropriate measure of distinguishability. Instead, in this Section we shall focus on optimizing a particular upper bound to this measure of distinguishability, the statistical overlap introduced in Section 2.2.2.

The “quantized” version of the statistical overlap is called the **quantum fidelity** and is defined by

\[
F(\hat{\rho}_0, \hat{\rho}_1) = \min_{\{E_b\}} \sum_b \sqrt{\text{tr}\hat{\rho}_0 \hat{E}_b} \sqrt{\text{tr}\hat{\rho}_1 \hat{E}_b}
\]  

(3.27)
Figure 3.1: Probability of error in guessing a photon’s polarization that is either horizontal or 45° from the horizontal. Error probability is plotted here as a function of measurement (i.e., radians from the horizontal) and number of measurement repetitions $M$ before the guess is made.
We shall show in this Section that
\[ F(\hat{\rho}_0, \hat{\rho}_1) = \text{tr} \sqrt{\hat{\rho}_1^{1/2} \hat{\rho}_0 \hat{\rho}_1^{1/2}}, \] (3.28)
where for any nonnegative operator \( \hat{A} \) we mean by \( \hat{A}^{1/2} \) (or \( \sqrt{\hat{A}} \)) the unique nonnegative operator such that \( \hat{A}^{1/2} \hat{A}^{1/2} = \hat{A} \).

The quantity on the right hand side of Eq. (3.28) has appeared before as the distance function
\[ d_B^2(\hat{\rho}_0, \hat{\rho}_1) = 2 - 2F(\hat{\rho}_0, \hat{\rho}_1) \] (3.29)
of Bures [80, 81], the generalized transition probability for mixed states
\[ \text{prob}(\hat{\rho}_0 \rightarrow \hat{\rho}_1) = (F(\hat{\rho}_0, \hat{\rho}_1))^2 \] (3.30)
of Uhlmann [7], and—in the same form as Uhlmann’s—Jozsa’s criterion [9] for “fidelity” of signals in a quantum communication channel. Note that Jozsa’s “fidelity” [9] is actually the square of the quantity called fidelity here. The fidelity was found to be of use within that context because it is symmetric in 0 and 1, because it is invariant under unitary operations, i.e.,
\[ F(\hat{U} \hat{\rho}_0 \hat{U}^\dagger, \hat{U} \hat{\rho}_1 \hat{U}^\dagger) = F(\hat{\rho}_0, \hat{\rho}_1), \] (3.31)
for any unitary operator \( \hat{U} \), because
\[ 0 \leq F(\hat{\rho}_0, \hat{\rho}_1) \leq 1 \] (3.32)
reaching 1 if and only if \( \hat{\rho}_0 = \hat{\rho}_1 \), and because
\[ (F(\hat{\rho}_0, \hat{\rho}_1))^2 = \langle \psi_1 | \hat{\rho}_0 | \psi_1 \rangle \] (3.33)
when \( \hat{\rho}_1 = |\psi_1\rangle \langle \psi_1| \) is a pure state.

The notion defined by Eq. (3.30) is particularly significant because of the auxiliary interpretation it gives the quantity in Eq. (3.28). Imagine another system B, described by an \( D \)-dimensional Hilbert space, attached to our given system. There are many pure states \( |\psi_0\rangle \) and \( |\psi_1\rangle \) on the composite system such that
\[ \text{tr}_B(|\psi_0\rangle \langle \psi_0|) = \hat{\rho}_0 \quad \text{and} \quad \text{tr}_B(|\psi_1\rangle \langle \psi_1|) = \hat{\rho}_1, \] (3.34)
where \( \text{tr}_B \) denotes a partial trace over System B’s Hilbert space. Such pure states are called “purifications” of the density operators \( \hat{\rho}_0 \) and \( \hat{\rho}_1 \). For these, the following theorem can be shown [7, 9].

**Theorem 3.1 (Uhlmann)** For all purifications \( |\psi_0\rangle \) and \( |\psi_1\rangle \) of \( \hat{\rho}_0 \) and \( \hat{\rho}_1 \), respectively,
\[ |\langle \psi_0 | \psi_1 \rangle| \leq \text{tr} \sqrt{\hat{\rho}_1^{1/2} \hat{\rho}_0 \hat{\rho}_1^{1/2}}. \] (3.35)
Moreover, equality is achievable in this expression by an appropriate choice of purifications.

That is to say, of all purifications of \( \hat{\rho}_0 \) and \( \hat{\rho}_1 \), the ones with the maximal modulus for their inner product have it actually equal to the quantum fidelity as defined here.

We should note that, in a roundabout way through the mathematical-physics literature (cf., for instance, in logical order [8], [82], [83], and [7]), one can put together a result quite similar in spirit to Eq. (3.28)—that is, a maximization like (3.4) but, instead of over all POVMs, restricted to orthogonal projection-valued measures. What is novel here is the explicit statistical interpretation, the simplicity and generality of the derivation, and the fact that it pinpoints the measurement by which Eq. (3.28) is attained.
3.3.1 The General Derivation

Before getting started, let us note that if \( \hat{\rho}_0 = |\psi_0\rangle\langle\psi_0| \) and \( \hat{\rho}_1 = |\psi_1\rangle\langle\psi_1| \) are pure states, the expression in Eq. (3.28) reduces to

\[
F(\hat{\rho}_0, \hat{\rho}_1) = \text{tr}(\sqrt{\langle\psi_1|\psi_1\rangle \hat{\rho}_1 \langle\psi_0|\psi_0\rangle \hat{\rho}_0}) = |\langle\psi_0|\psi_1\rangle| \sqrt{\text{tr}(\hat{\rho}_1)}.
\]

This already agrees with the expression derived by Wootters [85, 45, 8] for the optimal statistical overlap between pure states. Moreover, it indicates that Eq. (3.28) has a chance of being a general solution to Eq. (3.27).

The method we use for deriving Eq. (3.28) is to apply the Schwarz inequality to the statistical overlap in such a way that its specific conditions for equality can be met by a suitable measurement. First, however, it is instructive to consider a quick and dirty—and for this problem inappropriate—application of the Schwarz inequality; the difficulties encountered therein point naturally toward the correct proof. The Schwarz inequality for the operator inner product \( \text{tr}(\hat{A}^\dagger \hat{B}) \) is given by

\[
|\text{tr}(\hat{A}^\dagger \hat{B})|^2 \leq \text{tr}(\hat{A}^\dagger \hat{A}) \text{tr}(\hat{B}^\dagger \hat{B}),
\]

where equality is achieved if and only if \( \hat{B} = \mu \hat{A} \) for some constant \( \mu \).

Let \( \{\hat{E}_b\} \) be an arbitrary POVM and

\[
p_0(b) = \text{tr}(\hat{\rho}_0 \hat{E}_b) \quad \text{and} \quad p_1(b) = \text{tr}(\hat{\rho}_1 \hat{E}_b).
\]

By the cyclic property of the trace and this inequality, we must have for any \( b \),

\[
\sqrt{p_0(b)} \sqrt{p_1(b)} = \sqrt{\text{tr}(\hat{E}_b^{1/2} \hat{\rho}_0^{1/2})} \sqrt{\text{tr}(\hat{E}_b^{1/2} \hat{\rho}_1^{1/2})} \geq \left| \text{tr}(\hat{E}_b^{1/2} \hat{\rho}_0^{1/2}) \right| \left| \text{tr}(\hat{E}_b^{1/2} \hat{\rho}_1^{1/2}) \right|.
\]

The condition for attaining equality here is that

\[
\hat{E}_b^{1/2} \hat{\rho}_0^{1/2} = \mu_b \hat{E}_b^{1/2} \hat{\rho}_1^{1/2}.
\]

A subscript \( b \) has been placed on the constant \( \mu \) as a reminder of its dependence on the particular \( \hat{E}_b \) in this equation. From inequality (3.39), it follows by the linearity of the trace and the completeness property of POVMs that

\[
\sum_b \sqrt{p_0(b)} \sqrt{p_1(b)} \geq \sum_b \left| \text{tr}(\hat{E}_b^{1/2} \hat{\rho}_0^{1/2}) \right| \geq \left| \sum_b \text{tr}(\hat{E}_b^{1/2} \hat{\rho}_0^{1/2}) \right| \geq \left| \text{tr}(\hat{E}_b^{1/2} \hat{\rho}_0^{1/2}) \right|.
\]

50
The quantity \[ F_A(\hat{\rho}_0, \hat{\rho}_1) = \text{tr}\left(\hat{\rho}_0^{1/2} \hat{\rho}_1^{-1/2}\right) \] (3.43)
is thus a lower bound to \( F(\rho_0, \rho_1) \). For it actually to be the minimum, there must be a POVM such that, for all \( b \), Eq. (3.44) is satisfied and
\[
\text{tr}\left(\hat{\rho}_0^{1/2} \hat{E}_b \hat{\rho}_1^{1/2}\right) = \left|\text{tr}\left(\hat{\rho}_0^{1/2} \hat{E}_b \hat{\rho}_1^{1/2}\right)\right| e^{i\phi},
\] (3.44)
where \( \phi \) is an arbitrary phase independent of \( b \), so that the sum can be taken past the absolute values sign in Eq. (3.41) without effect.

These conditions, however, cannot be fulfilled by any POVM \( \{\hat{E}_b\} \) when \( \hat{\rho}_0 \) and \( \hat{\rho}_1 \) do not commute. This can be seen as follows. Suppose \( [\hat{\rho}_0, \hat{\rho}_1] \neq 0 \) and, for simplicity, let us suppose that \( \hat{\rho}_0 \) can be inverted. Then condition (3.44) can be written equivalently as
\[
\hat{E}_b^{1/2} \left(\mu_b \hat{1} - \hat{\rho}_1^{1/2} \hat{\rho}_0^{-1/2}\right) |\phi_q\rangle = 0.
\] (3.45)
The only way this can be satisfied is if we take the \( \hat{E}_b \) to be proportional to the projectors formed from the left-eigenvectors of \( \hat{\rho}_1^{1/2} \hat{\rho}_0^{-1/2} \) and let the \( \mu_b \) be the corresponding eigenvalues. This is seen easily.

The operator \( \hat{\rho}_1^{1/2} \hat{\rho}_0^{-1/2} \) is non-Hermitian by assumption. Thus, though it has \( D \) linearly independent left- and right-eigenvectors, they cannot be orthogonal. Let us denote the left-eigenvectors by \( \langle \psi_r \rangle \) and their corresponding eigenvalues by \( \sigma_r \); let us denote the right-eigenvectors and eigenvalues by \( |\phi_q\rangle \) and \( \lambda_q \). Then if Eq. (3.45) is to hold, we must have
\[
\hat{E}_b^{1/2} \left(\mu_b \hat{1} - \hat{\rho}_1^{1/2} \hat{\rho}_0^{-1/2}\right) |\phi_q\rangle = 0.
\] (3.46)
It follows that
\[
(\mu_b - \lambda_q) \hat{E}_b^{1/2} |\phi_q\rangle = 0
\] (3.47)
for all \( q \) and \( b \). Now assume—again for simplicity—that all the \( \lambda_q \) are distinct. If \( \hat{E}_b \) is not identically zero, then we must have that (modulo relabeling)
\[
\hat{E}_b^{1/2} |\phi_q\rangle = 0 \text{ for all } q \neq b \quad \text{and} \quad \mu_b = \lambda_q \text{ for } q = b.
\] (3.48)
This means that \( \hat{E}_b^{1/2} \) is proportional to the projector onto the one-dimensional subspace that is orthogonal to all the \( |\phi_q\rangle \) with \( q \neq b \). But since
\[
0 = \langle \psi_r | \hat{\rho}_1^{1/2} \hat{\rho}_0^{-1/2} |\phi_q\rangle - \langle \psi_r | \hat{\rho}_1^{1/2} \hat{\rho}_0^{-1/2} |\phi_q\rangle = (\sigma_r - \lambda_q) \langle \psi_r | \phi_q\rangle,
\] (3.49)
we have that (again modulo relabeling) \( |\psi_r\rangle \) is orthogonal to \( |\phi_q\rangle \) for \( q \neq r \) and \( \sigma_r = \lambda_q \) for \( q = r \). Therefore
\[
\hat{E}_b^{1/2} \propto |\psi_b\rangle \langle \psi_b|.
\] (3.50)
The reason Eq. (3.42) cannot be satisfied by any POVM is now apparent; it is just that the \( |\psi_b\rangle \) are nonorthogonal. When the \( |\psi_b\rangle \) are nonorthogonal, there are \( n \) positive constants \( \alpha_b (b = 1, \ldots, n) \) such that
\[
\sum_{b=1}^n |\psi_b\rangle \langle \psi_b| = \hat{1}.
\] (3.51)
For if there were, then the completeness relation would give rise to the equation

\[ \sum_{b=1}^{n} \alpha_b \langle \psi_b | \psi_c \rangle | \psi_b \rangle = | \psi_c \rangle \] (3.52)

so that

\[ \sum_{b \neq c} \alpha_b \langle \psi_b | \psi_c \rangle | \psi_b \rangle = (1 - \alpha_c) | \psi_c \rangle \] (3.53)

contradicting the fact that the \( | \psi_b \rangle \) are linearly independent but nonorthogonal. If \( \hat{\rho}_0 \) and \( \hat{\rho}_1 \) were commuting operators so that \( \hat{\rho}_1^{1/2} \hat{\rho}_0^{-1/2} \) were Hermitian, there would be no problem; for then all the eigenvectors would be mutually orthogonal. A complete set of orthonormal projectors necessarily sum to the identity operator.

The lesson from this example is that the naïve Schwarz inequality is not enough to prove Eq. (3.28): one must be careful to “build in” a way to attain equality by at least one POVM. Plainly the way to do this is to take advantage of the invariances of the trace operation. In particular, in the set of inequalities (3.39), we could just as well have written

\[ p_0(b) = \text{tr}(\hat{\rho}_0 \hat{E}_b) = \text{tr}(\hat{U} \hat{\rho}_0^{1/2} \hat{E}_b \hat{\rho}_0^{-1/2} \hat{U}^\dagger) \] (3.54)

for any unitary operator \( \hat{U} \) since \( \hat{U}^\dagger \hat{U} = \hat{1} \). Then, in exact analogy to the previous derivation, it follows that

\[
\sqrt{p_0(b)} \sqrt{p_1(b)} = \sqrt{\text{tr}\left( \left( \hat{E}_b^{1/2} \hat{\rho}_0^{1/2} \hat{U}^\dagger \right) \left( \hat{E}_b^{1/2} \hat{\rho}_0^{-1/2} \hat{U}^\dagger \right) \right)} \geq \left| \text{tr}\left( \left( \hat{E}_b^{1/2} \hat{\rho}_0^{1/2} \hat{U}^\dagger \right) \left( \hat{E}_b^{1/2} \hat{\rho}_0^{-1/2} \hat{U}^\dagger \right) \right) \right|
\]

\[ = \left| \text{tr}(\hat{U} \hat{\rho}_0^{1/2} \hat{E}_b \hat{\rho}_0^{-1/2}) \right|, \] (3.55)

where the condition for equality is now

\[ \hat{E}_b^{1/2} \hat{\rho}_0^{1/2} = \mu_b \hat{E}_b^{1/2} \hat{\rho}_0^{1/2} \hat{U}^\dagger. \] (3.56)

This equation, it turns out, can be satisfied by an appropriate choice for the unitary operator \( \hat{U} \).

To see this, let us first suppose that \( \hat{\rho}_0 \) and \( \hat{\rho}_1 \) are invertible. Then Eq. (3.56) is equivalent to

\[ \hat{E}_b^{1/2} \left( \hat{1} - \mu_b \hat{\rho}_0^{1/2} \hat{U}^\dagger \hat{\rho}_0^{-1/2} \right) = 0. \] (3.57)

Summing Eq. (3.53) on \( b \), we get

\[ \sum_b \sqrt{p_0(b)} \sqrt{p_1(b)} \geq \left| \text{tr}(\hat{U} \hat{\rho}_0^{1/2} \hat{\rho}_0^{-1/2}) \right| \] (3.58)

The final conditions for equality in this is that the \( \hat{E}_b \) satisfy both Eq. (3.57) and the requirement

\[ \text{tr}(\hat{U} \hat{\rho}_0^{1/2} \hat{E}_b \hat{\rho}_0^{1/2}) = \left| \text{tr}(\hat{U} \hat{\rho}_0^{1/2} \hat{E}_b \hat{\rho}_0^{1/2}) \right| e^{i\phi} \] (3.59)

for all \( b \), where again \( \phi \) is an arbitrary phase.
As in the last example, there can be no POVM \( \{ \hat{E}_b \} \) that satisfies condition (3.57) unless the operator \( \rho_0^{1/2} \hat{U} \rho_1^{-1/2} \) is Hermitian. An easy way to find a unitary \( \hat{U} \) that makes a solution to Eq. (3.57) possible is to note a completely different point about inequality (3.58). The unitary operator \( \hat{U} \) there is arbitrary; if there is to be a chance of attaining equality in (3.58), \( \hat{U} \) had better be chosen so as to maximize \( |\text{tr}(\hat{U} \rho_0^{1/2} \rho_1^{-1/2})| \). It turns out that that particular \( \hat{U} \) forces \( \rho_0^{1/2} \hat{U} \rho_1^{-1/2} \) to be Hermitian.

To demonstrate the last point, we need a result from the mathematical literature [9, 87, 75]: for any operator \( \hat{A} \),

\[
\max_{\hat{U}} |\text{tr}(\hat{U} \hat{A})| = \max_{\hat{U}} \text{Re}\left[\text{tr}(\hat{U} \hat{A})\right] = \text{tr}\sqrt{\hat{A}^\dagger \hat{A}}, \tag{3.60}
\]

where the maximum is taken over all unitary operators \( \hat{U} \). The set of operators \( \hat{U} \) that gives rise to the maximum must satisfy

\[
\hat{U} \hat{A} = \sqrt{\hat{A}^\dagger \hat{A}}. \tag{3.61}
\]

At least one such unitary operator is assured to exist by the so-called polar decomposition theorem. When \( \hat{A} \) is invertible, it is easy to see that

\[
\hat{U} = \sqrt{\hat{A}^\dagger \hat{A} \hat{A}^{-1}} \tag{3.62}
\]

has the desired properties and is unique. When \( \hat{A} \) is not invertible, \( \hat{U} \) is no longer unique, but can still be shown to exist [79, pp. 74–75].

So a unitary operator \( \hat{U}_c \) that gives rise to the tightest inequality in Eq. (3.58) can be taken to satisfy

\[
\hat{U}_c \rho_0^{1/2} \rho_1^{-1/2} = \sqrt{\left(\rho_0^{1/2} \rho_1^{-1/2}\right)^\dagger \left(\rho_0^{1/2} \rho_1^{-1/2}\right)} = \sqrt{\rho_1^{-1/2} \rho_0 \rho_0 \rho_1^{-1/2}} \tag{3.63}
\]

When \( \hat{\rho}_0 \) and \( \hat{\rho}_1 \) are both invertible, this equation is uniquely satisfied by

\[
\hat{U}_c \equiv \sqrt{\rho_1^{1/2} \hat{\rho}_0 \rho_1^{1/2} \rho_0^{-1/2} \rho_1^{-1/2}}. \tag{3.64}
\]

With this, Eq. (3.58) clearly takes the form needed to prove Eq. (3.27):

\[
\sum_b \sqrt{p_0(b) p_1(b)} \geq |\text{tr}(\hat{U}_c \rho_0^{1/2} \rho_1^{-1/2})| = \text{tr} \sqrt{\rho_1^{1/2} \hat{\rho}_0 \rho_1^{-1/2}}. \tag{3.65}
\]

Inserting this choice for \( \hat{U} \) into Eq. (3.57) gives the condition

\[
\hat{E}_b^{1/2} \left( \mathbb{1} - \mu_b \hat{M} \right) = 0, \tag{3.66}
\]

where the operator

\[
\hat{M} \equiv \rho_0^{1/2} \hat{U}_c \rho_0^{-1/2} = \rho_1^{-1/2} \sqrt{\rho_1 \rho_0 \rho_1^{1/2} \rho_0^{-1/2}} \tag{3.67}
\]
is indeed Hermitian and also nonnegative (as can be seen immediately from its symmetry). Thus there is a POVM \( \{ E^B_b \} \) that satisfies Eq. (3.57) for each \( b \): the \( E^B_b \) can be taken be projectors onto a basis \( |b\rangle \) that diagonalizes \( \hat{M} \). Here the \( \mu_b \) must be taken to be reciprocals of \( \hat{M} \)'s eigenvalues.

With the POVM \( \{ E^B_b \} \), Eq. (3.59) is automatically satisfied. Since the eigenvalues \( 1/\mu_b \) of \( \hat{M} \) are all nonnegative, one finds that

\[
\text{tr} \left( \hat{U}_c \hat{\rho}_0^{1/2} \hat{E}^B_b \hat{\rho}_1^{1/2} \right) = \text{tr} \left( \hat{\rho}_1 \hat{M} \hat{E}^B_b \right) = \frac{1}{\mu_b} \text{tr} \left( \hat{\rho}_1 \hat{E}^B_b \right) \geq 0 .
\]

This concludes the proof of Eq. (3.28) under the restriction that \( \hat{\rho}_0 \) and \( \hat{\rho}_1 \) be invertible.

When \( \hat{\rho}_0 \) and/or \( \hat{\rho}_1 \) are \emph{not} invertible, things are only slightly more difficult. Suppose \( \hat{\rho}_1 \) is not invertible; then there exists a projector \( \hat{\Pi}_{\text{null}} \) onto the null subspace of \( \hat{\rho}_1 \), i.e., \( \hat{\Pi}_{\text{null}} \) is a projector of maximal rank such that

\[
\hat{\Pi}_{\text{null}} \hat{\rho}_1 = 0 \quad \text{and} \quad \hat{\rho}_1 \hat{\Pi}_{\text{null}} = 0 .
\]

The projector onto the support of \( \hat{\rho}_1 \), i.e., the orthogonal complement to the null subspace, is defined by

\[
\hat{\Pi}_{\text{supp}} = \hat{1} - \hat{\Pi}_{\text{null}} .
\]

Clearly \( \hat{E}_{\text{null}} = \hat{\Pi}_{\text{null}} \) satisfies Eq. (3.56) if the associated constant \( \mu_{\text{null}} \) is chosen to be zero. Now let us construct a set of orthogonal projectors \( \hat{E}_b = |b\rangle \langle b| \) that span the support of \( \hat{\rho}_1 \) and satisfy Eqs. (3.56) and (3.59) with (3.63). This is done easily enough. Suppose the support of \( \hat{\rho}_1 \) is an \( m \)-dimensional subspace; the operator

\[
\hat{R}_1 = \hat{\Pi}_{\text{supp}} \hat{\rho}_1 \hat{\Pi}_{\text{supp}}
\]

is invertible on that subspace. Now consider any set of \( m \) orthogonal one-dimensional projectors \( \hat{\Pi}_b \) in the support of \( \hat{\rho}_1 \). If they are to satisfy Eq. (3.56), then they must also satisfy the equations created by sandwiching Eqs. (3.56) and (3.63) by the projector \( \hat{\Pi}_{\text{supp}} \):

\[
\hat{\Pi}_b \hat{R}_1^{1/2} = \mu_b \hat{\Pi}_b \left( \hat{\Pi}_{\text{supp}} \hat{\rho}_0^{1/2} \hat{U}_c \hat{\Pi}_{\text{supp}} \right) ,
\]

and

\[
\left( \hat{\Pi}_{\text{supp}} \hat{U}_c \hat{\rho}_0^{1/2} \hat{\Pi}_{\text{supp}} \right) \hat{R}_1^{1/2} = \hat{\Pi}_{\text{supp}} \sqrt{\rho_1^{1/2} \hat{\rho}_0 \rho_1^{1/2}} \hat{\Pi}_{\text{supp}} .
\]

Therefore, the \( \hat{\Pi}_b \) must satisfy

\[
h_{\Pi} = \frac{1}{\mu_b} \hat{\Pi}_b .
\]

Hereafter we may run through the same steps as in the invertible case. Because the operator on the left-hand side of Eq. (3.74) is a positive operator, there are indeed \( m \) orthogonal projectors on the support of \( \hat{\rho}_1 \) that satisfy the conditions for optimizing the statistical overlap. Taking the \( \hat{E}_b = \hat{\Pi}_b \) completes the proof.

A particular case of noninvertibility is when \( \hat{\rho}_0 = |\psi_0\rangle \langle \psi_0| \) and \( \hat{\rho}_1 = |\psi_1\rangle \langle \psi_1| \) are nonorthogonal pure states. Then Eq. (3.63) becomes

\[
\hat{U}_c |\psi_0\rangle \langle \psi_1| \langle \psi_1| = \sqrt{|\psi_1\rangle \langle \psi_1| |\psi_0\rangle \langle \psi_0| |\psi_1\rangle \langle \psi_1|} = |\langle \psi_0| \langle \psi_1| \langle \psi_1|.
\]

(3.75)
and Eq. (3.56) becomes
\[ |b\rangle\langle b|\psi_1\rangle = \mu_b |b\rangle\langle b|\psi_0\rangle \hat{U}_c^\dagger. \] (3.76)

If we redefine the phases of $|\psi_0\rangle$ and $|\psi_1\rangle$ so that $\langle \psi_0|\psi_1\rangle$ is positive, we have that
\[ \hat{U}_c|\psi_0\rangle = |\psi_1\rangle. \] (3.77)

Therefore, Eq. (3.76) implies
\[ \langle b|\psi_1\rangle = \mu_b \langle b|\psi_0\rangle. \] (3.78)

This equation specifies that any orthonormal basis $|b\rangle$ containing vectors $|0\rangle$ and $|1\rangle$ lying in the plane spanned by the vectors $|\psi_0\rangle$ and $|\psi_1\rangle$ and straddling them will form an optimal measurement basis. This follows because in this case all inner products $\langle b|\psi_1\rangle$ and $\langle b|\psi_0\rangle$ will be nonnegative; thus Eq. (3.78) has a solution with nonnegative $\mu_b$. This supplements the set of optimal measurements found in Ref. [3] and is easily confirmed to be true as follows. Let $\theta$ be the angle between $|\psi_0\rangle$ and $|\psi_1\rangle$ and let $\phi$ be the angle between $|0\rangle$ and $|\psi_0\rangle$. Then for this measurement,
\[
F(p_0, p_1) = \sqrt{\cos^2 \phi \cos^2 (\phi + \theta) + \cos^2(\phi - \frac{\pi}{4}) \cos^2(\phi + \theta - \frac{\pi}{2})} \\
= \cos \phi \cos(\phi + \theta) + \sin \phi \sin(\phi + \theta) \\
= \cos \theta,
\] (3.79)

which is completely independent of $\phi$. This verifies the result.

Equation (3.76) raises the interesting question of, more generally, what is the action of $\hat{U}_c$? Could it be that $\hat{U}_c$ always takes a basis diagonalizing $\hat{\rho}_0$ to a basis diagonalizing $\hat{\rho}_1$? This appears not to be the case, unfortunately. The question of a more geometric interpretation of $\hat{U}_c$ is an open one.

3.3.2 Properties

In this Subsection, we report a few interesting points about the measurement specified by $\hat{M}$ and the quantum distinguishability measure $F(\hat{\rho}_0, \hat{\rho}_1)$. The equation defining the statistical overlap is clearly invariant under interchanges of the labels 0 and 1. Therefore it must follow that
\[ F(\hat{\rho}_0, \hat{\rho}_1) = F(\hat{\rho}_1, \hat{\rho}_0). \] (3.80)

A neat way to see this directly is to note that the operators \( \hat{\rho}_0^{1/2} \hat{\rho}_1^{1/2} \) and \( \hat{\rho}_0^{1/2} \hat{\rho}_1^{1/2} \) have the same eigenvalue spectrum. For if $|b\rangle$ and $\lambda_b$ are an eigenvector and eigenvalue of $\hat{\rho}_0^{1/2} \hat{\rho}_1^{1/2}$, it follows that
\[
\lambda_b \left( \hat{\rho}_0^{1/2} \hat{\rho}_1^{1/2} |b\rangle \right) = \hat{\rho}_0^{1/2} \hat{\rho}_1^{1/2} \lambda_b |b\rangle \\
= \hat{\rho}_0^{1/2} \hat{\rho}_1^{1/2} \left( \hat{\rho}_0^{1/2} \hat{\rho}_1^{1/2} |b\rangle \right) \\
= \left( \hat{\rho}_0^{1/2} \hat{\rho}_1^{1/2} \right) \left( \hat{\rho}_0^{1/2} \hat{\rho}_1^{1/2} |b\rangle \right).
\] (3.81)

Hence,
\[
\text{tr} \sqrt{\hat{\rho}_0^{1/2} \hat{\rho}_1^{1/2}} = \sum_b \sqrt{\lambda_b} = \text{tr} \sqrt{\hat{\rho}_0^{1/2} \hat{\rho}_1^{1/2}},
\] (3.82)

and so $F(\hat{\rho}_0, \hat{\rho}_1) = F(\hat{\rho}_1, \hat{\rho}_0)$.  

55
By the same token, the derivation of Eq. (3.28) itself must remain valid if all the 0’s and 1’s in it are interchanged throughout. When $\hat{\rho}_0$ and $\hat{\rho}_1$ are invertible, however, this gives rise to a measurement specified by a basis diagonalizing

$$\hat{N} = \hat{\rho}_0^{-1/2} \sqrt{\rho_1 \rho_0^{-1/2}} \hat{\rho}_1^{-1/2} \hat{\rho}_0^{-1/2}.$$  \hfill (3.83)

It turns out that $\hat{M}$ and $\hat{N}$ can define the same measurement because not only do they commute, they are inverses of each other. This can be seen as follows. Let $\hat{A}$ be any operator and $\hat{V}$ be a unitary operator such that

$$\sqrt{\hat{A}^\dagger \hat{A}} = \hat{V}^\dagger \hat{A}.$$  \hfill (3.84)

Hence $\hat{A} = \hat{V} \sqrt{\hat{A}^\dagger \hat{A}}$ and also $\hat{A}^\dagger = \sqrt{\hat{A}^\dagger \hat{A}} \hat{V}^\dagger$. So

$$\left( \hat{V} \sqrt{\hat{A}^\dagger \hat{A}} \hat{V}^\dagger \right)^2 = \left( \hat{V} \sqrt{\hat{A}^\dagger \hat{A}} \right) \left( \sqrt{\hat{A}^\dagger \hat{A}} \hat{V}^\dagger \right) = \hat{A} \hat{A}^\dagger,$$  \hfill (3.85)

and therefore, because $\hat{V} \sqrt{\hat{A}^\dagger \hat{A}} \hat{V}^\dagger$ is a nonnegative operator,

$$\sqrt{\hat{A} \hat{A}^\dagger} = \hat{V} \sqrt{\hat{A}^\dagger \hat{A}} \hat{V}^\dagger = \hat{V} \hat{A}^\dagger.$$  \hfill (3.86)

In particular, if

$$\sqrt{\hat{\rho}_1 \rho_0^{-1/2} \hat{\rho}_0^{-1/2}} = \hat{U}_c \hat{\rho}_0^{-1/2} \hat{\rho}_1^{-1/2},$$  \hfill (3.87)

then

$$\sqrt{\hat{\rho}_0^{-1/2} \hat{\rho}_1 \hat{\rho}_0^{-1/2}} = \hat{U}_c^\dagger \hat{\rho}_1 \hat{\rho}_0^{-1/2}.$$  \hfill (3.88)

Therefore, the desired property follows at once,

$$\hat{M} \hat{N} = \hat{\rho}_1^{-1/2} \left( \hat{U}_c \hat{\rho}_0^{1/2} \hat{\rho}_1^{-1/2} \right) \hat{\rho}_1^{-1/2} \rho_0^{-1/2} \left( \hat{U}_c^\dagger \hat{\rho}_1 \hat{\rho}_0^{-1/2} \right) \hat{\rho}_0^{-1/2}$$

$$= \hat{\rho}_1^{-1/2} \hat{U}_c \hat{U}_c^\dagger \hat{\rho}_1^{-1/2}$$

$$= \mathbb{1}.$$  \hfill (3.89)

We may also note an interesting expression for $\hat{M}$’s eigenvalues that arises from the last result. Let the eigenvalues and eigenvectors of $\hat{M}$ be denoted by $m_b$ and $|b\rangle$; in this notation $\hat{E}_b^B = |b\rangle \langle b|$. Then we can write two expressions for $m_b$:

$$m_b \langle b| \hat{\rho}_1 |b\rangle = \langle b| \hat{\rho}_1 \hat{M} |b\rangle$$

$$= \langle b| \hat{\rho}_1^{1/2} \hat{U}_c \hat{\rho}_0^{-1/2} |b\rangle,$$  \hfill (3.90)

and

$$\frac{1}{m_b} \langle b| \hat{\rho}_0 |b\rangle = \langle b| \hat{\rho}_0 \hat{N} |b\rangle$$

$$= \langle b| \hat{\rho}_0^{1/2} \hat{U}_c^\dagger \hat{\rho}_1^{1/2} |b\rangle$$

$$= \left( \langle b| \hat{\rho}_0^{1/2} \hat{U}_c \hat{\rho}_0^{-1/2} |b\rangle \right)^*.$$  \hfill (3.91)
Because the left hand sides of these equations are real numbers, so are the right hand sides; in particular, combining Eqs. (3.90) and (3.91), we get

\[ m_b = \left( \frac{(b|\hat{\rho}_b|b)}{(b|\hat{\rho}_1|b)} \right)^{1/2} = \left( \frac{\text{tr}\hat{\rho}_0 \hat{E}_b}{\text{tr}\hat{\rho}_1 \hat{E}_b} \right)^{1/2}. \] (3.92)

The optimal measurement operator \( \hat{M} \) can be considered a sort of operator analog to the classical likelihood ratio, for its squared eigenvalues are the ratio of two probabilities. This fact gives rise to an interesting expression for the Kullback-Leibler relative information between \( \hat{\rho}_0 \) and \( \hat{\rho}_1 \) with respect to this measurement:

\[ K_B(\hat{\rho}_0/\hat{\rho}_1) = \sum_b (\text{tr}\hat{\rho}_0 \hat{E}_b) \ln \left( \frac{\text{tr}\hat{\rho}_0 \hat{E}_b}{\text{tr}\hat{\rho}_1 \hat{E}_b} \right) \]
\[ = 2 \text{tr} \left( \hat{\rho}_0 \sum_b (\ln m_b) \hat{E}_b \right) \]
\[ = 2 \text{tr} \left( \hat{\rho}_0 \ln \left( \hat{\rho}_1^{-1/2} \sqrt{\hat{\rho}_1^{1/2} \hat{\rho}_0 \hat{\rho}_1^{1/2} \hat{\rho}_1^{-1/2}} \right) \right). \] (3.93)

This, of course, will generally not be the maximum of the Kullback-Leibler information over all measurements, but it does provide a lower bound for the maximum value. Moreover, a quantity quite similar to this arises naturally in the context of still another measure of quantum distinguishability studied by Braunstein [88, 89]. In yet another guise, it appears in the work of Nagaoka [90].

There are two other representations for the quantum fidelity \( F(\hat{\rho}_0, \hat{\rho}_1) \) that can be worked out simply with the techniques developed here. The first is

\[ F(\hat{\rho}_0, \hat{\rho}_1) = \sqrt{\min_{\hat{G}} \text{tr}(\hat{\rho}_0 \hat{\hat{G}}) \text{tr}(\hat{\rho}_1 \hat{\hat{G}}^{-1})}, \] (3.94)

when \( \hat{\rho}_0 \) and \( \hat{\rho}_1 \) are invertible, and where the minimum is taken over all invertible positive operators \( \hat{G} \). This representation, in analogy to the representation of fidelity as the optimal statistical overlap, also comes about via the Schwarz inequality. Let us show this.

Let \( \hat{G} \) be any invertible positive operator and let \( \hat{U} \) be any unitary operator. Using the cyclic property of the trace and the Schwarz inequality, we have that

\[ \text{tr}(\hat{\rho}_0 \hat{\hat{G}}) \text{tr}(\hat{\rho}_1 \hat{\hat{G}}^{-1}) = \text{tr} \left( \left( \hat{U} \hat{\rho}_0^{1/2} \hat{G}^{1/2} \right) \left( \hat{U} \hat{\rho}_0^{1/2} \hat{G}^{1/2} \right) \right) \text{tr} \left( \left( \hat{\rho}_1^{1/2} \hat{G}^{-1/2} \right) \left( \hat{\rho}_1^{1/2} \hat{G}^{-1/2} \right) \right) \]
\[ \geq \left| \text{tr} \left( \left( \hat{U} \hat{\rho}_0^{1/2} \hat{G}^{1/2} \right) \left( \hat{\rho}_1^{1/2} \hat{G}^{-1/2} \right) \right) \right|^2 \]
\[ = \left| \text{tr} \left( \hat{U}^{\dagger} \hat{\rho}_1^{1/2} \hat{\rho}_0^{-1/2} \right) \right|^2. \] (3.95)

Since \( \hat{U} \) is arbitrary, we may use this freedom to make the inequality as tight as possible. To do this we choose

\[ \hat{U}^{\dagger} \hat{\rho}_1^{1/2} \hat{\rho}_0^{-1/2} = \sqrt{\hat{\rho}_1^{1/2} \hat{\rho}_0^{-1/2} \hat{\rho}_1^{1/2} \hat{\rho}_0^{-1/2}}. \] (3.96)
to get that
\[
\text{tr}(\hat{\rho}_0 \hat{G}) \text{tr}(\hat{\rho}_1 \hat{G}^{-1}) \geq F(\hat{\rho}_0, \hat{\rho}_1)^2.
\] (3.97)

To find a particular \( \hat{G} \) that achieves equality in this, we need merely study the condition for equality in the Schwarz inequality; in this case we must have
\[
\hat{U} \hat{\rho}_0^{1/2} \hat{G}^{1/2} = \alpha \hat{\rho}_1^{-1/2} \hat{G}^{-1/2}.
\] (3.98)

The solution \( \hat{G} \) to this equation is unique and easy to find,
\[
\hat{G} = \alpha \hat{\rho}_0^{-1/2} \sqrt{\hat{\rho}_0^{1/2} \hat{\rho}_1 \hat{\rho}_0^{-1/2}} \hat{\rho}_0^{-1/2}.
\] (3.99)

The constraint that \( \hat{G} \) be a positive operator further restricts \( \alpha \) to be a positive real number. Thus the optimal operator \( \hat{G} \) is proportional to the operator \( \hat{N} \) given by Eq. (3.83). The choice for \( \hat{G} \) given by Eq. (3.99) demonstrates that Eq. (3.94) does in fact hold. This is easy to verify by noting the fact that \( \hat{N}^{-1} = \hat{M} \).

The second representation is more literally concerned with the Bures distance defined by Eq. (3.29). It is [7]
\[
d_B^2(\hat{\rho}_0, \hat{\rho}_1) = \min \text{tr}\left( (\hat{W}_0 - \hat{W}_1)(\hat{W}_0 - \hat{W}_1)^\dagger \right),
\] (3.100)

where the minimum is taken over all operators \( \hat{W}_0 \) and \( \hat{W}_1 \) such that
\[
\hat{W}_0 \hat{W}_0^\dagger = \hat{\rho}_0 \quad \text{and} \quad \hat{W}_1 \hat{W}_1^\dagger = \hat{\rho}_1.
\] (3.101)

This is seen easily by noting that Eq. (3.101) requires, by the operator polar decomposition theorem, that
\[
\hat{W}_0 = \hat{\rho}_0^{1/2} \hat{U}_0 \quad \text{and} \quad \hat{W}_1 = \hat{\rho}_1^{1/2} \hat{U}_1
\] (3.102)

for some unitary operators \( \hat{U}_0 \) and \( \hat{U}_1 \). Then the right hand side of Eq. (3.101) becomes
\[
\min_{\hat{U}_0, \hat{U}_1} \text{tr}\left( (\hat{W}_0 - \hat{W}_1)(\hat{W}_0 - \hat{W}_1)^\dagger \right) = \min_{\hat{U}_0, \hat{U}_1} \text{tr}\left( \hat{W}_0 \hat{W}_0^\dagger - \hat{W}_0 \hat{W}_1^\dagger - \hat{W}_1 \hat{W}_0^\dagger + \hat{W}_1 \hat{W}_1^\dagger \right)
= \text{tr}(\hat{\rho}_0) + \text{tr}(\hat{\rho}_1) - 2 \max_{\hat{U}_0, \hat{U}_1} \text{Re}\left[ \text{tr}\left( \hat{W}_0 \hat{W}_1^\dagger \right) \right]
= 2 - 2 \max_{\hat{V}} \text{Re}\left[ \text{tr}\left( \hat{V} \hat{\rho}_1^{-1/2} \hat{\rho}_0^{-1/2} \right) \right]
= 2 - 2 F(\hat{\rho}_0, \hat{\rho}_1).
\] (3.103)

The last step in this follows from Eq. (3.61) and demonstrates the truth of Eq. (3.100).

Finally, we should mention something about the measurement specified by \( \hat{M} \), as it might appear in the larger context. A very general theory of operator means has been developed by Kubo and Ando [12, 13] in which the notion of a geometric mean [14] plays a special role. The geometric mean between two positive operators \( \hat{A} \) and \( \hat{B} \) is defined by
\[
\hat{A} \# \hat{B} = \hat{A}^{1/2} \sqrt{\hat{A}^{-1/2} \hat{B} \hat{A}^{-1/2}} \hat{A}^{1/2}.
\] (3.104)

More generally an operator mean is any mapping \( (\hat{A}, \hat{B}) \mapsto \hat{A} \sigma \hat{B} \) from operators on a \( D \)-dimensional Hilbert space to a \( D' \)-dimensional space such that
1. $\alpha (A \sigma B) = (\alpha A) \sigma (\alpha B)$ for any nonnegative constant $\alpha$,
2. $\tilde{A} \sigma \tilde{A} = \tilde{A}$,
3. $\tilde{A} \sigma \tilde{B} \geq \tilde{A}' \sigma \tilde{B}'$ whenever $\tilde{A} \geq \tilde{A}'$ and $\tilde{B} \geq \tilde{B}'$,
4. a certain continuity condition is satisfied, and
5. $(\tilde{T} \dagger \tilde{A} \sigma \tilde{B}) \tilde{T} \geq \tilde{T} \dagger (\tilde{A} \sigma \tilde{B}) \tilde{T}$ for every operator $\tilde{T}$.

Another characterization of the geometric mean is that (in any representation) it is the matrix $\tilde{X}$ such that the matrix (on a $D^2$-dimensional space) defined by

\[
\begin{pmatrix}
\tilde{A} & \tilde{X} \\
\tilde{X} & \tilde{B}
\end{pmatrix}
\]

is maximized in the matrix sense.

In this notation, the optimal measurement operator $\tilde{M}$ for statistical overlap is

\[
\tilde{M} = \rho_1^{-1} \# \rho_0.
\]

The significance of this correspondence, however, is yet to be determined.

### 3.3.3 The Two-Dimensional Case

In this Subsection, we derive a useful expression for the measurement $\{\tilde{E}_B^B\}$ in a case of particular interest, two-dimensional Hilbert spaces. Here the best strategy for finding the basis projectors $\tilde{E}_B^B$ is not to directly diagonalize the operator $\tilde{M}$, but rather to focus on variational methods. The great simplification for two-dimensional Hilbert spaces is that the signal states $\tilde{\rho}_0$ and $\tilde{\rho}_1$ may be represented as vectors within the unit ball of $\mathbb{R}^3$, the so-called Bloch sphere:

\[
\tilde{\rho}_0 = \frac{1}{2}(1 + \tilde{a} \cdot \tilde{\sigma}) \quad \text{and} \quad \tilde{\rho}_1 = \frac{1}{2}(1 + \tilde{b} \cdot \tilde{\sigma}),
\]

where $\tilde{a} \equiv |\tilde{a}| \leq 1$, $\tilde{b} \equiv |\tilde{b}| \leq 1$, and $\tilde{\sigma}$ is the Pauli spin vector. This follows because the identity operator $\mathbb{1}$ and the (trace-free) Pauli operators $\tilde{\sigma} = (\tilde{\sigma}_x, \tilde{\sigma}_y, \tilde{\sigma}_z)$, i.e.,

\[
\tilde{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \tilde{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \tilde{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},
\]

form a basis for the vector space of $2 \times 2$ Hermitian operators. In this representation the signal states are pure if $\tilde{a}$ and $\tilde{b}$ have unit modulus. More generally, the eigenvalues of $\tilde{\rho}_0$ are given by $\frac{1}{2}(1 - a)$ and $\frac{1}{2}(1 + a)$ and similarly for $\tilde{\rho}_1$. Consider an orthogonal projection-valued measurement corresponding to the unit Bloch vector $\tilde{n}/n$ and its antipode $-\tilde{n}/n$; for this measurement, the possible outcomes can be labeled simply $+1$ and $-1$. It is a trivial matter, using the identity

\[
(\tilde{a} \cdot \tilde{\sigma})(\tilde{n} \cdot \tilde{\sigma}) = (\tilde{a} \cdot \tilde{n}) \mathbb{1} + i \tilde{\sigma} \cdot (\tilde{a} \times \tilde{n}),
\]

to show that

\[
p_0(b) = \frac{1}{2} \left( 1 \pm \frac{\tilde{a} \cdot \tilde{n}}{n} \right) \quad \text{and} \quad p_1(b) = \frac{1}{2} \left( 1 \pm \frac{\tilde{b} \cdot \tilde{n}}{n} \right).
\]
The statistical overlap, i.e., \( F(p_0, p_1) \), with respect to this measurement can thus be written as
\[
W(\vec{n}) \equiv \frac{1}{2} \sqrt{\left(1 + \vec{a} \cdot \frac{\vec{n}}{n}\right)\left(1 + \vec{b} \cdot \frac{\vec{n}}{n}\right)} + \frac{1}{2} \sqrt{\left(1 - \vec{a} \cdot \frac{\vec{n}}{n}\right)\left(1 - \vec{b} \cdot \frac{\vec{n}}{n}\right)}.
\] (3.111)

The optimal projector for expression (3.111) can be found by varying it with respect to all vectors \( \vec{n} \), i.e., by setting \( \delta W(\vec{n}) = 0 \). Using
\[
\delta n = \delta \left(\sqrt{\vec{n} \cdot \vec{n}}\right) = \frac{1}{2n} \delta (\vec{n} \cdot \vec{n}) = \frac{1}{2n} \left((\delta \vec{n}) \cdot \vec{n} + \vec{n} \cdot (\delta \vec{n})\right) = \frac{\vec{n}}{n} \cdot (\delta \vec{n}) ,
\] (3.112)
one finds after a bit of algebra that the optimal \( \vec{n} \) must lie in the plane spanned by \( \vec{a} \) and \( \vec{b} \) and satisfy the equation
\[
(a^2 - b^2) n^2 - (1 - b^2) (\vec{a} \cdot \vec{n})^2 + (1 - a^2) (\vec{b} \cdot \vec{n})^2 = 0 .
\] (3.113)

A vector \( \vec{n}_B \) satisfying these two requirements is
\[
\vec{n}_B = \frac{\vec{a}}{\sqrt{1 - a^2}} - \frac{\vec{b}}{\sqrt{1 - b^2}} .
\] (3.114)

It might be noted that the variational equation \( \delta W(\vec{n}) = 0 \) also generates the measurement with respect to which \( \hat{\rho}_0 \) and \( \hat{\rho}_1 \) are the least distinguishable; this is the measurement specified by the Bloch vector \( \vec{n}_0 \) orthogonal to the vector \( \vec{d} = \vec{b} - \vec{a} \).

If \( \vec{n}_B \) is plugged back into Eq. (3.111), one finds after quite some algebra that
\[
F(\hat{\rho}_0, \hat{\rho}_1) = \frac{1}{\sqrt{2}} \left(1 + \vec{a} \cdot \vec{b} + \sqrt{1 - a^2} \sqrt{1 - b^2}\right)^{1/2} .
\] (3.115)

(This expression does not match Hübner’s expression in Ref. [81] because of his convention that the Bloch sphere is of radius \( \frac{1}{2} \).)

### 3.4 The Quantum Rényi Overlaps

Recall that the quantum Rényi overlap of order \( \alpha \) (for \( 0 < \alpha < 1 \)) is defined by
\[
F_\alpha(\hat{\rho}_0/\hat{\rho}_1) \equiv \min_{\{E_b\}} \sum_b \left(\text{tr}(\hat{\rho}_0 E_b)\right)^\alpha \left(\text{tr}(\hat{\rho}_1 E_b)\right)^{1-\alpha} .
\] (3.116)

This measure of quantum distinguishability, though it has no compelling operational meaning, proves to be a convenient testing ground for optimization techniques more elaborate than so far encountered. Equation (3.116) is more unwieldy than the quantum statistical overlap, but not so transcendental in character as to contain a logarithm like the Kullback-Leibler and mutual informations. One can still maintain a serious hope that an explicit expression for it is possible.

Moreover, if an explicit expression can be found for Eq. (3.116), then one would have a direct route to the quantum Kullback information through either the Rényi relative information of order \( \alpha \) [36, 37]
\[
K_\alpha(p_0/p_1) = \frac{1}{\alpha - 1} \ln \left(\sum_{b=1}^n p_0(b)^\alpha p_1(b)^{1-\alpha}\right) ,
\] (3.117)
or the relative information of type $\alpha$ of Rathie and Kannappan [95, 66]

$$K^\alpha(p_0/p_1) = \left(e^{\alpha-1} - 1\right)^{-1} \left(\sum_{b=1}^{n} p_0(b)^{\alpha} p_1(b)^{1-\alpha} - 1\right).$$ (3.118)

Both these quantities converge to the Kullback-Leibler relative information in the limit $\alpha \to 1$, as can be seen easily by using l’Hospital’s rule. Therefore, one just needs to find $F^\alpha(\hat{\rho}_0/\hat{\rho}_1)$ and take the limit $\alpha \to 1$ to get the quantum Kullback information.

The brightest ray of hope for finding an explicit expression for $F^\alpha(\hat{\rho}_0/\hat{\rho}_1)$ is that the quantum fidelity was found via an application of the Schwarz inequality. There is a closely related inequality in the mathematical literature known as the Hölder inequality [96, 97] that—at first sight at least—would appear to be of use in the same way for this context. This inequality is that, for any two sequences $a_k$ and $b_k$ of complex numbers, $k = 1, \ldots, n$,

$$\sum_{k=1}^{n} |a_k b_k| \leq \left(\sum_{k=1}^{n} |a_k|^p\right)^{1/p} \left(\sum_{k=1}^{n} |b_k|^q\right)^{1/q},$$ (3.119)

when $p, q > 1$ with

$$\frac{1}{p} + \frac{1}{q} = 1.$$ (3.120)

Equality is achieved in Eq. (3.119) if and only if there exists a constant $c$ such that

$$|b_k| = c|a_k|^{p-1}.$$ (3.121)

The standard Schwarz inequality is the special case of this for $p = 2$.

One would like to use some appropriate operator analog to the Hölder inequality in much the same way as the operator-Schwarz inequality was used for optimizing the statistical overlap: use it to bound the quantum Rényi overlap and then search out the conditions for achieving equality—perhaps again by taking advantage of the invariances of the trace. In particular, one would like to find something of the form

$$\left(\text{tr}(\hat{\rho}_0 \hat{E}_b)\right)^\alpha \left(\text{tr}(\hat{\rho}_1 \hat{E}_b)\right)^{1-\alpha} \geq \text{tr}\left(f(\hat{\rho}_0, \hat{\rho}_1; \alpha) \hat{E}_b\right),$$ (3.122)

with a function $f(\hat{\rho}_0, \hat{\rho}_1; \alpha)$ that is independent of the POVM $\{\hat{E}_b\}$. In this way, the linearity of the trace and the completeness of the $\hat{E}_b$ could be used in the same fashion as before.

Unfortunately—even after an exhaustive literature search—an inequality sufficiently strong to carry through the optimization has yet to be found. Nevertheless, for future endeavors, we report the most promising lines of attack found so far.

For the first demonstration, we need to list the standard operator-Hölder inequality [98, 99, 100]

$$|\text{tr}(\hat{A} \hat{B})| \leq \left(\text{tr}(\hat{A}^\dagger \hat{A})^{p/2}\right)^{1/p} \left(\text{tr}(\hat{B}^\dagger \hat{B})^{q/2}\right)^{1/q},$$ (3.123)

and the Araki inequality [101, 102],

$$\text{tr}\left(\hat{C}^{1/2} \hat{D} \hat{C}^{1/2}/2\right) \leq \text{tr}\left(\hat{C}^{r/2} \hat{D}^{r/2}\right),$$ (3.124)

for $\hat{C}$ and $\hat{D}$ positive operators and $r \geq 1$. These two inequalities can get us to something “close” to Eq. (3.122), though not quite linear in the $\hat{E}_b$. Let us show how this is done. Suppose positive
$p$ and $q$ satisfy Eq. (3.124). Then

$$
\left( \text{tr}(\hat{\rho}_0 \hat{E}_b) \right)^{\frac{1}{p}} \left( \text{tr}(\hat{\rho}_1 \hat{E}_b) \right)^{\frac{1}{q}} = \left( \text{tr} \left( \left( \hat{E}_b \right)^{\frac{1}{q}} \left( \hat{\rho}_0 \right)^{\frac{1}{p}} \left( \hat{E}_b \right)^{\frac{1}{q}} \right) \right)^{\frac{1}{p}} \left( \text{tr} \left( \left( \hat{E}_b \right)^{\frac{1}{q}} \left( \hat{\rho}_1 \right)^{\frac{1}{q}} \left( \hat{E}_b \right)^{\frac{1}{q}} \right) \right)^{\frac{1}{q}} \\
\geq \left( \text{tr} \left( \hat{E}_b \hat{\rho}_0 \hat{E}_b \right) \right)^{\frac{1}{p}} \left( \text{tr} \left( \hat{E}_b \hat{\rho}_1 \hat{E}_b \right) \right)^{\frac{1}{q}} \\
\geq \left| \text{tr} \left( \hat{E}_b \hat{\rho}_0 \hat{E}_b \right) \right| \\
\geq \left| \text{tr} \left( \hat{E}_b \hat{\rho}_0 \hat{E}_b \hat{\rho}_1 \right) \right| .
$$

(3.125)

The upshot is a bound that is “almost” linear in the $\hat{E}_b$. There are other variations on this theme, but they are lacking in the same respect.

A second way to tackle this problem via the Hölder inequality is at the eigenvalue level. To set this problem up, let us use the notation $\lambda_i(\hat{A})$ to denote the eigenvalues of any Hermitian operator $\hat{A}$, when numbered so that they form a nonincreasing sequence, i.e.,

$$
\lambda_1(\hat{A}) \geq \lambda_2(\hat{A}) \geq \cdots \geq \lambda_D(\hat{A}) .
$$

With this, we may write down a theorem, originally due to Richter [103, 104], that places a bound on the trace of a product of two operators

$$
\sum_{i=1}^{D} \lambda_i(\hat{A}) \lambda_{D-i+1}(\hat{B}) \leq \text{tr}(\hat{A}\hat{B}) \leq \sum_{i=1}^{D} \lambda_i(\hat{A}) \lambda_i(\hat{B}) .
$$

(3.127)

Using this and the Hölder inequality for numbers, one immediately obtains,

$$
\left( \text{tr}(\hat{\rho}_0 \hat{E}_b) \right)^{\frac{1}{p}} \left( \text{tr}(\hat{\rho}_1 \hat{E}_b) \right)^{\frac{1}{q}} \geq \left( \sum_{i=1}^{D} \lambda_i(\hat{\rho}_0) \lambda_{D-i+1}(\hat{E}_b) \right)^{\frac{1}{p}} \left( \sum_{i=1}^{D} \lambda_i(\hat{\rho}_1) \lambda_{D-i+1}(\hat{E}_b) \right)^{\frac{1}{q}} \\
\geq \sum_{i=1}^{D} \lambda_i(\hat{\rho}_0)^{\frac{1}{q}} \lambda_i(\hat{\rho}_1)^{\frac{1}{q}} \lambda_{D-i+1}(\hat{E}_b)
$$

(3.128)

This is—in a certain sense—linear in the operator $\hat{E}_b$. Regardless of this, however, the bound given by Eq. (3.128), is far too loose. For instance, if the $\hat{E}_b$ are one-dimensional projectors, this bound reduces to the product $\lambda_D(\hat{\rho}_0)^{\frac{1}{q}} \lambda_D(\hat{\rho}_1)^{\frac{1}{q}}$ and so gives rise to

$$
\sum_{b=1}^{D} \left( \text{tr}(\hat{\rho}_0 \hat{E}_b) \right)^{\frac{1}{p}} \left( \text{tr}(\hat{\rho}_1 \hat{E}_b) \right)^{\frac{1}{q}} \geq D \lambda_D(\hat{\rho}_0)^{\frac{1}{q}} \lambda_D(\hat{\rho}_1)^{\frac{1}{q}} .
$$

(3.129)

This can hardly be a tight bound, disregarding as it does all the other structure of the operators $\hat{\rho}_0$ and $\hat{\rho}_1$ and their relation to each other.

Could it be that an optimal POVM for the Rényi overlap can always be taken to be an orthogonal projection-valued measurement? Chances of this are strong, given that that was the case for the
statistical overlap. In case of this, let us point out the following. Suppose $\hat{A}$ is an invertible positive operator with spectral decomposition $\hat{A} = \sum_b a_b \hat{\Pi}_b$. Then applying the Hölder inequality again, we have

$$
\left( \frac{\text{tr}(\hat{\rho}_0 \hat{A}^p)}{\text{tr}(\hat{\rho}_1 \hat{A}^{-q})} \right)^\frac{i}{p} \geq \left( \sum_b a_b^p \text{tr}(\hat{\rho}_0 \hat{\Pi}_b) \right)^\frac{1}{p} \left( \sum_b a_b^{-q} \text{tr}(\hat{\rho}_1 \hat{\Pi}_b) \right)^\frac{1}{q}.
$$

(3.130)

Therefore, as it was for the case of the quantum statistical overlap, it may well be that

$$
\min_{\hat{A} > 0} \left( \frac{\text{tr}(\hat{\rho}_0 \hat{A}^p)}{\text{tr}(\hat{\rho}_1 \hat{A}^{-q})} \right)^\frac{1}{p} = \left( \sum_i \lambda_i \hat{\rho}_0 \right)^{\frac{1}{p}} \left( \sum_i \lambda_i \hat{\rho}_1 \right)^{\frac{1}{q}}.
$$

(3.131)

Let us point out a bound for this quantity. Note that, for any positive invertible operator $\hat{A}$,

$$
\lambda_{D-i+1}(\hat{A}^{-1}) = \left( \lambda_i(\hat{A}) \right)^{-1}.
$$

(3.132)

Using the Richter and Hölder inequalities, we have that

$$
\left( \frac{\text{tr}(\hat{\rho}_0 \hat{A}^p)}{\text{tr}(\hat{\rho}_1 \hat{A}^{-q})} \right)^\frac{i}{q} \geq \left( \sum_{i=1}^D \lambda_{D-i+1}(\hat{\rho}_0) \lambda_i(\hat{A})^p \right)^\frac{1}{p} \left( \sum_{i=1}^D \lambda_i(\hat{\rho}_1) \lambda_i(\hat{A}^{-q}) \right)^\frac{1}{q}
$$

$$
\geq \sum_{i=1}^D \lambda_{D-i+1}(\hat{\rho}_0) \lambda_i(\hat{\rho}_1)^\frac{1}{q}.
$$

(3.133)

This gives a nice lower bound, though it is most certainly not tight—as can be seen from that fact that it does not reproduce the quantum fidelity when $p = 2$.

Let us now mention another method for lower bounding the quantum Rényi overlap that does not appear to be related to a Hölder inequality at all. This one relies on an inequality of Ando [93] concerning the operator means introduced in Section (3.3.2). For any operator mean $\sigma$,

$$
\left( \text{tr}(\hat{C} \hat{A}) \right) \sigma \left( \text{tr}(\hat{C} \hat{B}) \right) \geq \text{tr} \left( \hat{C} (\hat{A} \sigma \hat{B}) \right),
$$

(3.134)

where $\hat{A}$, $\hat{B}$, and $\hat{C}$ are all positive operators. We can use this in the following way. Note that the mapping $\#_\alpha$ defined by

$$
\hat{A} \#_\alpha \hat{B} = \hat{A}^{1/2} \left( \hat{A}^{-1/2} \hat{B} \hat{A}^{-1/2} \right)^\alpha \hat{A}^{1/2}
$$

(3.135)

satisfies all the properties of an operator mean [92]. When $\hat{A}$ and $\hat{B}$ are scalars, and so commute, this operator mean reduces to

$$
\hat{A} \#_\alpha \hat{B} = \hat{B}^\alpha \hat{A}^{-\alpha}.
$$

(3.136)
Therefore, for any POVM \( \{ \hat{E}_b \} \), we can write the inequality
\[
\sum_b \left( \text{tr}(\hat{\rho}_0 \hat{E}_b) \right)^\alpha \left( \text{tr}(\hat{\rho}_1 \hat{E}_b) \right)^{1-\alpha} \geq \sum_b \text{tr} \left( \hat{E}_b (\hat{\rho}_1 ^{\#_\alpha} \hat{\rho}_0) \right) = \text{tr} \left( \hat{\rho}_1^{1/2} \left( \hat{\rho}_1^{-1/2} \hat{\rho}_0 \hat{\rho}_1^{-1/2}\right)^\alpha \hat{\rho}_1^{1/2} \right). \tag{3.137}
\]
Therefore one obtains a lower bound on the quantum Rényi overlap of order \( \alpha \). Again the bound is not as tight as it might be because it does not reproduce the result known for \( \alpha = \frac{1}{2} \).

Finally, we should point out that Hasegawa \([105, 106]\) has studied the quantity
\[
H_\alpha(\hat{\rho}_0/\hat{\rho}_1) = \frac{4}{1-\alpha^2} \text{tr} \left( \left( 1 - \frac{1+\alpha}{2} \hat{\rho}_0 \right) \hat{\rho}_1 \right), \tag{3.138}
\]
in the context of distinguishing quantum states. The connection between this and Eq. (3.116) (if there is any) is not known.

### 3.5 The Accessible Information

A binary quantum communication channel is defined by its signal states \( \{ \hat{\rho}_0, \hat{\rho}_1 \} \) and their prior probabilities
\[
\pi_0 = 1 - t \quad \text{and} \quad \pi_1 = t, \tag{3.139}
\]
for \( 0 \leq t \leq 1 \). Consider a measurement \( \{ \hat{E}_b \} \) on the channel. The probability of an outcome \( b \) when the message state is \( k \) \( (k = 0, 1) \) is
\[
p_k(b) = \text{tr}(\hat{\rho}_k \hat{E}_b). \tag{3.140}
\]
The unconditioned probability distribution for the outcomes is
\[
p(b) = \text{tr}(\hat{\rho} \hat{E}_b), \tag{3.141}
\]
for
\[
\hat{\rho} = (1-t)\hat{\rho}_0 + t\hat{\rho}_1 = \hat{\rho}_0 + t\hat{\Delta} = \hat{\rho}_1 - (1-t)\hat{\Delta}, \tag{3.142}
\]
where the difference operator \( \hat{\Delta} \) is defined by
\[
\hat{\Delta} = \hat{\rho}_1 - \hat{\rho}_0. \tag{3.143}
\]
The Shannon mutual information \([10, 60]\) for the channel, with respect to the measurement \( \{ \hat{E}_b \} \), is defined to be
\[
J(p_0, p_1; t) \equiv H(p) - (1-t)H(p_0) - tH(p_1) = (1-t)K(p_0/p) + tK(p_1/p), \tag{3.144}
\]
where
\[
H(q) = - \sum_b q(b) \ln q(b) \tag{3.145}
\]
64
is the Shannon information \([11, 60, 66]\) of the probability distribution \(q(b)\). Because a natural logarithm has been used in this definition, information here is quantified in terms of “nats” rather than the more commonly used unit of “bits.” The accessible information \([107, 108]\) is the mutual information maximized over all measurements \(\{\hat{E}_b\}\):

\[
I(\hat{\rho}_0|\hat{\rho}_1) = \max_{\{\hat{E}_b\}} \sum_b \left( - \text{tr}(\hat{\rho}\hat{E}_b) \ln(\text{tr}(\hat{\rho}\hat{E}_b)) \right) + (1 - t) \text{tr}(\hat{\rho}_0\hat{E}_b) \ln(\text{tr}(\hat{\rho}_0\hat{E}_b)) + t \text{tr}(\hat{\rho}_1\hat{E}_b) \ln(\text{tr}(\hat{\rho}_1\hat{E}_b)) \right)
\]

\[= \max_{\{\hat{E}_b\}} \sum_b \left( \pi_0 \text{tr}(\hat{\rho}_0\hat{E}_b) \ln\left( \frac{\text{tr}(\hat{\rho}_0\hat{E}_b)}{\text{tr}(\hat{\rho}\hat{E}_b)} \right) + \pi_1 \text{tr}(\hat{\rho}_1\hat{E}_b) \ln\left( \frac{\text{tr}(\hat{\rho}_1\hat{E}_b)}{\text{tr}(\hat{\rho}\hat{E}_b)} \right) \right) .
\]

(3.146)

In this Section we will often use the alternative notations \(J\) and \(I\) for the mutual and accessible informations; this notation is more compact while still making explicit the dependence of these quantities on the prior probabilities.

The significance of expression (3.144), explained in great detail in Chapter 2, can be summarized in the following way. Imagine for a moment that the receiver actually does know which message \(m_k\) was sent, but nevertheless performs the measurement \(\{\hat{E}_b\}\) on it. Regardless of this knowledge, the receiver will not be able to predict the exact outcome of his measurement; this is just because of quantum indeterminism—the most he can say is that outcome \(b\) will occur with probability \(p_k(b)\). A different way to summarize this is that even with the exact message known, the receiver will gain information via the unpredictable outcome \(b\). That information, however, has nothing to do with the message itself. The residual information gain is a signature of quantum indeterminism, now quantified by the Shannon information \(H(p_k)\) of the outcome distribution. Now return to the real scenario, where the receiver actually does not know which message was sent. The amount of residual information the receiver can expect to gain in this case is \((1 - t)H(\hat{\rho}_0) + tH(\hat{\rho}_1)\). This quantity, however, is not identical to the information the receiver can expect to gain in toto. That is because the receiver must describe the quantum system encoding the message by the mean density operator \(\hat{\rho}\); this reflects his lack of knowledge about the preparation. For this state, the expected amount of information gain in a measurement of \(\{\hat{E}_b\}\) is \(H(p)\). This time some of the information will have to do with the message itself, rather than being due to quantum indeterminism. The natural quantity for describing the information gained exclusively about the message itself (i.e., not augmented through quantum indeterminism) is just the mutual information Eq. (3.144).

### 3.5.1 The Holevo Bound

The problems associated with actually finding \(I(t)\) and the measurement that gives rise to it are every bit as difficult as those in maximizing the Kullback-Leibler information, perhaps more so—for here it is not only the logarithm that confounds things, but also the fact that \(\hat{\rho}_0\) and \(\hat{\rho}_1\) are “coupled” through the mean density operator \(\hat{\rho}\). Outside of a very few isolated examples, namely the case where \(\hat{\rho}_0\) and \(\hat{\rho}_1\) are pure states and the case where they are 2 \(\times\) 2 density operators with equal determinant and equal prior probabilities \([109, 110]\), explicit expressions for \(I(t)\) have never been calculated. Moreover no general algorithms for approximating this quantity appear to exist as yet. There is a result, due to Davies \([4, 111]\), stating that there always exists an optimal measurement \(\{\hat{E}_b^D\}\) of the form

\[
\hat{E}_b^D = \alpha_b|\psi_b\rangle\langle\psi_b| \quad b = 1, \ldots, N ,
\]

(3.147)
where the number of terms in this is bracketed by

\[ D \leq N \leq D^2 \]  

(3.148)

for signal states on a \( D \)-dimensional Hilbert space. This theorem, however, does not pin down the measurement any further than that. The most useful general statements about \( I(t) \) have been in the form of bounds: an upper bound first conjectured in print by Gordon \([112]\) in 1964 (though there may also have been some discussion of it by Forney \([113]\) in 1962) and proven by Holevo \([3]\) in 1973 (though Levitin did announce a similar but more restricted result \([114]\) in 1969), and a lower bound first conjectured by Wootters \([115]\) and proven by Jozsa, Robb, and Wootters \([6]\). These bounds, however, are of little use in pinpointing the measurement that gives rise to \( I(t) \). In what follows, we simplify the derivation of the Holevo bound via a variation of the methods used in the Section 3.3. This simplification has the advantage of specifying a measurement, the use of which immediately gives rise to a new lower bound to \( I(t) \). We also supply an explicit expression for a still-tighter upper bound whose existence is required within the original Holevo derivation. Since Holevo’s original derivation, various improved versions have also appeared \([116, 117]\). The improvements until now, however, have been in proving the upper bound for more general situations: infinite dimensional Hilbert spaces, infinite numbers of messages states and infinite numbers of measurement outcomes. In contrast, in this section and throughout the remainder of the report, we retain the finiteness assumptions made by Holevo; the aim here is to build a deeper understanding of the issues involved in finding approximations to the accessible information.

The Holevo upper bound to \( I(t) \) is given by

\[ I(t) \leq S(\hat{\rho}) - (1 - t)S(\hat{\rho}_0) - tS(\hat{\rho}_1) \equiv S(t) \]  

(3.149)

where

\[ S(\hat{\rho}) = -\text{tr}(\hat{\rho} \ln \hat{\rho}) = -\sum_{j=1}^{D} \lambda_j \ln \lambda_j \]  

(3.150)

is the von Neumann entropy \([118]\) of the density operator \( \hat{\rho} \), whose eigenvalues are \( \lambda_j, j = 1, \ldots, D \). Equality is achieved in this bound if and only if \( \hat{\rho}_0 \) and \( \hat{\rho}_1 \) commute.

The Jozsa-Robb-Wootters lower bound to \( I(t) \) is formally quite similar to the Holevo upper bound. For later reference, we write it out explicitly:

\[ I(t) \geq Q(\hat{\rho}) - (1 - t)Q(\hat{\rho}_0) - tQ(\hat{\rho}_1) \equiv Q(t) \]  

(3.151)

where

\[ Q(\hat{\rho}) = -\sum_{j=1}^{D} \left( \prod_{k \neq j} \frac{\lambda_j}{\lambda_j - \lambda_k} \right) \lambda_j \ln \lambda_j \]  

(3.152)

is the “sub-entropy” \([119, 120]\) of the density operator \( \hat{\rho} \). The formal similarity between Eqs. (3.149) and (3.151) becomes even more apparent if \( S(\hat{\rho}) \) and \( Q(\hat{\rho}) \) are represented as contour integrals \([3, 6, 121]\):\n
\[ S(\hat{\rho}) = -\frac{1}{2\pi i} \oint_C (\ln z) \text{tr} \left( \left( \hat{1} - z^{-1} \hat{\rho} \right)^{-1} \right) dz \]  

(3.153)

and

\[ Q(\hat{\rho}) = -\frac{1}{2\pi i} \oint_C (\ln z) \det \left( \left( \hat{1} - z^{-1} \hat{\rho} \right)^{-1} \right) dz \]  

(3.154)

where the contour \( C \) encloses all the nonzero eigenvalues of \( \hat{\rho} \).
The key to deriving the Holevo bound is in realizing the importance of properties of $J(t)$ and $S(t)$ as functions of $t$. Note that

$$J(0) = J(1) = S(0) = S(1) = 0.$$  \hspace{1cm} (3.155)

Moreover, both $J(t)$ and $S(t)$ are downwardly convex, as can be seen by working out their second derivatives. For $J(t)$ a straightforward calculation gives

$$J''(t) = -\sum_b \frac{\left(\text{tr}(\hat{\Delta}\hat{E}_b)\right)^2}{\text{tr}(\hat{\rho}\hat{E}_b)}.$$  \hspace{1cm} (3.156)

For $S(t)$ it is easiest to proceed by using the contour integral representation of $S(\hat{\rho})$. By differentiating within the integral and using the operator identity

$$\frac{d}{dt} \hat{A}^{-1} = -\hat{A}^{-1} \frac{d\hat{A}}{dt} \hat{A}^{-1}$$  \hspace{1cm} (3.157)

(which comes simply from the fact that $\hat{A}^{-1} \hat{A} = \hat{1}$), one finds

$$\frac{d}{dt} S(\hat{\rho}) = -\frac{1}{2\pi i} \oint_C (z \ln z) \text{tr} \left( (z \hat{1} - \hat{\rho})^{-1} \Delta (z \hat{1} - \hat{\rho})^{-1} \right) dz,$$  \hspace{1cm} (3.158)

and

$$\frac{d^2}{dt^2} S(\hat{\rho}) = -\frac{2}{2\pi i} \oint_C (z \ln z) \text{tr} \left( (z \hat{1} - \hat{\rho})^{-2} \Delta (z \hat{1} - \hat{\rho})^{-1} \right) dz.$$  \hspace{1cm} (3.159)

Therefore, if $|j\rangle$ is the eigenvector of $\hat{\rho}$ with eigenvalue $\lambda_j$ and $\Delta_{jk} = \langle j|\hat{\Delta}|k\rangle$, we can write

$$S''(t) = -\sum_{\{j,k: \lambda_j + \lambda_k \neq 0\}} \Phi(\lambda_j, \lambda_k) |\Delta_{jk}|^2,$$  \hspace{1cm} (3.160)

where

$$\Phi(\lambda_j, \lambda_k) = \frac{2}{2\pi i} \oint_C \frac{z \ln z}{(z - \lambda_j)(z - \lambda_k)} dz.$$  \hspace{1cm} (3.161)

An application of Cauchy’s integral theorem gives

$$\Phi(x, y) = \frac{\ln x - \ln y}{x - y} \quad \text{if} \quad x \neq y,$$  \hspace{1cm} (3.162)

and

$$\Phi(x, x) = \frac{1}{x}.$$  \hspace{1cm} (3.163)

Expressions (3.156) and (3.160) are thus clearly nonpositive.

The statement that $S(t)$ is an upper bound to $J(t)$ for any $t$ is equivalent to the property that, when plotted versus $t$, the curve for $S(t)$ has a more negative curvature than the curve for $J(t)$ regardless of which POVM $\{\hat{E}_b\}$ is used in its definition. This has to be because $S(t)$ must climb higher than $J(t)$ to be an upper bound for it. The meat of the derivation is in showing the inequality

$$S''(t) \leq J''(t) \leq 0 \quad \text{for any POVM} \ \{\hat{E}_b\}.$$  \hspace{1cm} (3.164)

Holevo does this by demonstrating the existence of a function $L''(t)$, independent of $\{\hat{E}_b\}$, such that

$$S''(t) \leq L''(t) \quad \text{and} \quad L''(t) \leq J''(t).$$  \hspace{1cm} (3.165)
From this it follows, upon enforcing the boundary condition
\[ L(0) = L(1) = 0, \] (3.166)
that
\[ I(t) \leq L(t) \leq S(t). \] (3.167)

(It should be noted that \( L(t) \) is not explicitly computed in Ref. [5]; it is only shown to exist via the expression for its second derivative.)

At this point a fairly drastic simplification can be made to the original proof. An easy way to get at such a function \( L''(t) \) is simply to minimize \( J''(t) \) over all POVMs \( \{ \hat{E}_b \} \) and to define the result to be the function \( L''(t) \). Thereafter one can work to show that \( S''(t) \leq L''(t) \). This is decidedly more tractable than extremizing the mutual information \( J(t) \) itself because no logarithms appear in \( J''(t) \); there can be hope for a solution by means of standard algebraic inequalities such as the Schwarz inequality. This approach, it turns out, generates exactly the same function \( L''(t) \) as used by Holevo in the original proof, though the two derivations appear to have little to do with each other. The difference of real importance here is that this approach pinpoints the measurement that actually minimizes \( I''(t) \). This measurement, though it generally does not maximize \( J(t) \) itself, necessarily does provide a lower bound to the accessible information \( I(t) \).

The problem of minimizing Eq. (3.156) is formally identical to the problem considered by Braunstein and Caves [122]: the expression for \(-I''(t)\) is of the same form as the Fisher information optimized there. The steps are as follows. The idea is to think of the numerator within the sum (3.156) as analogous to the left hand side of the Schwarz inequality:
\[ |\text{tr}(\hat{\Delta} \hat{E}_b)|^2 \leq |\text{tr}(\hat{\Delta} \hat{E}_b G_{\hat{C}}(\hat{\Delta})\hat{E}_b)|^2. \] (3.168)

One would like to use this inequality in such a way that the \( \text{tr}(\hat{\rho} \hat{E}_b) \) term in the denominator is cancelled and only an expression linear in \( \hat{E}_b \) is left; for then, upon summing over the index \( b \), the completeness property for POVMs will leave the final expression independent of the given measurement.

These ideas are formalized by introducing a “lowering” super-operator \( G_{\hat{C}}, \) (i.e., a mapping from operators to operators that depends explicitly on a third operator \( \hat{C} \)) with the property that for any operators \( \hat{A} \) and \( \hat{B} \) and any positive operator \( \hat{C} \),
\[ \text{tr}(\hat{A} \hat{B}) \leq |\text{tr}(\hat{C} \hat{B} G_{\hat{C}}(\hat{A}))| \leq |\text{tr}(\hat{C} \hat{B} G_{\hat{C}}(\hat{A})\hat{B} G_{\hat{C}}(\hat{A})^\dagger)| \]. (3.169)

There are many examples of such super-operators; perhaps the simplest example is
\[ G_{\hat{C}}(\hat{A}) = \hat{A} \hat{C}^{-1}, \] (3.170)
when \( \hat{C} \) is invertible. In any case, for these super-operators, one can derive—via simple applications of the Schwarz inequality—that
\[
\left( \text{tr}(\hat{\Delta} \hat{E}_b) \right)^2 \leq \left| \text{tr}(\hat{\rho} \hat{E}_b G_{\hat{\rho}}(\hat{\Delta})) \right|^2 \\
= \left| \text{tr}\left((\hat{E}_b^{1/2} \hat{\rho}^{1/2}) \hat{E}_b^{1/2} G_{\hat{\rho}}(\hat{\Delta}) \hat{\rho}^{1/2}) \right) \right|^2 \\
\leq \text{tr}(\hat{\rho} \hat{E}_b) \text{tr}\left(\hat{E}_b \left(G_{\hat{\rho}}(\hat{\Delta}) \hat{\rho} G_{\hat{\rho}}(\hat{\Delta})^\dagger\right)\right) \] (3.171)
\[(\text{tr}(\hat{\Delta}\hat{E}_b))^2 \leq \left| \text{tr}\left(\hat{\rho}^{1/2}\hat{E}_b\mathcal{G}_{\hat{\rho}^{1/2}}\right)\right|^2 \]
\[
= \left| \text{tr}\left((\mathcal{E}_b^{1/2}\hat{\rho}^{1/2})^\dagger(\mathcal{E}_b^{1/2}\mathcal{G}_{\hat{\rho}^{1/2}})\right)\right|^2 \]
\[
\leq \text{tr}(\hat{\rho}\hat{E}_b)\text{tr}\left(\hat{E}_b\left(\mathcal{G}_{\hat{\rho}^{1/2}}\mathcal{G}_{\hat{\rho}^{1/2}}\right)^\dagger\right). \tag{3.172} \]

By \(\mathcal{G}_C(\hat{A})^\dagger\), we mean simply the Hermitian conjugate to the operator \(\mathcal{G}_C(\hat{A})\). The conditions for equality in these are that the super-operators \(\mathcal{G}_\hat{\rho}\) and \(\mathcal{G}_{\hat{\rho}^{1/2}}\) give equality in the first steps and, moreover, saturate the Schwarz inequality via
\[
\hat{E}_b^{1/2}\mathcal{G}_\hat{\rho}(\hat{\Delta})\hat{\rho}^{1/2} = \mu_b\hat{E}_b^{1/2}\hat{\rho}^{1/2}, \tag{3.173} \]
and
\[
\hat{E}_b^{1/2}\mathcal{G}_{\hat{\rho}^{1/2}}(\hat{\Delta}) = \mu_b\hat{E}_b^{1/2}\hat{\rho}^{1/2}, \tag{3.174} \]
respectively.

Using inequalities (3.171) and (3.172) in Eq. (3.156) for \(J''(t)\) immediately gives the lower bounds
\[
J''(t) \geq -\text{tr}\left(\mathcal{G}_\hat{\rho}(\hat{\Delta})\hat{\rho}\mathcal{G}_\hat{\rho}(\hat{\Delta})^\dagger\right), \tag{3.175} \]
and
\[
J''(t) \geq -\text{tr}\left(\mathcal{G}_{\hat{\rho}^{1/2}}(\hat{\Delta})\mathcal{G}_{\hat{\rho}^{1/2}}(\hat{\Delta})^\dagger\right). \tag{3.176} \]

The problem now, much like in Section 3.3, is to choose a super-operator \(\mathcal{G}_C\) or in such a way that equality can be attained in either Eq. (3.173) or Eq. (3.174).

The super-operator \(\mathcal{L}_\hat{\rho}\) that does the trick for minimizing Eq. (3.156) is defined by its action on an operator \(\hat{A}\) through
\[
\frac{1}{2}\left(\hat{\rho}\mathcal{L}_\hat{\rho}(\hat{A}) + \mathcal{L}_\hat{\rho}(\hat{A})\hat{\rho}\right) = \hat{A}. \tag{3.177} \]
This equation is a special case of the operator equation known as the Lyapunov equation \[78\]:
\[
\hat{B}\hat{X} + \hat{X}\hat{C} = \hat{D}. \tag{3.178} \]

The Lyapunov equation has a solution for all \(\hat{D}\) if and only if no eigenvalue of \(\hat{B}\) and no eigenvalue of \(\hat{C}\) sum to zero. Thus when \(\hat{\rho}\) has zero eigenvalues, \(\mathcal{L}_\hat{\rho}(\hat{A})\) is not well defined for a general operator \(\hat{A}\). For the case of interest here, however, where \(\hat{A} = \hat{\Delta}\), \(\mathcal{L}_\hat{\rho}(\hat{A})\) does exist regardless of whether \(\hat{\rho}\) has zero eigenvalues or not. This can be seen by constructing a solution.

Let \(|j\rangle\) be an orthonormal basis that diagonalizes \(\hat{\rho}\) and let \(\lambda_j\) be the associated eigenvalues. Note that if \(\lambda_j = 0\), then
\[
0 = \langle j|\hat{\rho}|j\rangle = (1 - t)\langle j|\hat{\rho}_0|j\rangle + t\langle j|\hat{\rho}_1|j\rangle. \tag{3.179} \]
Therefore, if \(0 < t < 1\), we must have that both \(\langle j|\hat{\rho}_0|j\rangle = 0\) and \(\langle j|\hat{\rho}_1|j\rangle = 0\). So if \(\lambda_j = 0\), then \(\hat{\rho}_0^{1/2}|j\rangle = 0\) and \(\hat{\rho}_1^{1/2}|j\rangle = 0\). In particular, sandwiching Eq. (3.177) between eigenvectors of \(\hat{\rho}\), we find that
\[
\frac{1}{2}(\lambda_j + \lambda_k)\mathcal{L}_\hat{\rho}(\hat{\Delta})_{jk} = \Delta_{jk}. \tag{3.180} \]
has a solution for $L_{\rho}(\hat{\Delta})_{jk} = \langle j|L_{\rho}(\hat{\Delta})|k\rangle$ because $\Delta_{jk} = \langle j|\hat{\Delta}|k\rangle$ vanishes whenever $\lambda_j + \lambda_k = 0$. With this $L_{\rho}(\hat{\Delta})$ becomes

$$L_{\rho}(\hat{\Delta}) \equiv \sum_{\{j,k|\lambda_j + \lambda_k \neq 0\}} \frac{2}{\lambda_j + \lambda_k} \Delta_{jk} |j\rangle \langle k| ,$$

(3.181)

where we have conveniently set the terms in the null subspace of $\hat{\rho}$ to be zero. (For further discussion of why Eq. (3.181) is the appropriate extension of $L_{\rho}(\hat{\Delta})$ to the zero-eigenvalue subspaces of $\hat{\rho}$, see Ref. [122]; note that $L_{\rho}$ is denoted there by $R_{\rho}^{-1}$.) Eq. (3.181) demonstrates that $L_{\rho}(\hat{\Delta})$ can be taken to be a Hermitian operator.

The super-operator $L_{\rho}$ is easily seen to satisfy the defining property of a “lowering” super-operator, Eq. (3.177), because, for Hermitian $\hat{A}$ and $\hat{B}$,

$$|\text{tr}(\hat{\rho}\hat{A}L_{\rho}(\hat{B}))| \geq \text{Re}[\text{tr}(\hat{\rho}\hat{A}L_{\rho}(\hat{B}))] = \frac{1}{2} \left[ \text{tr}(\hat{\rho}\hat{A}L_{\rho}(\hat{B})) + \text{tr}(\hat{\rho}\hat{A}L_{\rho}(\hat{B}))^* \right]$$

$$= \frac{1}{2} \left[ \text{tr}(\hat{\rho}\hat{A}L_{\rho}(\hat{B})) + \text{tr}(L_{\rho}(\hat{B})\hat{A}\hat{\rho}) \right]$$

$$= \text{tr}\left(\hat{A} \frac{1}{2} (L_{\rho}(\hat{B})\hat{\rho} + \hat{\rho}L_{\rho}(\hat{B})) \right)$$

$$= \text{tr}(\hat{A}\hat{B}) .$$

(3.182)

The desired optimization is via Eq. (3.175):

$$J''(t) \geq -\text{tr}(L_{\rho}(\hat{\Delta})\hat{\rho}L_{\rho}(\hat{\Delta}))$$

$$= -\text{tr}(\hat{\Delta}L_{\rho}(\hat{\Delta}))$$

$$= -\sum_{\{j,k|\lambda_j + \lambda_k \neq 0\}} \frac{2}{\lambda_j + \lambda_k} |\Delta_{jk}|^2 .$$

(3.183)

Equality can be satisfied in Eq. (3.183) if

$$\text{Im}[\text{tr}(\hat{\rho}\hat{E}_bL_{\rho}(\hat{\Delta}))] = 0 \text{ for all } b ,$$

(3.184)

and, from Eq. (3.173),

$$L_{\rho}(\hat{\Delta})\hat{E}_b^{1/2} = \mu_b \hat{E}_b^{1/2} \text{ for all } b .$$

(3.185)

The second of these can be met easily by choosing the operators $\hat{E}_b = \hat{E}_b^F = |b\rangle\langle b|$ to be projectors onto an eigenbasis for the Hermitian operator $L_{\rho}(\hat{\Delta})$ and choosing the constants $\mu_b$ to be the eigenvalues of $L_{\rho}(\hat{\Delta})$. The first condition then follows simply by Eq. (3.183) being satisfied. For

$$\text{tr}(\hat{\rho}\hat{E}_bL_{\rho}(\hat{\Delta})) = \text{tr}(\hat{\rho}\hat{E}_b^{1/2}\hat{E}_b^{1/2}L_{\rho}(\hat{\Delta}))$$

$$= \mu_b \text{tr}(\hat{\rho}\hat{E}_b) ,$$

(3.186)

which is clearly a real number.
The function $L''(t)$ can now be defined as

$$L''(t) = -\text{tr}\left(\hat{\Delta}L\rho(\hat{\Delta})\right).$$

This, as stated above, is exactly the function $L''(t)$ used by Holevo, but obtained there by other means. Again, among other things, what is new here is that the derivation above gives a way of associating a measurement with the function $L''(t)$. This measurement may be used to define a new lower bound to the accessible information $I(t)$; this bound we shall call $M(t)$.

The next step in the derivation of Eq. (3.149), to show that $S''(t) \leq L''(t)$; i.e., that

$$\sum_{\{j,k|\lambda_j + \lambda_k \neq 0\}} \frac{2}{\lambda_j + \lambda_k} |\Delta_{jk}|^2 \geq \sum_{\{j,k|\lambda_j + \lambda_k \neq 0\}} \Phi(\lambda_j, \lambda_k) |\Delta_{jk}|^2.$$  (3.188)

This can be accomplished by demonstrating the arithmetic inequality \[123, 124\]. We reiterate Holevo’s method of proof in particular. The case for $\Phi(x,x)$ is easy: equality is satisfied automatically. Suppose now that $x \neq y$ for $0 < x, y \leq 1$ and let

$$s = \frac{x - y}{x + y},$$

Then

$$x = \frac{1}{2}(x + y)(1 + s) \quad \text{and} \quad y = \frac{1}{2}(x + y)(1 - s),$$

and $0 < |s| < 1$. Hence

$$\ln x - \ln y = \ln(1 + s) - \ln(1 - s)$$

has a convergent Taylor series expansion about $s = 0$. In particular, one has

$$\frac{1}{2}(x + y) \Phi(x, y) = 1 + \sum_{n=1}^{\infty} \frac{1}{(2n + 1)} s^{2n}.$$  (3.193)

Since this expansion contains only even powers of $s$, it follows immediately that Eq. (3.189) holds, with equality if and only if $\hat{\rho}_0$ and $\hat{\rho}_1$ commute. The “if” side of the statement is trivial; one need only choose the $\hat{E}_k$ to be projectors onto a common basis diagonalizing both $\hat{\rho}_0$ and $\hat{\rho}_1$. Then one has immediately that

$$J(t) = I(t) = S(\hat{\rho}) - (1 - t)S(\hat{\rho}_0) - tS(\hat{\rho}_1).$$

(3.194)

For the noncommuting case, if we can show that $L(t)$ is strictly less than $S(t)$, then our work will be done.

We do this by showing that $L(t) = S(t)$ implies that $\hat{\rho}_0$ and $\hat{\rho}_1$ commute. Taking two derivatives of the supposition, we must have that $S''(t) = L''(t)$. Note, from Eq. (3.188) and the properties of $\Phi(x, y)$, that this holds if and only if

$$|\Delta_{jk}|^2 = 0 \quad \text{for all } k \neq j.$$  (3.195)

71
The latter condition implies that \( \hat{\rho}_0 \) and \( \hat{\rho}_1 \) commute. This is seen easily, for note that Eq. (3.195) implies

\[
0 = \sum_{k,j} (\lambda_j - \lambda_k)^2 |\Delta_{jk}|^2
\]

\[
= \sum_{k,j} (\lambda_j - \lambda_k)^2 \tr(\hat{\Pi}_k \hat{\Delta} \hat{\Pi}_j \hat{\Delta})
\]

\[
= \sum_{k,j} \tr(\hat{\Pi}_k (\hat{\rho} \hat{\Delta} - \hat{\Delta} \hat{\rho}) \hat{\Pi}_j (\hat{\Delta} \hat{\rho} - \hat{\rho} \hat{\Delta}))
\]

\[
= \tr((\hat{\Delta} \hat{\rho} - \hat{\rho} \hat{\Delta})^\dagger (\hat{\Delta} \hat{\rho} - \hat{\rho} \hat{\Delta})).
\]

(3.196)

This implies \( \hat{\Delta} \hat{\rho} - \hat{\rho} \hat{\Delta} = 0 \) and thus \([\rho_0, \rho_1] = 0\). This completes the proof.

### 3.5.2 The Lower Bound \( M(t) \)

Now we focus on deriving an explicit expression for the lower bound \( M(t) \) to the accessible information. This bound takes on a surprisingly simple form. Moreover, as we shall see for the two dimensional case, this lower bound can be quite close to the accessible information and sometimes actually equal to it.

For simplicity, let us suppose \( \hat{\rho}_0 \) and \( \hat{\rho}_1 \) are invertible. We start by rewriting, in the manner of Eq. (3.93), the mutual information as

\[
J(t) = \tr((1-t)\hat{\rho}_0 \sum_b (\ln \alpha_b) \hat{E}_b + t \hat{\rho}_1 \sum_b (\ln \beta_b) \hat{E}_b),
\]

(3.197)

where

\[
\alpha_b = \frac{\tr(\hat{\rho}_0 \hat{E}_b)}{\tr(\hat{\rho} \hat{E}_b)} \quad \text{and} \quad \beta_b = \frac{\tr(\hat{\rho}_1 \hat{E}_b)}{\tr(\hat{\rho} \hat{E}_b)}.
\]

(3.198)

The lower bound \( M(t) \) is defined by inserting the projectors \( \hat{E}_b^F \) onto a basis that diagonalizes \( \mathcal{L}_{\hat{\rho}}(\hat{\Delta}) \) into this formula. This expression simplifies because of a curious fact: even though \( \hat{\rho}_0 \) and \( \hat{\rho}_1 \) need not commute, \( \mathcal{L}_{\hat{\rho}}(\hat{\rho}_0) \) and \( \mathcal{L}_{\hat{\rho}}(\hat{\rho}_1) \) necessarily do commute. This follows from the linearity of the \( \mathcal{L}_{\hat{\rho}} \) super-operator:

\[
\mathcal{L}_{\hat{\rho}}(\hat{\rho}_0) = \mathcal{L}_{\hat{\rho}}(\hat{\rho} - t\hat{\Delta})
\]

\[
= \hat{1} - t\mathcal{L}_{\hat{\rho}}(\hat{\Delta}),
\]

(3.199)

and

\[
\mathcal{L}_{\hat{\rho}}(\hat{\rho}_1) = \mathcal{L}_{\hat{\rho}}(\hat{\rho} + (1-t)\hat{\Delta})
\]

\[
= \hat{1} + (1-t)\mathcal{L}_{\hat{\rho}}(\hat{\Delta}).
\]

(3.200)

Thus the projectors \( \hat{E}_b^F \) that diagonalize \( \mathcal{L}_{\hat{\rho}}(\hat{\Delta}) \) also clearly diagonalize both \( \mathcal{L}_{\hat{\rho}}(\hat{\rho}_0) \) and \( \mathcal{L}_{\hat{\rho}}(\hat{\rho}_1) \).

Therefore, if \( |b\rangle \) is such that \( \hat{E}_b^F = |b\rangle \langle b| \) and \( \alpha_{Fb} \) is the associated eigenvalue of \( \mathcal{L}_{\hat{\rho}}(\hat{\rho}_0) \), then the definition of \( \mathcal{L}_{\hat{\rho}}(\hat{\rho}_0) \), Eq. (3.177), requires that

\[
\alpha_{Fb} = \frac{\langle b| \hat{\rho}_0 |b\rangle}{\langle b| \hat{\rho} |b\rangle} = \frac{\tr(\hat{\rho}_0 \hat{E}_b^F)}{\tr(\hat{\rho} \hat{E}_b^F)}.
\]

(3.201)
Thus the operator $\mathcal{L}_\hat{\rho}(\hat{\rho}_0)$, much like the operator $\hat{M} = \hat{\rho}_1^{-1/2} \sqrt{\hat{\rho}_1^{1/2} \hat{\rho}_0 \hat{\rho}_1^{1/2} \hat{\rho}_1^{-1/2}}$, can be considered an operator analog to the classical likelihood ratio. Similarly, for the eigenvalues $\beta_{F_b}$ of $\mathcal{L}_\hat{\rho}(\hat{\rho}_1)$, we must have

$$\beta_{F_b} = \frac{\text{tr}(\hat{\rho}_1 \hat{E}_b^F)}{\text{tr}(\hat{\rho} \hat{E}_b^F)}.$$  \hfill (3.202)

Hence $M(t)$ takes the simple form

$$M(t) = \text{tr}\left( (1-t) \hat{\rho}_0 \ln(\mathcal{L}_\rho(\hat{\rho}_0)) + t \hat{\rho}_1 \ln(\mathcal{L}_\rho(\hat{\rho}_1)) \right).$$  \hfill (3.203)

As an aside, we note that one can also obtain by this method a lower bound to the quantum Kullback information (in the vein of Eq. (3.93)). Using the measurement basis that diagonalizes $\mathcal{L}_\hat{\rho}(\hat{\rho}_1)$ in the classical Kullback-Leibler relative information, we have, via the steps above, the expression

$$K_F(\hat{\rho}_0/\hat{\rho}_1) \equiv \text{tr}\left( \hat{\rho}_0 \ln(\mathcal{L}_\rho(\hat{\rho}_1)) \right),$$  \hfill (3.204)

whenever $\mathcal{L}_\hat{\rho}(\hat{\rho}_1)$ is well defined.

There is a close relation between the lowering super-operator discussed here and the optimal measurement operator $\hat{M}$ for statistical overlap found in Section 3.3. This can be seen by noting that for small $\epsilon$

$$\sqrt{\hat{A} + \epsilon \hat{B}} \approx \sqrt{\hat{A} + \frac{1}{2} \mathcal{L}_{\hat{A}^{1/2}}(\hat{B})},$$  \hfill (3.205)

when $\hat{A}$ is invertible (as can be seen by squaring the left and right hand sides), and for any operator $\hat{B}$ that commutes with $\hat{\rho}$,

$$\mathcal{L}_\rho(\hat{B} \hat{A} \hat{B}) = \hat{B} \mathcal{L}_\rho(\hat{A}) \hat{B}.$$  \hfill (3.206)

Then, when

$$\hat{\rho}_0 = \hat{\rho}_1 + \delta \hat{\rho},$$  \hfill (3.207)

so that the two density operators to be distinguished are close to each other,

$$\hat{M} = \hat{\rho}_1^{-1/2} \sqrt{\hat{\rho}_1^{1/2} (\hat{\rho}_1 + \delta \hat{\rho}) \hat{\rho}_1^{1/2} \hat{\rho}_1^{-1/2}} \approx 1 + \frac{1}{2} \mathcal{L}_{\hat{\rho}_1}(\delta \hat{\rho}).$$  \hfill (3.208)

Thus the measurement bases defined by $\hat{M}$ and $\mathcal{L}_{\hat{\rho}_1}(\hat{\rho}_1)$ in this limit can be taken to be the same.

Equations (3.204) and (3.93), it should be noted, are both distinct from that quantity usually considered the quantum analog to the Kullback-Leibler information in the literature [125, 126]. That quantity, given by

$$K_U(\hat{\rho}_0/\hat{\rho}_1) \equiv \text{tr}\left( \hat{\rho}_0 \ln \hat{\rho}_0 - \hat{\rho}_0 \ln \hat{\rho}_1 \right),$$  \hfill (3.209)

is not a lower bound to the maximum Kullback-Leibler information. In fact, the Holevo upper bound to the mutual information is easily seen to be expressible in terms of it:

$$I(t) \leq (1-t)K_U(\hat{\rho}_0/\hat{\rho}) + tK_U(\hat{\rho}_1/\hat{\rho}).$$  \hfill (3.210)
3.5.3 The Upper Bound $L(t)$

The upper bound $L(t)$ has not yet yielded a form as sleek as the one found for $M(t)$. All that need be done in principle, of course, is integrate Eq. (3.187) twice and apply the boundary conditions $L(0) = L(1) = 0$. The trouble lies in that, whereas general methods exist for differentiating operators with respect to parameters [127, 128, 129, 130, 131, 132], methods for the inverse problem of integration are nowhere to be found. The main problem here reduces to finding a tractable representation for $L_\hat{\rho}(\hat{\Delta})$. This has turned out to be a difficult matter in spite of the fact that Eq. (3.177) is a special case of the Lyapunov equation and has been studied widely in the mathematical literature.

Though there are convenient ways for finding numerical expressions for $L_\hat{\rho}(\hat{\Delta})$ [133] (even when the matrices involved are 1000-dimensional [134]), this is of no help to our integration problem. On the other hand, there do exist various methods for obtaining an exact expression for $L_\hat{\rho}(\hat{\Delta})$ in a basis that does not depend on $t$ [135, 136, 137, 138, 139]. These expressions can be integrated in principle. However the representations so found appear to have no compact form that makes obvious the algorithm for their calculation.

Two of the more useful representations for $L_\hat{\rho}(\hat{A})$ [140, 141] might appear to be, a contour integral representation (when $\hat{\rho}$ is invertible),

\[
L_\hat{\rho}(\hat{A}) = \frac{2}{2\pi i} \oint (z\hat{1} - \hat{\rho})^{-1} \hat{A}(z\hat{1} + \hat{\rho})^{-1} dz ,
\]

(3.211)

where the contour contains the pole at $z = \lambda_j$ for all eigenvalues $\lambda_j$ of $\hat{\rho}$, but does not contain the pole at $z = -\lambda_j$ for any $j$, and, more generally, a Riemann integral representation,

\[
L_\hat{\rho}(\hat{A}) = \int_0^\infty e^{-\hat{\rho}u/2} \hat{A} e^{-\hat{\rho}u/2} du .
\]

(3.212)

Both of these expressions can be checked easily enough by writing them out in a basis that diagonalizes $\hat{\rho}$.

However, these two representations really lead nowhere. Seemingly the best one can do with them is use them to derive a doubly infinite (to be explained momentarily) Fourier sine series expansion for $L(t)$:

\[
L(t) = \sum_{m=1}^\infty b_m \sin(m\pi t) .
\]

(3.213)

This unfortunately does not have the compelling conciseness of Eq. (3.203), but at least it does automatically satisfy the boundary conditions. Perhaps one can hope that only the first few terms in Eq. (3.213) are significant.

Luckily it turns out that there are better, somewhat nonstandard representations of $L_\hat{\rho}$ to work with. Nevertheless, before working toward a better representation, we go through the exercise of building the Fourier expansion to illustrate the difficulties encountered. The idea is to start off with a Taylor expansion for $L''(t)$ about $t = 0$ and then use that in finding the coefficients $b_m$—these being given by the standard Fourier algorithm,

\[
b_m = -\frac{2}{(m\pi)^2} \int_0^1 L''(t) \sin(m\pi t) dt .
\]

(3.214)

The Taylor series expansion for $L''(t)$ is

\[
L''(t) = -\sum_{n=0}^\infty \frac{t^n}{n!} \left[ \text{tr} \left( \hat{\Delta} \frac{d^n}{dt^n} L_\hat{\rho}(\hat{\Delta}) \right) \right]_{t=0} .
\]

(3.215)
Now using the operator-inverse differentiation formula Eq. (3.157) within the integral of Eq. (3.211), one finds the following. Differentiating once with respect to \( t \) generates one term of the form
\[
(z \hat{1} - \hat{\rho})^{-1} \hat{\Delta} (z \hat{1} - \hat{\rho})^{-1} \hat{\Delta} (z \hat{1} + \hat{\rho})^{-1} = \hat{\Delta}^{-1} \left[ \hat{\Delta} (z \hat{1} - \hat{\rho})^{-1} \right]^2 \left[ \hat{\Delta} (z \hat{1} + \hat{\rho})^{-1} \right] \tag{3.216}
\]
and one term of the form
\[
-(z \hat{1} - \hat{\rho})^{-1} \hat{\Delta} (z \hat{1} + \hat{\rho})^{-1} \hat{\Delta} (z \hat{1} + \hat{\rho})^{-1} = -\hat{\Delta}^{-1} \left[ \hat{\Delta} (z \hat{1} - \hat{\rho})^{-1} \right] \left[ \hat{\Delta} (z \hat{1} + \hat{\rho})^{-1} \right]^2 . \tag{3.217}
\]
Differentiating again generates two terms of the form
\[
\hat{\Delta}^{-1} \left[ \hat{\Delta} (z \hat{1} - \hat{\rho})^{-1} \right]^3 \left[ \hat{\Delta} (z \hat{1} + \hat{\rho})^{-1} \right] , \tag{3.218}
\]
two of the form
\[
-\hat{\Delta}^{-1} \left[ \hat{\Delta} (z \hat{1} - \hat{\rho})^{-1} \right]^2 \left[ \hat{\Delta} (z \hat{1} + \hat{\rho})^{-1} \right]^2 , \tag{3.219}
\]
and two of the form
\[
\hat{\Delta}^{-1} \left[ \hat{\Delta} (z \hat{1} - \hat{\rho})^{-1} \right] \left[ \hat{\Delta} (z \hat{1} + \hat{\rho})^{-1} \right]^3 . \tag{3.220}
\]
The pattern quickly becomes apparent; in general, one has:
\[
\hat{\Delta} \frac{d^n}{dt^n} L_{\hat{\rho}}(\hat{\Delta}) = 2(n!) \sum_{k=0}^n (-1)^k D_{\hat{\rho}}(n; k) , \tag{3.221}
\]
where
\[
D_{\hat{\rho}}(n; k) = \frac{1}{2\pi i} \oint \left[ \hat{\Delta} (z \hat{1} - \hat{\rho})^{-1} \right]^{n+1-k} \left[ \hat{\Delta} (z \hat{1} + \hat{\rho})^{-1} \right]^{k+1} dz . \tag{3.222}
\]
Putting Eqs. (3.214) through (3.222) together, one arrives at an expression for the expansion coefficients,
\[
b_m = \frac{2}{m^3 \pi^3} \sum_{n=0}^{\infty} (n!) \left[ b(n; m) - (-1)^m \sum_{j=0}^n \frac{1}{(n-j)!} b(j; m) \right] \sum_{k=0}^n (-1)^k \text{tr} \left( D_{\hat{\rho}}(n; k) \right) , \tag{3.223}
\]
where
\[
b(j; m) = (-1)^{j/2} [1 + (-1)^j (m\pi)^{-j} . \tag{3.224}
\]
The calculation of the terms \( \text{tr} \left( D_{\hat{\rho}}(n; k) \right) \) in this expansion is straightforward but tedious. Because each \( b_m \) itself can only be written in terms of an infinite series, the Fourier sine series here is dubbed a doubly infinite series.

**A Better Way**

It turns out that one integration of the operator \( L_{\hat{\rho}}(\hat{\Delta}) \) is enough to give an explicit expression for \( L(t) \) instead of the two integrations naively called for in the definition of \( L''(t) \):
\[
L(t) = -\text{tr} \left( \hat{\Delta} \int \int \int' \int'' L_{\hat{\rho}(t')}(\hat{\Delta}) dt'' dt' \right) + c_1 t + c_2 , \tag{3.225}
\]
where now we are making the integration variable in $\hat{\rho}(t)$ explicit. This reduction to one integration greatly simplifies things already, and we develop it now. The point can be seen from an integration by parts:

$$
\int_t^t \hat{\rho}(t') \mathcal{L}_{\hat{\rho}(t')}(\hat{\Delta}) \, dt' = \int_t^t \hat{\rho}(t') \left( \frac{d}{dt'} \int_t^t \mathcal{L}_{\hat{\rho}(t')}(\hat{\Delta}) \, dt'' \right) \, dt'
$$

$$
= \int_t^t \left\{ \frac{d}{dt'} \left( \hat{\rho}(t') \int_t^t \mathcal{L}_{\hat{\rho}(t')}(\hat{\Delta}) \, dt'' \right) - \hat{\Delta} \int_t^t \mathcal{L}_{\hat{\rho}(t')}(\hat{\Delta}) \, dt'' \right\} \, dt'
$$

$$
= \hat{\rho}(t) \int_t^t \mathcal{L}_{\hat{\rho}(t')}(\hat{\Delta}) \, dt' - \hat{\Delta} \int_t^t \int_t^t \mathcal{L}_{\hat{\rho}(t')}(\hat{\Delta}) \, dt'' \, dt'. \quad (3.226)
$$

Similarly

$$
\int_t^t \mathcal{L}_{\hat{\rho}(t')}(\hat{\Delta}) \hat{\rho}(t') \, dt' = \left( \int_t^t \mathcal{L}_{\hat{\rho}(t')}(\hat{\Delta}) \, dt' \right) \hat{\rho}(t) - \left( \int_t^t \int_t^t \mathcal{L}_{\hat{\rho}(t')}(\hat{\Delta}) \, dt'' \, dt' \right) \hat{\Delta}. \quad (3.227)
$$

Adding these expressions together and using the fact that

$$
\hat{\rho} \mathcal{L}_{\hat{\rho}}(\hat{\Delta}) + \mathcal{L}_{\hat{\rho}}(\hat{\Delta}) \hat{\rho} = 2 \hat{\Delta},
$$

we get,

$$
\int_t^t \int_t^t \frac{1}{2} \left( \hat{\Delta} \mathcal{L}_{\hat{\rho}(t')}(\hat{\Delta}) + \mathcal{L}_{\hat{\rho}(t')}(\hat{\Delta}) \hat{\Delta} \right) \, dt'' \, dt'
$$

$$
= \frac{1}{2} \left( \hat{\rho} \int_t^t \mathcal{L}_{\hat{\rho}(t')}(\hat{\Delta}) \, dt' \right) + \left( \int_t^t \mathcal{L}_{\hat{\rho}(t')}(\hat{\Delta}) \, dt' \right) \hat{\rho} - t\hat{\Delta} + \eta, \quad (3.228)
$$

where $\eta$ is a constant operator. Therefore, using the linearity and the cyclic property of the trace, we obtain

$$
L(t) = -\mathrm{tr} \left( \hat{\rho} \int_t^t \mathcal{L}_{\hat{\rho}(t')}(\hat{\Delta}) \, dt' \right) + c_1 t + c_2. \quad (3.230)
$$

**Kronecker Product Methods**

There is another way of looking at the equation defining $\mathcal{L}_{\hat{\rho}}(\hat{\Delta})$ [Eq. (3.177)] which leads to a way of calculating the operator

$$
\hat{H} = \int_t^t \mathcal{L}_{\hat{\rho}}(\hat{\Delta}) \, dt'. \quad (3.231)
$$

The resulting expression is not particularly elegant, but it does give an operational way of carrying out this integral.

The method is to think of Eq. (3.177) quite literally as a set of simultaneous linear equations, the solution of which defines the matrix elements of $\mathcal{L}_{\hat{\rho}}$. Once one realizes this, then there is some hope that Eq. (3.177) may be rearranged to be of a form more amenable to standard linear algebraic techniques. This can be accomplished by introducing the notion of *vec*’ing a matrix [142, 143, 132].
The operation of vec’ing a matrix is that of forming a vector by stacking all its columns on top each other. That is to say, if the elements of a matrix $A$ are given by $A_{ij}$, $1 \leq i, j \leq D$, i.e.,

$$A = \begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1D} \\ A_{21} & A_{22} & \cdots & A_{2D} \\ \vdots & \vdots & \ddots & \vdots \\ A_{D1} & A_{D2} & \cdots & A_{DD} \end{bmatrix}, \quad (3.232)$$

then the (column) vector associated with the vec operation on $A$ is given by

$$\text{vec}(A) = \begin{bmatrix} A_{11} \\ A_{21} \\ \vdots \\ A_{D1} \\ A_{12} \\ A_{22} \\ \vdots \\ A_{D2} \\ \vdots \\ A_{DD} \end{bmatrix}. \quad (3.233)$$

Note that the vec operation is not a simple mapping from operators to vectors because it is basis dependent.

We shall need two simple properties of the vec operation. The first, that it is linear, is obvious. The second is not obvious, but quite simple to derive [132, p. 255]: for any three matrices $A$, $B$, and $X$,

$$\text{vec}(AXB) = (B^T \otimes A)\text{vec}(X), \quad (3.234)$$

where $B^T$ denotes the transpose of $B$ and $\otimes$ denotes the Kronecker or direct product defined by

$$A \otimes B = \begin{bmatrix} A_{11}B & A_{12}B & \cdots & A_{1DB} \\ A_{21}B & A_{22}B & \cdots & A_{2DB} \\ \vdots & \vdots & \ddots & \vdots \\ A_{D1}B & A_{D2}B & \cdots & A_{DDB} \end{bmatrix}. \quad (3.235)$$

Choosing a particular representation for the operators in the Lyapunov equation Eq. (3.178) and letting $I$ be the identity matrix, we see that it can be rewritten as

$$BXI + IXC = D. \quad (3.236)$$

Using Eq. (3.234) on this, we have finally that it is equivalent to the system of linear equations given by

$$\left(I \otimes B + C^T \otimes I\right)\text{vec}(X) = \text{vec}(D). \quad (3.237)$$

A combination of matrices like on the left hand side of this is called the Kronecker sum of $B$ and $C^T$ and is denoted by $B \oplus C^T$. Therefore, using this notation, when $B \oplus C^T$ is invertible we have

$$\text{vec}(X) = \left(B \oplus C^T\right)^{-1}\text{vec}(D). \quad (3.238)$$

Let us now apply these facts and notations toward finding an explicit representation for the operator $\hat{H}$ in Eq. (3.231). We start by picking a particular basis $|j\rangle$, independent of $t$, in which to
express the operators $\hat{\rho}_0, \hat{\rho}_1, \hat{\Delta}, \mathcal{L}_\rho(\hat{\Delta})$, and $\hat{H}$. Let us denote the matrix representations of these by the same symbol but with the hat removed, except for $\mathcal{L}_\rho(\hat{\Delta})$ which we represent by a matrix $X$. Since all these matrices are Hermitian, we have that $\rho^\dagger = \rho^*$, etc., where the $*$ just means complex conjugation. (As an aside, note that for any Hermitian matrix $A$, the matrix $A^*$ is also Hermitian. Moreover, for any positive semidefinite matrix $B$, the matrix $B^*$ is positive semidefinite. This follows because any positive semidefinite matrix $B$ can be written in the form $B = UDU^\dagger$ for some diagonal matrix $D = D^*$ and some unitary matrix $U$. Therefore $B^* = (U^*)D(U^*)^\dagger$ is a positive semidefinite matrix because $U^*$ is a unitary matrix.) Then, for invertible $\hat{\rho}_0$ and $\hat{\rho}_1$, we have immediately that

$$\text{vec}(X) = 2 \left( \rho \oplus \rho^* \right)^{-1} \text{vec}(\Delta),$$

where the matrix $\rho \oplus \rho^*$ is positive definite. Finding the matrix $H$ simply corresponds to unvec’ing the vector

$$2 \left( \int t' \left( \rho \oplus \rho^* \right)^{-1} dt' \right) \text{vec}(\Delta).$$

(3.240)

Our problem thus reduces to evaluating the operator integral in Eq. (3.240). For this purpose, we rearrange the integrand as follows:

$$\left( \rho \oplus \rho^* \right)^{-1} = \left( \left( \rho_0 \oplus \rho_0^* \right) + t \left( \Delta \oplus \Delta^* \right) \right)^{-1} = \tilde{\rho}_0^{-1/2} \left( \tilde{I} + t \left( \tilde{\rho}_0^{-1/2} \tilde{\Delta} \tilde{\rho}_0^{-1/2} \right) \right)^{-1} \tilde{\rho}_0^{-1/2},$$

(3.241)

where

$$\tilde{\rho}_0 = \rho_0 \oplus \rho_0^* \quad \text{and} \quad \tilde{\Delta} = \Delta \oplus \Delta^*,$$

and $\tilde{I}$ is the appropriate sized identity matrix. If we suppose that $\tilde{\Delta}$ is invertible, Eq. (3.241) can be integrated immediately. This is because the matrices $\tilde{I}$ and $\tilde{\rho}_0^{-1/2} \tilde{\Delta} \tilde{\rho}_0^{-1/2}$ commute. Thus

$$\int t' \left( \tilde{I} + t' \left( \tilde{\rho}_0^{-1/2} \tilde{\Delta} \tilde{\rho}_0^{-1/2} \right) \right)^{-1} dt' = \left( \tilde{\rho}_0^{-1/2} \tilde{\Delta} \tilde{\rho}_0^{-1/2} \right)^{-1} \ln \left( \tilde{I} + t \left( \tilde{\rho}_0^{-1/2} \tilde{\Delta} \tilde{\rho}_0^{-1/2} \right) \right),$$

(3.243)

and so

$$\text{vec}(H) = 2 \tilde{\rho}_0^{-1/2} \left( \tilde{\rho}_0^{-1/2} \tilde{\Delta} \tilde{\rho}_0^{-1/2} \right)^{-1} \ln \left( \tilde{I} + t \left( \tilde{\rho}_0^{-1/2} \tilde{\Delta} \tilde{\rho}_0^{-1/2} \right) \right) \tilde{\rho}_0^{-1/2} \text{vec}(\Delta).$$

(3.244)

The logarithm in this is well defined because the operators in its argument are invertible [132, p. 474].

Eq. (3.244) contains the algorithm for calculating $\hat{H}$ in the given basis. This then may be used in conjunction with Eq. (3.239) to calculate $L(t)$. An interesting open question is whether there exists a basis in which to represent the operators $\hat{\rho}_0, \hat{\rho}_1$, etc., so that the matrix appearing in the logarithm above is diagonal. If so, this would greatly simplify the computation of $L(t)$.  

78
3.5.4 The Two-Dimensional Case

In this Subsection we consider the important special case of binary communication channels on two-dimensional Hilbert spaces. Here the new bounds are readily expressible in terms of elementary functions and, moreover, the optimal orthogonal projection-valued measurement can be found via a variational calculation (just as was possible with the statistical overlap). With this case, one can gain a feel for how tightly the new bounds delimit the true accessible information $I(t)$.

Let the signal states $\hat{\rho}_0$ and $\hat{\rho}_1$ again be represented by two vectors within the Bloch sphere, i.e.,

$$\hat{\rho}_0 = \frac{1}{2} \left( \mathbb{1} + \vec{a} \cdot \vec{\sigma} \right) \quad \text{and} \quad \hat{\rho}_1 = \frac{1}{2} \left( \mathbb{1} + \vec{b} \cdot \vec{\sigma} \right).$$

The total density matrix for the channel can then be written as

$$\hat{\rho} = \frac{1}{2} \left( \mathbb{1} + \vec{c} \cdot \vec{\sigma} \right),$$

where

$$\vec{c} = (1 - t) \vec{a} + t \vec{b}$$

$$= \vec{a} + t \vec{d}$$

$$= \vec{b} - (1 - t) \vec{d}$$

and

$$\vec{d} = \vec{b} - \vec{a}.$$  

(3.247)

For an orthogonal projection-valued measurement specified by the Bloch vector $\vec{n}/n$, the mutual information takes the form

$$J(t; \vec{n}) = (1 - t) \frac{1}{2n} \left[ (n + \vec{a} \cdot \vec{n}) \ln \left( \frac{n + \vec{a} \cdot \vec{n}}{n + \vec{c} \cdot \vec{n}} \right) + (n - \vec{a} \cdot \vec{n}) \ln \left( \frac{n - \vec{a} \cdot \vec{n}}{n - \vec{c} \cdot \vec{n}} \right) \right] + t \frac{1}{2n} \left[ (n + \vec{b} \cdot \vec{n}) \ln \left( \frac{n + \vec{b} \cdot \vec{n}}{n + \vec{c} \cdot \vec{n}} \right) + (n - \vec{b} \cdot \vec{n}) \ln \left( \frac{n - \vec{b} \cdot \vec{n}}{n - \vec{c} \cdot \vec{n}} \right) \right].$$

(3.250)

The optimal projector is found by varying expression (3.249) over all vectors $\vec{n}$. The resulting equation for the optimal $\vec{n}$ is

$$0 = (1 - t) \ln \left( \frac{n + \vec{c} \cdot \vec{n}}{n - \vec{c} \cdot \vec{n}} \right) \frac{\vec{a}_\perp}{(n + \vec{a} \cdot \vec{n})(n - \vec{a} \cdot \vec{n})} + t \ln \left( \frac{n + \vec{b} \cdot \vec{n}}{n - \vec{b} \cdot \vec{n}} \right) \frac{\vec{b}_\perp}{(n + \vec{b} \cdot \vec{n})(n - \vec{b} \cdot \vec{n})},$$

(3.252)

where

$$\vec{a}_\perp = \vec{a} - \left( \vec{a} \cdot \frac{\vec{n}}{n} \right) \frac{\vec{n}}{n}$$

and

$$\vec{b}_\perp = \vec{b} - \left( \vec{b} \cdot \frac{\vec{n}}{n} \right) \frac{\vec{n}}{n}.$$
are vectors perpendicular to $\vec{n}$. Equation (3.252) is unfortunately a transcendental equation and as such generally has no explicit solution. That is really no problem, however, for given any particular $\vec{a}$, $\vec{b}$, and $t$, a numerical solution for $\vec{n}$ can easily be computed. Nevertheless, it is of some interest to classify the cases in which one can actually write out an explicit solution to Eq. (3.252). There are four nontrivial situations where this is possible:

1. a classical channel, where $\hat{\rho}_0$ and $\hat{\rho}_1$ commute (i.e., $\vec{a}$ and $\vec{b}$ are parallel),
2. $\hat{\rho}_0$ and $\hat{\rho}_1$ are both pure states (i.e., $a = b = 1$),
3. $a = b$ and $t = \frac{1}{2}$, and
4. $t$ is explicitly determined by $\hat{\rho}_0$ and $\hat{\rho}_1$ according to

$$t = \left(1 + \sqrt{\frac{1 - b^2}{1 - a^2}}\right)^{-1}.$$  (3.255)

In case (1), taking $\vec{n}/n$ parallel to $\vec{a}$ and $\vec{b}$ causes $\vec{a}_\perp$ and $\vec{b}_\perp$ to vanish. When conditions (2)–(4) are fulfilled, Eq. (3.252) can be solved by requiring that the arguments of the logarithms be multiplicative inverses, i.e.,

$$\frac{(n + \vec{c} \cdot \vec{n})}{(n - \vec{c} \cdot \vec{n})} = \frac{(n + a \cdot \vec{n})}{(n - a \cdot \vec{n})},$$  (3.256)

and choosing $\vec{n}$ such that

$$(1 - t)\vec{a}_\perp = t\vec{b}_\perp.$$  (3.257)

Cases (2) and (3), reported previously by Levitin [109], are limits of case (4).

The condition of Eq. (3.257) in the exactly solvable cases (2)–(4) is equivalent to the requirement that

$$\vec{n} = t\vec{b} - (1 - t)\vec{a}.$$  (3.258)

This is of significance because, for arbitrary $t$, the measurement that minimizes the probability of error measure of distinguishability studied in Section 3.2 is just the measurement specified by Eq. (3.258) [70, 27]. Thus, in the cases where the optimal information gathering measurement can be written explicitly, it coincides with the optimal error probability measurement. Now, simply rewriting $t$ and $1 - t$ in terms of the vectors $\vec{a}$, $\vec{b}$, and $\vec{c}$, the vector (3.258) becomes,

$$\vec{n} = \frac{\vec{a} \cdot (\vec{a} - \vec{c})}{\vec{a} \cdot (\vec{a} - \vec{b})} \vec{b} - \frac{\vec{b} \cdot (\vec{b} - \vec{c})}{\vec{b} \cdot (\vec{b} - \vec{a})} \vec{a}.$$  (3.259)

In cases (1)–(3) this can be seen to reduce to

$$\vec{n}_0 = (1 - \vec{a} \cdot \vec{c}) \vec{b} - (1 - \vec{b} \cdot \vec{c}) \vec{a}$$

$$= \vec{a} + \vec{c} \times (\vec{c} \times \vec{a}).$$  (3.260)

(It should be kept in mind that in going from Eqs. (3.258) to (3.259) to (3.260) the length of $\vec{n}$ has been allowed to vary.)
Case (2), and consequently the orthogonal projection-valued measurement set by Eq. (3.260), is of particular interest in communication theory. This is because two pure states in any Hilbert space span only a two-dimensional subspace of that Hilbert space. Hence Eq. (3.260) remains valid as the optimal orthogonal projection-valued measurement for a pure-state binary channel in a Hilbert space of any dimension. Moreover, Levitin [110] has shown that in this case the optimal orthogonal projection-valued measurement is indeed the actual optimal measurement.

Let us write out this case in more standard notation. Suppose $\hat{\rho}_0 = \vert \psi_0 \rangle \langle \psi_0 \vert$ and $\hat{\rho}_1 = \vert \psi_1 \rangle \langle \psi_1 \vert$ and let

$$q \equiv \vert \langle \psi_0 \vert \psi_1 \rangle \vert^2 = \text{tr}(\hat{\rho}_0 \hat{\rho}_1) = \frac{1}{2} \left( 1 + \vec{a} \cdot \vec{b} \right).$$

(3.261)

Then, because $a = b = 1$ here, the optimal measurement given by Eq. (3.258) has norm

$$n = \sqrt{1 - 4t(1 - t)q}.$$  

(3.262)

Using this and some algebra, the expression for the accessible information $I(t)$ reduces to

$$I(t) = \frac{1}{2n} \left\{ (1 - t) \left[ (n + 1 - 2tq) \ln \left( \frac{1 + n}{2(1 - t)} \right) + (n - 1 + 2tq) \ln \left( \frac{1 - n}{2(1 - t)} \right) \right] 
+ t \left[ (n + 1 - 2(1 - t)q) \ln \left( \frac{1 + n}{2t} \right) + (n - 1 + 2(1 - t)q) \ln \left( \frac{1 - n}{2t} \right) \right] \right\}$$

(3.263)

This confirms Levitin’s expression in Ref. [109] though this version is significantly more compact.

With this much known about the exact solutions, let us return to the question of how well the bounds $M(t)$, $L(t)$, etc., fare in comparison. For a measurement specified by the Bloch vector $\vec{n}/n$, the second derivative of the mutual information takes the form

$$J''(t) = -\frac{(\vec{d} \cdot \vec{n})^2}{n^2 - (\vec{c} \cdot \vec{n})^2}.$$  

(3.264)

The vector $\vec{n}$ that minimizes this is again given easily enough by a variational calculation: the equation specifying the nontrivial solution is

$$\left( n^2 - (\vec{c} \cdot \vec{a})^2 \right) \vec{a} - (\vec{d} \cdot \vec{n}) \left( \vec{n} - (\vec{d} \cdot \vec{n}) \vec{c} \right) = 0.$$  

(3.265)

After a bit of algebra one finds its solution to be given by none other than

$$\vec{n}_0 = \left( 1 - \vec{a} \cdot \vec{c} \right) \vec{b} - \left( 1 - \vec{b} \cdot \vec{c} \right) \vec{a},$$  

(3.266)

the vector given by Eq. (3.260): this time, however, the expression is valid for all $\vec{a}$, $\vec{b}$, and $t$. Inserting this vector into expressions (3.250) and (3.251) produces the lower bound $M(t)$,

$$M(t) = (1 - t) K(\hat{\rho}_0/\hat{\rho}; \vec{n}_0) + t K(\hat{\rho}_1/\hat{\rho}; \vec{n}_0).$$  

(3.267)
The upper bound $L(t)$ is found by integrating $J''(t)$ back up but with this particular measurement in place; that is to say, by integrating

$$L''(t) = -\left(d^2 + \frac{1}{1-c^2} (\vec{c} \cdot \vec{d})^2\right). \quad (3.268)$$

The result, upon requiring the boundary conditions $L(0) = L(1) = 0$, is

$$L(t) = \frac{\delta}{2d^2} \left(-\left(\delta - \vec{c} \cdot \vec{d}\right) \ln\left(\delta - \vec{c} \cdot \vec{d}\right) - \left(\delta + \vec{c} \cdot \vec{d}\right) \ln\left(\delta + \vec{c} \cdot \vec{d}\right) + \beta_1 t + \beta_2\right), \quad (3.269)$$

where

$$\beta_2 = \left(\delta - \vec{a} \cdot \vec{d}\right) \ln\left(\delta - \vec{a} \cdot \vec{d}\right) + \left(\delta + \vec{a} \cdot \vec{d}\right) \ln\left(\delta + \vec{a} \cdot \vec{d}\right), \quad (3.270)$$

and

$$\beta_1 = \left(\delta - \vec{b} \cdot \vec{d}\right) \ln\left(\delta - \vec{b} \cdot \vec{d}\right) + \left(\delta + \vec{b} \cdot \vec{d}\right) \ln\left(\delta + \vec{b} \cdot \vec{d}\right) - \beta_2, \quad (3.271)$$

and

$$\delta = \sqrt{\left(1 - \vec{a} \cdot \vec{b}\right)^2 - (1 - a^2)(1 - b^2)}$$

$$\delta = \sqrt{d^2 - \left|\vec{c} \times \vec{d}\right|^2}$$

$$= \sqrt{d^2 - \left|\vec{a} \times \vec{b}\right|^2}. \quad (3.272)$$

In contrast, the Jozsa-Robb-Wootters lower bound and the Holevo upper bound are given by Eqs. (3.151) and (3.149), respectively, where in Bloch vector representation

$$Q(\hat{\rho}) = \frac{1}{4c} \left((1-c)^2 \ln\left(\frac{1-c}{2}\right) - (1+c)^2 \ln\left(\frac{1+c}{2}\right)\right), \quad (3.273)$$

and

$$S(\hat{\rho}) = -\frac{1}{2}(1-c) \ln\left(\frac{1-c}{2}\right) - \frac{1}{2}(1+c) \ln\left(\frac{1+c}{2}\right), \quad (3.274)$$

and similarly for $Q(\hat{\rho}_0)$, $S(\hat{\rho}_0)$, etc. The extent to which the bounds $M(t)$ and $L(t)$ are tighter than the bounds $Q(t)$ and $S(t)$ and the degree to which they conform to the exact numerical answer $I(t)$ is illustrated by a typical example in Fig. 3.2.

### 3.5.5 Other Bounds

#### Another Bound from the Schwarz Inequality

Because of the difficulties in constructing a concise expression for $L(t)$, it is worthwhile to look at another upper bound to $I(t)$ derived from the Schwarz inequality. This is a bound derived from the second usage of lowering operators $G_{\hat{\rho}}$, i.e., that in Eq. (3.176), but with $L_{\hat{\rho}}$ in particular. We can immediately write

$$J''(t) \geq -\text{tr}\left(L_{\hat{\rho}} (\hat{\Delta})^2\right) = N''(t), \quad (3.275)$$

since $L_{\hat{\rho}} (\hat{\Delta})$ is Hermitian and guaranteed to exist for the same reason $L_{\hat{\rho}}(\hat{\Delta})$ does. The right hand side of this, when integrated twice and required to meet the boundary conditions

$$N(0) = N(1) = 1, \quad (3.276)$$

82
Figure 3.2: The Holevo upper bound $S(t)$, the upper bound $L(t)$, the information $I(t)$ extractable by optimal orthogonal projection-valued measurement (found numerically), the lower bound $M(t)$, and the Jozsa-Robb-Wootters lower bound $Q(t)$, all for the case that $\hat{\rho}_0$ is pure ($a = 1$), $\hat{\rho}_1$ is mixed with $b = 2/3$, and the angle between the two Bloch vectors is $\pi/3$.  

83
gives a new upper bound $N(t)$.

Since the bound derived from Eq. (3.275) is necessarily worse than $L(t)$, this would be of little interest if it were not for the following fact. Consider any positive operator $\hat{X}$ that depends on a parameter $t$. Then

$$
\frac{d\hat{X}}{dt} = \frac{d}{dt} \left( \sqrt{\hat{X}} \sqrt{\hat{X}} \right) = \sqrt{\hat{X}} \frac{d\sqrt{\hat{X}}}{dt} + \frac{d\sqrt{\hat{X}}}{dt} \sqrt{\hat{X}}.
$$

(3.277)

Thus,

$$
\frac{d\sqrt{\hat{X}}}{dt} = 2 L^{X^{1/2}} \left( \frac{d\hat{X}}{dt} \right),
$$

(3.278)

and specifically,

$$
N''(t) = -\frac{1}{4} \text{tr} \left[ \left( \frac{d\sqrt{\hat{\rho}}}{dt} \right)^2 \right].
$$

(3.279)

The simplicity of this expression would apparently give hope that there may be some way of integrating it explicitly.

The reason it would be useful to find $N(t)$ is that, though it cannot be as tight as the $L(t)$ bound, it still beats the Holevo bound $S(t)$. This can be seen as follows. In a basis $|j\rangle$ diagonalizing $\hat{\rho}$,

$$
N''(t) = -\sum_{\{j,k\mid \lambda_j + \lambda_k \neq 0\}} \left( \frac{2}{\lambda_j + \lambda_k} \right)^2 |\Delta_{jk}|^2.
$$

(3.280)

Now, as in the proof of the Holevo bound, $S(t) \geq N(t)$ requires that

$$
\Phi(x, y) \geq \left( \frac{2}{\sqrt{x} + \sqrt{y}} \right)^2.
$$

(3.281)

This can be shown very simply. The case for $\Phi(x, x)$ is again automatic. Suppose $0 < x, y \leq 1$ and $x \neq y$. We already know that $\Phi(x, y) \geq 2/(x + y)$. Consequently,

$$
\Phi(\sqrt{x}, \sqrt{y}) \geq \frac{2}{\sqrt{x} + \sqrt{y}}.
$$

(3.282)

But that is to say,

$$
\frac{1}{2}(\ln x - \ln y) \geq \frac{2}{\sqrt{x} + \sqrt{y}}.
$$

(3.283)

Multiplying both sides of this by $2/(\sqrt{x} + \sqrt{y})$ gives the desired result.

Unfortunately, despite the seeming simplicity of Eq. (3.279), little progress has been made toward its general integration. This in itself may be an indication that the simplicity is only apparent. This can be seen with the example of $2 \times 2$ density operators. Let us report enough of these results to make this point convincing.

The operator $\sqrt{\hat{\rho}}$ can represented with the help of the unit operator and the Pauli matrices as

$$
\sqrt{\hat{\rho}} = r_0 \mathbf{1} + \vec{r} \cdot \vec{\sigma},
$$

(3.284)
where the requirement that $\sqrt{\hat{\rho}}$ squares to give the representation of $\hat{\rho}$ in Eq. (3.240) forces
\[ r_0^2 + r^2 = \frac{1}{2} \quad (3.285) \]
and
\[ 2r_0 \vec{r} = \frac{1}{2} \vec{c} \quad (3.286) \]
These two requirements go together to give a quartic equation specifying $r_0$. Since $\sqrt{\hat{\rho}}$ must be a positive operator, its eigenvalues $r_0 + r$ and $r_0 - r$ must both be positive. Hence, picking the largest value of $r_0$ consistent with the quartic equation, we find
\[ r_0 = \frac{1}{2} \left( 1 + \sqrt{1 - c^2} \right)^{1/2} \quad (3.287) \]
and
\[ \vec{r} = \frac{1}{4r_0} \vec{c} \quad (3.288) \]
Taking the derivative of these quantities with respect to $t$, we find that
\[ N''(t) = -\frac{1}{2} \left( \left( r_0' \right)^2 + \vec{r}' \cdot \vec{r}' \right) \quad (3.289) \]
which reduces after quite some algebra to
\[ N''(t) = -\frac{1}{32r_0^2} \left( \frac{\vec{d} \cdot \vec{c}}{1 - c^2} \left( 1 - \frac{1}{8r_0^2} \right) + d^2 \right) \quad (3.290) \]
and really cannot be reduced any further. Clearly this is a considerable mess as a function of $t$, and the actual expression for $N(t)$ is far worse.

**A Bound Based on Jensen’s Inequality**

Still another upper bound to the accessible information can be built from the technique developed to find the function $L''(t)$. This bound makes crucial use of the concavity of the logarithm function.

For simplicity, let us suppose that both $\hat{\rho}_0$ and $\hat{\rho}_1$ are invertible. Recall the representation, given by Eq. (3.144), of the mutual information as the average of two Kullback-Leibler relative informations. For each of these terms, we have two different bounds that come Jensen’s inequality [97], i.e., for any probability distribution $q(b)$,
\[ \sum_b q(b) \ln x_b \leq \ln \left( \sum_b q(b)x_b \right) \quad (3.291) \]
The first bound is that
\[ K(p_i/p) = \sum_b p_i(b) \ln \left( \frac{p_i(b)}{p(b)} \right) \leq \ln \left( \sum_b p_i(b)^2 \right) \quad (3.292) \]
85
The second is that
\[
K(p_i/p) = - \sum_b p_i(b) \ln \left( \frac{p(b)}{p_i(b)} \right)
\]
\[
= -2 \sum_b p_i(b) \ln \left( \frac{p(b)}{p_i(b)} \right)^{1/2}
\]
\[
\geq -2 \ln \left( \sum_b \sqrt{p_i(b)p(b)} \right)
\]  \[(3.293)\]

Therefore, it follows that the quantum Kullback information \( K(\hat{\rho}_i/\hat{\rho}) \) is bounded by
\[
-2 \ln \left( \min_{E_b} \sum_b \sqrt{\text{tr}(\hat{\rho}_i E_b) \text{tr}(\hat{\rho} E_b)} \right) \leq K(\hat{\rho}_i/\hat{\rho}) \leq \ln \left( \max_{E_b} \sum_b \left( \frac{\text{tr}(\hat{\rho}_i E_b)}{\text{tr}(\hat{\rho} E_b)} \right)^2 \right) .
\]  \[(3.294)\]

These bounds can be evaluated explicitly by the techniques of Sections \ref{sec:3.3} and \ref{sec:3.5.1}. Namely, we have
\[
-2 \ln \left( \min_{E_b} \sum_b \sqrt{\text{tr}(\hat{\rho}_i E_b) \text{tr}(\hat{\rho} E_b)} \right) \leq K(\hat{\rho}_i/\hat{\rho}) \leq \ln \left( \max_{E_b} \sum_b \left( \frac{\text{tr}(\hat{\rho}_i E_b)}{\text{tr}(\hat{\rho} E_b)} \right)^2 \right) .
\]  \[(3.295)\]

(The upper bound is assured to exist in the form stated because \( \mathcal{L}_\rho(\hat{\rho}_i) \) is itself well defined; this follows because the \( \hat{\rho}_i \) are assumed invertible.)

One of these bounds may be used to upper bound the accessible information. In particular, since the maximum of a sum is less than or equal to the sum of the maxima, it follows that
\[
I(t) \leq (1 - t) \ln \left( \text{tr}(\hat{\rho}_0 \mathcal{L}_\rho(\hat{\rho}_0)) \right) + t \ln \left( \text{tr}(\hat{\rho}_1 \mathcal{L}_\rho(\hat{\rho}_1)) \right) \equiv R(t).
\]  \[(3.296)\]

To see how the bound \( R(t) \) looks for 2-dimensional density operators, note that in this case \( \mathcal{L}_\rho(\hat{\rho}_0) \) can be written in terms of Bloch vectors as \[144\]
\[
\mathcal{L}_\rho(\hat{\rho}_0) = S_0 \mathbf{1} + \vec{R}_0 \cdot \vec{\sigma},
\]  \[(3.297)\]
where
\[
S_0 = \frac{1}{1 - c^2} \left( 1 - \vec{a} \cdot \vec{c} \right),
\]  \[(3.298)\]
and
\[
\vec{R}_0 = \vec{a} - S_0 \vec{c}.
\]  \[(3.299)\]
A similar representation holds for \( \mathcal{L}_\rho(\hat{\rho}_1) \); one need only substitute \( \vec{b} \) for \( \vec{a} \) above. Then, we get
\[
\text{tr}(\hat{\rho}_0 \mathcal{L}_\rho(\hat{\rho}_0)) = S_0 + \vec{a} \cdot \vec{R}_0
\]
\[
= \frac{1}{1 - c^2} \left( 1 - \vec{a} \cdot \vec{c} \right)^2 + a^2 ,
\]  \[(3.300)\]
and similarly
\[
\text{tr}(\hat{\rho}_1 \mathcal{L}_\rho(\hat{\rho}_1)) = \frac{1}{1 - c^2} \left( 1 - \vec{b} \cdot \vec{c} \right)^2 + b^2 .
\]  \[(3.301)\]
Substituting these into Eq. \ref{eq:3.296} gives the desired result.
A Bound Based on Purifications

Imagine that states $\hat{\rho}_0$ and $\hat{\rho}_1$ come from a partial trace over some subsystem of a larger Hilbert space prepared in either a pure state $|\tilde{\psi}_0\rangle$ or $|\tilde{\psi}_1\rangle$. That is to say, let $|\tilde{\psi}_0\rangle$ and $|\tilde{\psi}_1\rangle$ be purifications of $\hat{\rho}_0$ and $\hat{\rho}_1$, respectively. Then any measurement POVM $\{\hat{E}_b\}$ on the original Hilbert space can be thought of as a measurement POVM $\{\hat{E}_b \otimes \hat{1}\}$ on the larger Hilbert space that ignores the extra subsystem. In particular, we will have that the measurement outcome statistics can be rewritten as

$$\text{tr}(\rho_s \hat{E}_b) = \text{tr}\left(|\tilde{\psi}_s\rangle\langle\tilde{\psi}_s| \left(\hat{E}_b \otimes \hat{1}\right)\right),$$

for $s = 0, 1$. (The trace on the left side of this equation is taken over only the original Hilbert space; the trace on the right side is taken over the larger Hilbert space in which the purifications live.) Similarly, we have for the average density operator $\hat{\rho}$ that

$$\text{tr}(\rho \hat{E}_b) = \text{tr}\left(\hat{\rho}^{AB} \left(\hat{E}_b \otimes \hat{1}\right)\right),$$

where

$$\hat{\rho}^{AB} = (1 - t) |\tilde{\psi}_0\rangle\langle\tilde{\psi}_0| + t |\tilde{\psi}_1\rangle\langle\tilde{\psi}_1|$$

is the average density operator of the purifications.

Let us now denote the mutual information for the ensemble consisting of $\hat{\rho}_0$ and $\hat{\rho}_1$ with respect to the measurement $\{\hat{E}_b\}$ by

$$J(\hat{\rho}_0, \hat{\rho}_1; \{\hat{E}_b\}).$$

It follows then that

$$I(\hat{\rho}_0 | \hat{\rho}_1) = \max_{\{\hat{E}_b\}} J(\hat{\rho}_0, \hat{\rho}_1; \{\hat{E}_b\})$$

$$= \max_{\{\hat{E}_b\}} J\left(|\tilde{\psi}_0\rangle, |\tilde{\psi}_1\rangle; \{\hat{E}_b \otimes \hat{1}\}\right)$$

$$\leq \max_{\{\hat{F}_c\}} J\left(|\tilde{\psi}_0\rangle, |\tilde{\psi}_1\rangle; \{\hat{F}_c\}\right)$$

$$= I\left(|\tilde{\psi}_0\rangle | \tilde{\psi}_1\rangle\right).$$

That is to say, the accessible information of the original ensemble of states must be less than or equal to the accessible information of the ensemble of purifications.

This is of great interest because we already know how to calculate the accessible information for two pure states. It is given by Eq. (3.263) with

$$q = \left|\langle \tilde{\psi}_0 | \tilde{\psi}_1 \rangle\right|^2.$$

This observation immediately gives an infinite number of new upper bounds to the accessible information—one for each possible set of purifications. The one of most interest, of course, is the smallest upper bound in this class.

Clearly then, the larger the overlap between the purifications $|\tilde{\psi}_0\rangle$ and $|\tilde{\psi}_1\rangle$, the tighter the bound will be. For the larger the overlap, the less the distinguishability that will have been added to the purifications above and beyond that of the original states. We need only recall from Section 3.3 that the largest possible overlap between purifications is given by

$$q = \left|\langle \tilde{\psi}_0 | \tilde{\psi}_1 \rangle\right|^2 = \left(\text{tr}\sqrt{\hat{\rho}_1^{1/2} \hat{\rho}_0 \hat{\rho}_1^{1/2}}\right)^2.$$

87
Use of this $q$ in Eq. (3.263) gives the best upper bound based on purifications. This bound we shall denote by $P(t)$. When $\hat{\rho}_0$ and $\hat{\rho}_1$ are both very close to being pure states, this bound can be very tight.

### 3.5.6 Photo Gallery

In the following pages, several plots compare the bounds on accessible information derived in the previous sections. The plots were generated by Mathematica™ with the following code.

```mathematica
(* Initial Notation *)
av = aa { 1, 0, 0 }
bv = bb { Cos[theta], Sin[theta], 0 }
dv = bv - av
cv = av + t*dv
a = Sqrt[av.av]
b = Sqrt[bv.bv]
c = Sqrt[cv.cv]
d = Sqrt[dv.dv]

(* ********************************************************* *)
(* Holevo Upper Bound *)
SC = -( (1-c)*Log[(1-c)/2] + (1+c)*Log[(1+c)/2] )/2
SB = -( (1-b)*Log[(1-b)/2] + (1+b)*Log[(1+b)/2] )/2
SA = -( (1-a)*Log[(1-a)/2] + (1+a)*Log[(1+a)/2] )/2
SS = SC - (1-t)*SA - t*SB

(* ********************************************************* *)
(* Jozsa-Robb-Wootters Lower Bound *)
QC = ( ((1-c)^2)*Log[(1-c)/2] - ((1+c)^2)*Log[(1+c)/2] )/(4*c)
QB = ( ((1-b)^2)*Log[(1-b)/2] - ((1+b)^2)*Log[(1+b)/2] )/(4*b)
QA = ( ((1-a)^2)*Log[(1-a)/2] - ((1+a)^2)*Log[(1+a)/2] )/(4*a)
QQ = QC - (1-t)*QA - t*QB

(* ********************************************************* *)
(* Lower Bound M(t) *)
mv = (1 - av.cv)*bv - (1 - bv.cv)*av
m = Sqrt[mv.mv]
MA = ( (m + av.mv)*Log[(m + av.mv)/(m + cv.mv)] +
     (m - av.mv)*Log[(m - av.mv)/(m - cv.mv)] )/(2*m)
MB = ( (m + bv.mv)*Log[(m + bv.mv)/(m + cv.mv)] +
     (m - bv.mv)*Log[(m - bv.mv)/(m - cv.mv)] )/(2*m)
MM = (1-t)*MA + t*MB

(* ********************************************************* *)
(* Upper Bound L(t) *)
Ld = Sqrt[ (1 - av.bv)^2 - (1 - a^2)*(1 - b^2) ]
LA = (Ld - av.dv)*Log[Ld - av.dv] + (Ld + av.dv)*Log[Ld + av.dv]
LL = ( Ld/(2*d^2) )* ( LC + t*LB + LA )

(* ********************************************************* *)
```

88
\[(*) \text{Upper Bound } R(t) \text{ Based On Jensen's Inequality *)}\]

\[
RA = a^2 + \frac{(1 - av.cv)^2}{(1 - c^2)} \\
RB = b^2 + \frac{(1 - bv.cv)^2}{(1 - c^2)} \\
RR = (1-t)\log[RA] + t\log[RB] 
\]

\[(* \quad \text{*********************************************************************** *)}\]

\[(*) \text{Upper Bound } P(t) \text{ Based On Purifications *)}\]

\[
qq = \frac{(1 + av.bv + \sqrt{1-a^2}\sqrt{1-b^2})}{2} \\
p = \sqrt{1 - 4*t*(1-t)*qq} \\
PA = (p + 1 - 2*t*qq)\log\left(\frac{1 + p}{2*(1-t)}\right) + (p - 1 + 2*t*qq)\log\left(\frac{1 - p}{2*(1-t)}\right) \\
PB = (p + 1 - 2*(1-t)*qq)\log\left(\frac{1 + p}{2*t}\right) + (p - 1 + 2*(1-t)*qq)\log\left(\frac{1 - p}{2*t}\right) \\
PP = \frac{( (1-t)*PA + t*PB )}{2*p} 
\]

### 3.6 The Quantum Kullback Information

The \textit{quantum Kullback information} for a density operator \( \hat{\rho}_0 \) relative to density operator \( \hat{\rho}_1 \) is defined to be

\[
K(\hat{\rho}_0/\hat{\rho}_1) \equiv \max_{\{E_b\}} \sum_b \text{tr}(\hat{\rho}_0\hat{E}_b) \ln\left(\frac{\text{tr}(\hat{\rho}_0\hat{E}_b)}{\text{tr}(\hat{\rho}_1\hat{E}_b)}\right), \tag{3.309}
\]

where the maximization is taken over all POVMs \( \{\hat{E}_b\} \). This quantity is significant because it details a notion of distinguishability for quantum states most notably in the following way. (For other interpretations of the Kullback-Leibler relative information, see Chapter 2.)

Suppose \( N \gg 1 \) copies of a quantum system are prepared identically to be in state \( \hat{\rho}_1 \). If a POVM \( \{\hat{E}_b : b = 1, \ldots, n\} \) is measured on each of these, the most likely frequencies for the various outcomes \( b \) will be those given by the probability estimates \( p_1(b) = \text{tr}(\hat{\rho}_1\hat{E}_b) \) themselves. All other frequencies beside this “natural” set will become less and less likely for large \( N \) as statistical fluctuations in the frequencies eventually damp away. In fact, any set of outcome frequencies \( \{f(b)\} \)—distinct from the “natural” ones \( \{p_1(b)\} \)—will become exponentially less likely with the number of measurements according to

\[
e^{-NK(f/p_1) - n\ln(N+1)} \leq \text{PROB}\left(\text{freq} = \{f(b)\} \left| \text{prob} = \{p_1(b)\}\right.\right) \leq e^{-NK(f/p_1)}, \tag{3.310}
\]

where

\[
K(f/p_1) = \sum_{b=1}^{n} f(b) \ln\left(\frac{f(b)}{p_1(b)}\right) \tag{3.311}
\]

is the Kullback-Leibler relative information \([\text{II}]\) between the distributions \( f(b) \) and \( p_1(b) \). Therefore the quantity \( K(f/p_1) \), which controls the leading behavior of this exponential decline, says something about how dissimilar the frequencies \( \{f(b)\} \) are from the “natural” ones \( \{p_1(b)\} \).

Now suppose instead that the measurements are performed on quantum systems identically prepared in the state \( \hat{\rho}_0 \). The outcome frequencies most likely to appear in this scenario are those specified by the distribution \( p_0(b) = \text{tr}(\hat{\rho}_0\hat{E}_b) \). Therefore the particular POVM \( \hat{E}_b^0 \) satisfying Eq. (3.309) has the following interpretation. It is the measurement for which the natural frequencies of outcomes for state \( \hat{\rho}_0 \) are maximally distinct from those for measurements on \( \hat{\rho}_1 \), given that \( \hat{\rho}_1 \) is actually controlling the statistics. In this sense, Eq. (3.309) gives an operationally defined (albeit asymmetric) notion of distinguishability for quantum states.
Figure 3.3: All the bounds to accessible information studied here, for the case that $\hat{\rho}_0$ is pure ($a = 1$), $\hat{\rho}_1$ is mixed with $b = 2/3$, and the angle between the two Bloch vectors is $\pi/4$. 
Figure 3.4: All the bounds to accessible information studied here, for the case that \( \hat{\rho}_0 \) and \( \hat{\rho}_1 \) are pure states \( (a = b = 1) \) and the angle between the two Bloch vectors is \( \pi/4 \). For this case, \( M(t) = P(t) = I(t) \).
Figure 3.5: All the bounds to accessible information studied here, for the case that $\hat{\rho}_0$ and $\hat{\rho}_1$ are mixed states with $a = \frac{4}{5}$ and $b = \frac{9}{10}$ and the angle between the two Bloch vectors is $\pi/3$. 
Figure 3.6: All the bounds to accessible information studied here, for the case that $\hat{\rho}_0$ and $\hat{\rho}_1$ are pure states ($a = b = 1$) and the angle between the two Bloch vectors is $\pi/3$. For this case, $M(t) = P(t) = I(t)$. 

93
Figure 3.7: The bounds $S(t)$, $L(t)$, $M(t)$, and $P(t)$ for the case that $\hat{\rho}_0$ and $\hat{\rho}_1$ are mixed states with $a = \frac{9}{10}$ and $b = \frac{3}{5}$ and the angle between the two Bloch vectors is $\pi/5$. 
Figure 3.8: The bounds $S(t)$, $L(t)$, $M(t)$, and $P(t)$ for the case that $\hat{\rho}_0$ and $\hat{\rho}_1$ are mixed states with $a = b = \frac{2}{3}$ and the angle between the two Bloch vectors is $\pi/4$. 

95
The main difficulty with Eq. (3.309) as a notion of distinguishability is that one would like an explicit, convenient expression for it—not simply the empty definer given there. Chances for that, however, are very slim. For just by looking at the $2 \times 2$ density operator case, one can see that the POVM optimal for this criterion must satisfy a transcendental equation. For instance, by setting the variation of Eq. (3.250) to zero, we see that an optimal orthogonal projection-measurement $\vec{n}$ must satisfy,

$$
\ln \left( \frac{(n + \vec{a} \cdot \vec{n})(n - \vec{c} \cdot \vec{n})}{(n - \vec{a} \cdot \vec{n})(n + \vec{c} \cdot \vec{n})} \right) \vec{a}_\perp + 2n \left( \frac{\vec{c} \cdot \vec{n} - \vec{a} \cdot \vec{n}}{n^2 - (\vec{c} \cdot \vec{n})^2} \right) \vec{c}_\perp = 0 ,
$$

(3.312)

where the vectors $\vec{a}_\perp$ and $\vec{c}_\perp$ are defined as in Eq. (3.253). This may well not have an explicit solution in general. We are again forced to study bounds rather than exact solutions just as was the case for accessible information.

So far, several bounds to the quantum Kullback information have come along incidentally. There are the lower bounds given by Eqs. (3.93) and (3.204), which will soon be revisited in Section 3.6.2. And there are the upper and lower bounds due to Jensen’s inequality given in Eq. (3.295). In the remainder of this Section, we shall detail a few more bounds, both upper and lower.

### 3.6.1 The Umegaki Relative Information

The Umegaki relative information between $\hat{\rho}_0$ and $\hat{\rho}_1$ is defined by

$$
K_U(\hat{\rho}_0 / \hat{\rho}_1) \equiv \text{tr} \left( \hat{\rho}_0 \ln \hat{\rho}_0 - \hat{\rho}_0 \ln \hat{\rho}_1 \right).
$$

(3.313)

This concept was introduced by Umegaki in 1962 [125], and a large literature exists concerning it. Some authors have gone so far as to label it the “proper” notion of a relative information for two quantum states [145, 126].

As we have already seen, the Holevo upper bound to mutual information is easily expressible in terms of Eq. (3.313). This turns out to be no surprise because, indeed, this quantity is an upper bound to the quantum Kullback information itself [146]. This will be demonstrated directly from the Holevo bound in this Section.

For simplicity, let us assume that both $\hat{\rho}_0$ and $\hat{\rho}_1$ are invertible. Let $\{\hat{E}_b\}$ be any POVM and $p_0(b)$ and $p_1(b)$ be the probability distributions it generates. Suppose $0 < t < 1$. Then the Holevo bound Eq. (3.210) can be rewritten as

$$
K(p_0/p) + \frac{t}{1-t}K(p_1/p) \leq K_U(\hat{\rho}_0 / \hat{\rho}) + \frac{t}{1-t}K_U(\hat{\rho}_1 / \hat{\rho}) .
$$

(3.314)

Taking the limit of this as $t$ approaches 1, we obtain

$$
K(p_0/p_1) + \lim_{t \to 1} \frac{t}{1-t}K(p_1/p) \leq K_U(\hat{\rho}_0 / \hat{\rho}_1) + \lim_{t \to 1} \frac{t}{1-t}K_U(\hat{\rho}_1 / \hat{\rho}) .
$$

(3.315)

It turns out that the limits yet to be evaluated vanish; let us show this. Note that, trivially,

$$
\lim_{t \to 1} (1-t) = \lim_{t \to 1} K(p_1/p) = \lim_{t \to 1} K_U(\hat{\rho}_1 / \hat{\rho}) = 0.
$$

(3.316)

Therefore we must use l’Hospital’s rule to evaluate the desired limits. In the first case, this readily gives

$$
\lim_{t \to 1} \frac{t}{1-t}K(p_1/p) = -\lim_{t \to 1} \left( K(p_1/p) + t \frac{d}{dt} K(p_1/p) \right)
$$
\[
= \sum_b \left( \lim_{t \to 1} \frac{\text{tr}(\hat{\rho}_b \hat{E}_b)}{\text{tr}(\hat{\rho} \hat{E}_b)} \text{tr}(\hat{\Delta} \hat{E}_b) \right)
\]
\[
= \sum_b \text{tr}(\hat{\Delta} \hat{E}_b)
\]
\[
= \text{tr}(\hat{\Delta}) = 0.
\] (3.317)

The second case is slightly more difficult. l’Hôpital’s rule gives
\[
\lim_{t \to 1} \frac{t - 1}{t} K_U(\hat{\rho}_1/\hat{\rho}) = -\lim_{t \to 1} \left( K_U(\hat{\rho}_1/\hat{\rho}) + t \frac{d}{dt} K_U(\hat{\rho}_1/\hat{\rho}) \right)
\]
\[
= \lim_{t \to 1} \frac{d}{dt} \text{tr}(\hat{\rho}_1 \ln \hat{\rho}) ,
\] (3.318)
but there is still some work required to evaluate the last expression.

Recall that the operator \( \ln \hat{\rho} \) may be represented by a contour integral,
\[
\ln \hat{\rho} = \frac{1}{2\pi i} \oint_C \ln z (z \mathbb{1} - \hat{\rho})^{-1} dz,
\] (3.319)
where the contour \( C \) encloses all the eigenvalues of \( \hat{\rho} \) (for all possible values of \( t \)). Then
\[
\frac{d}{dt} \ln \hat{\rho} = \frac{1}{2\pi i} \oint_C \ln z (z \mathbb{1} - \hat{\rho})^{-1} \Delta (z \mathbb{1} - \hat{\rho})^{-1} dz,
\] (3.320)
so that
\[
\lim_{t \to 1} \frac{d}{dt} \text{tr}(\hat{\rho}_1 \ln \hat{\rho}) = \frac{1}{2\pi i} \oint_C \ln z \left( (z \mathbb{1} - \hat{\rho}_1)^{-1} \hat{\rho}_1 (z \mathbb{1} - \hat{\rho}_1)^{-1} \Delta \right) dz
\]
\[
= \sum_{k=1}^D \lambda_k \Delta_{kk} \frac{1}{2\pi i} \oint_C \frac{\ln z}{(z - \lambda_k)^2} dz ,
\] (3.321)
where \( \lambda_k \) are the eigenvalues of \( \hat{\rho}_1 \) and \( \Delta_{kk} \) are the matrix elements of \( \hat{\Delta} \) in a basis that diagonalizes \( \hat{\rho}_1 \). By the Cauchy integral theorem, however,
\[
\frac{1}{2\pi i} \oint_C \frac{\ln z}{(z - \lambda_k)^2} dz = \frac{1}{\lambda_k}.
\] (3.322)

Therefore
\[
\lim_{t \to 1} \frac{d}{dt} \text{tr}(\hat{\rho}_1 \ln \hat{\rho}) = \sum_{k=1}^D \Delta_{kk}
\]
\[
= \text{tr}(\hat{\Delta}) = 0.
\] (3.323)

This proves that the Kullback-Leibler relative information for any measurement is bounded above by the Umegaki relative information. In particular, this places an upper bound on the quantum Kullback information,
\[
K(\hat{\rho}_0/\hat{\rho}_1) \leq K_U(\hat{\rho}_0/\hat{\rho}_1) .
\] (3.324)
Moreover, since the Holevo bound on mutual information is achievable if and only if \( \hat{\rho}_0 \) and \( \hat{\rho}_1 \) commute, it follows that there is equality in this bound if and only the density operators commute.
3.6.2 One Million One Lower Bounds

It appears to be productive to ask, among other things, if there is any systematic procedure for generating successively tighter lower bounds to $K(\hat{\rho}_0/\hat{\rho}_1)$. In particular, one would like to know if there is a procedure for finding lower bounds of the form

$$\text{tr}\left(\hat{\rho}_0 \ln \hat{\Lambda}(\hat{\rho}_0/\hat{\rho}_1)\right), \quad (3.325)$$

where $\hat{\Lambda}(\hat{\rho}_0/\hat{\rho}_1)$ is a Hermitian operator that depends (asymmetrically) on $\hat{\rho}_0$ and $\hat{\rho}_1$.

We already know of two such bounds. The first [147, 148] is given by Eq. (3.204),

$$K_F(\hat{\rho}_0/\hat{\rho}_1) \equiv \text{tr}\left(\hat{\rho}_0 \ln \left(\hat{\rho}_1 \hat{\rho}_1^{-1/2} \hat{\rho}_0 \hat{\rho}_1^{1/2} \hat{\rho}_1^{-1/2}\right)\right), \quad (3.326)$$

where $\hat{\rho}_1$ is an operator $\hat{X}$ satisfying the equation

$$\hat{X} \hat{\rho}_1 + \hat{\rho}_1 \hat{X} = 2 \hat{\rho}_0. \quad (3.327)$$

The second [149, 150] is given by Eq. (3.93),

$$K_B(\hat{\rho}_0/\hat{\rho}_1) \equiv 2 \text{tr}\left(\hat{\rho}_0 \ln \left(\hat{\rho}_1^{-1/2} \sqrt{\hat{\rho}_1^{-1/2} \hat{\rho}_0 \hat{\rho}_1^{-1/2} \hat{\rho}_1^{-1/2}}\right)\right). \quad (3.328)$$

Both these bounds come quite close to the exact answer defined by Eq. (3.6) when $\hat{\rho}_0$ and $\hat{\rho}_1$ are $2 \times 2$ density operators [150]. Nevertheless, these approximations may not fare so well for density operators of higher dimensionality.

The trick in finding expressions (3.326) and (3.328) was in noting that the eigenvalues $\lambda_b$ of the operators

$$\hat{\Lambda}_1 \equiv \hat{L}(\hat{\rho}_0) \quad (3.329)$$

and

$$\hat{\Lambda}_2 \equiv \hat{\rho}_1^{-1/2} \sqrt{\hat{\rho}_1^{-1/2} \hat{\rho}_0 \hat{\rho}_1^{-1/2} \hat{\rho}_1^{-1/2}} \quad (3.330)$$

can be written in the form

$$\lambda_b^p = \frac{\text{tr}(\hat{\rho}_0 \hat{E}_b)}{\text{tr}(\hat{\rho}_1 \hat{E}_b)}, \quad (3.331)$$

where the $\hat{E}_b = |b\rangle\langle b|$ are projectors onto the one-dimensional subspaces spanned by eigenvectors $|b\rangle$ of $\hat{\Lambda}_p$, $p = 1$ or 2 respectively. Using this fact, one simply notes that

$$\text{tr}\left(\hat{\rho}_0 \ln \hat{\Lambda}_p\right) = \text{tr}\left(\hat{\rho}_0 \sum_b \ln \lambda_b^p \hat{E}_b\right) \quad (3.332)$$

Eq. (3.331) is derived easily from the defining equation for $\hat{\Lambda}_1$: one just notes that for an eigenvector $|b\rangle$ of $\hat{\Lambda}_1$

$$\langle b|\hat{\Lambda}_1 \hat{\rho}_1 |b\rangle + \langle b|\hat{\rho}_1 \hat{\Lambda}_1 |b\rangle = 2\langle b|\hat{\rho}_0 |b\rangle \quad \Rightarrow \quad 2\lambda_b \langle b|\hat{\rho}_1 |b\rangle = 2\langle b|\hat{\rho}_0 |b\rangle \quad (3.333)$$
The corresponding fact for $\hat{\Lambda}_2$ was derived from more complex considerations in Section 3.3. A much simpler way to see it is by noting that $\hat{\Lambda}_2$ satisfies the matrix quadratic equation

$$\hat{X}\hat{\rho}_1\hat{X} = \hat{\rho}_0 .$$

(This can be seen by inspection.) Then along similar lines as above, if one takes $|b\rangle$ to be an eigenvector of $\hat{\Lambda}_2$, one gets

$$\langle b|\hat{\Lambda}_2\hat{\rho}_1\hat{\Lambda}_2|b\rangle = \langle b|\hat{\rho}_0|b\rangle \iff \lambda_b^2\langle b|\hat{\rho}_1|b\rangle = \langle b|\hat{\rho}_0|b\rangle .$$

Now that the common foundation for both lower bounds (3.326) and (3.328) is plain, we are led to ask whether there are any other operators $\hat{\Lambda}(\hat{\rho}_0/\hat{\rho}_1)$ whose eigenvalues have a similar form, i.e.,

$$\lambda_b\left(\hat{\Lambda}(\hat{\rho}_0/\hat{\rho}_1)\right) \equiv \frac{\text{tr}(\hat{\rho}_0\hat{E}_b)}{\text{tr}(\hat{\rho}_1\hat{E}_b)} ,$$

where $\lambda_b(\hat{X})$ denotes the $b$’th eigenvalue of the operator $\hat{X}$. If so, then

$$\ln\hat{\Lambda}(\hat{\rho}_0/\hat{\rho}_1) = \sum_b \ln\left(\frac{\text{tr}(\hat{\rho}_0\hat{E}_b)}{\text{tr}(\hat{\rho}_1\hat{E}_b)}\right)\hat{E}_b ,$$

and we get the desired result, Eq. (3.325), via the steps in Eq. (3.332).

Posed in this way, the solution to the question becomes quickly apparent. It is found by generalizing the defining equations for the operators $\hat{\Lambda}_1$ and $\hat{\Lambda}_2$. For instance, consider the Hermitian operator $\hat{X}$ defined by

$$\frac{1}{2}(\hat{\rho}_1\hat{X} + \hat{X}\hat{\rho}_1) + (1 - \alpha)\hat{\rho}_1\hat{X} = \hat{\rho}_0 ,$$

If its eigenvectors and eigenvalues are $|b\rangle$ and $\lambda_b$, one obtains (by the same method as before)

$$\frac{\langle b|\hat{\rho}_0|b\rangle}{\langle b|\hat{\rho}_1|b\rangle} = \lambda_b^2 + \lambda_b .$$

Therefore, the operator

$$\hat{\Lambda} = \hat{X}^2 + \hat{X}$$

has eigenvalues $(\text{tr}\hat{\rho}_0\hat{E}_b)/(\text{tr}\hat{\rho}_1\hat{E}_b)$, and we obtain another lower bound

$$\text{tr}\left(\hat{\rho}_0\ln(\hat{X}^2 + \hat{X})\right)$$

to the quantum Kullback information.

More interestingly, however, is that we now have a method for inserting parameters into the bound which can be varied to obtain an “optimal” bound. For instance, we could instead consider the solutions $\hat{X}_\alpha$ to the (parameterized) operator equation

$$\frac{1}{2}\alpha(\hat{\rho}_1\hat{X}_\alpha + \hat{X}_\alpha\hat{\rho}_1) + (1 - \alpha)\hat{\rho}_1\hat{X}_\alpha = \hat{\rho}_0 ,$$

and thus get the best bound of this form by

$$\max_{\alpha}\text{tr}\left(\hat{\rho}_0\ln((1 - \alpha)\hat{X}_\alpha^2 + \alpha\hat{X}_\alpha)\right) .$$
This bound has no choice but to be at least as good or better than the bounds $K_F(\hat{\rho}_0/\hat{\rho}_1)$ and $K_B(\hat{\rho}_0/\hat{\rho}_1)$ simply because Eq. (3.342) interpolates between the measurements defining them in the first place. Moreover Eq. (3.342) is still within the realm of equations known to the mathematical community; methods for its solution exist [151, 152, 153, 154].

This pretty much builds the picture. More generally, one has measurements defined by

$$\frac{1}{2} \sum_{ij} \alpha_{ij} \left( \hat{X}^i \hat{\rho}_1 \hat{X}^j + \hat{X}^j \hat{\rho}_1 \hat{X}^i \right) = \hat{\rho}_0$$

(3.344)

giving rise to lower bounds to the Quantum Kullback of the form

$$\text{tr} \left( \hat{\rho}_0 \ln \left( \sum_{ij} \alpha_{ij} \hat{X}^{i+j} \right) \right).$$

(3.345)

(Here $i$ and $j$ may range anywhere from 0 up to values for which the $\alpha_{ij}$ are no longer freely specifiable.) These may then be varied over all the parameters $\alpha_{ij}$ to find the best bound allowable at that order. To the extent that solutions to Eq. (3.344) can be found, even numerically, better lower bounds to the Quantum Kullback information can be generated.

### 3.6.3 Upper Bound Based on Ando’s Inequality and Other Bounds from the Literature

Another way to get an upper bound on the quantum Kullback information is by examining Eq. (3.137), the bound on the quantum Rényi overlap due to Ando’s inequality. With this, one immediately has

$$\frac{1}{\alpha - 1} \ln \left( \sum_{b=1}^{n} p_0(b)^{\alpha} p_1(b)^{1-\alpha} \right) \leq \frac{1}{\alpha - 1} \ln \text{tr} \left( \hat{\rho}_1^{1/2} \left( \hat{\rho}_1^{-1/2} \hat{\rho}_0 \hat{\rho}_1^{-1/2} \right)^{\alpha} \hat{\rho}_1^{1/2} \right).$$

(3.346)

However, as $\alpha \to 1$, the left hand side of this inequality converges to the Kullback-Leibler information. Therefore if we can evaluate the right hand side of this in the limit, we will have generated a new bound. Using l’Hospital’s rule, we get

$$\lim_{\alpha \to 1} \text{RHS} =$$

$$= \lim_{\alpha \to 1} \left[ \text{tr} \left( \hat{\rho}_1^{1/2} \left( \hat{\rho}_1^{-1/2} \hat{\rho}_0 \hat{\rho}_1^{-1/2} \right)^{\alpha} \hat{\rho}_1^{1/2} \right) \right]^{-1} \left[ \text{tr} \left( \hat{\rho}_1^{1/2} \left( \hat{\rho}_1^{-1/2} \hat{\rho}_0 \hat{\rho}_1^{-1/2} \right)^{\alpha} \ln \left( \hat{\rho}_1^{-1/2} \hat{\rho}_0 \hat{\rho}_1^{-1/2} \right) \hat{\rho}_1^{1/2} \right) \right].$$

(3.347)

Therefore, one arrives at the relatively asymmetric upper bound to the quantum Kullback information given by

$$K(\hat{\rho}_0/\hat{\rho}_1) \leq \text{tr} \left( \left( \hat{\rho}_1^{1/2} \hat{\rho}_0 \hat{\rho}_1^{-1/2} \right) \ln \left( \hat{\rho}_1^{-1/2} \hat{\rho}_0 \hat{\rho}_1^{-1/2} \right) \right).$$

(3.348)

Note that when $\rho_0$ and $\rho_1$ commute, this reduces to the Umegaki relative information.

Finally, we note that the last property of reducing to the Umegaki relative entropy is not an uncommon property of many known upper bounds to it. For instance it is known [155] that for every $p > 0$,

$$K_U(\hat{\rho}_0/\hat{\rho}_1) \leq \frac{1}{p} \text{tr} \left( \hat{\rho}_0 \ln \left( \hat{\rho}_1^{p/2} \hat{\rho}_0^{-p/2} \right) \right),$$

(3.349)
and all of these have this property. Alternatively, so do the lower bounds Eqs. (3.204) and (3.93) to the quantum Kullback information derived earlier, as well as the lower bound [155] given by

$$K(\hat{\rho}_0/\hat{\rho}_1) \geq \text{tr} \left( \hat{\rho}_0 \ln \left( \hat{\rho}_1^{-1/2} \hat{\rho}_0 \hat{\rho}_1^{-1/2} \right) \right). \quad (3.350)$$

This may or may not lessen the importance of the Umegaki upper bound, depending upon one’s taste.
Chapter 4

Distinguishability in Action

“Something only really happens when an observation is being made . . . . Between the observations nothing at all happens, only time has, ‘in the interval,’ irreversibly progressed on the mathematical papers!”

—Wolfgang Pauli
Letter to Markus Fierz
30 March 1947

4.1 Introduction

In the preceding chapters, we went to great lengths to define and calculate various notions of distinguishability for quantum mechanical states. These notions are of intrinsic interest for their associated statistical problems. However, we might still wish for a larger payoff on the work invested. This is what this Chapter is about. Here, we present the briefest of sketches of what can be accomplished by using some of the measures of distinguishability already encountered. The applications concern two questions that lie much closer to the foundations of quantum theory than was our previous concern.

“Quantum mechanical measurements disturb the states of quantum systems in uncontrollable ways.” Statements like this are uttered in almost every beginning quantum mechanics course—it is part of the folklore of the theory. But what does this really mean? How is it to be quantified? The next two sections outline steps toward answers to these questions.

4.2 Inference vs. Disturbance of Quantum States: Extended Abstract

Suppose an observer obtains a quantum system secretly prepared in one of two standard but nonorthogonal quantum states. Quantum theory dictates that there is no measurement he can use to certify which of the two states was actually prepared. This is well known and has already been discussed many times in the preceding chapters. A simple, but less recognized, corollary to this is that no interaction used for performing such an information-gathering measurement can leave both states unchanged in the process. If the observer could completely regenerate the unknown
quantum state after measurement, then—by making further nondisturbing information-gathering measurements on it—he would be able eventually to infer the state’s identity after all.

This consistency argument is enough to establish a tension between inference and disturbance in quantum theory. What it does not capture, however, is the extent of the tradeoff between these two quantities. In this Section, we shall lay the groundwork for a quantitative study that goes beyond the qualitative nature of this tension. \footnote{This Section is based on a manuscript disseminated during the “Quantum Computation 1995” workshop held at the Institute for Scientific Interchange (Turin, Italy); as such, it contains a small redundancy with the previous Chapters.} Namely, we will show how to capture in a formal way the idea that, depending upon the particular measurement interaction, there can be a tradeoff between the disturbance of the quantum states and the acquired ability to make inferences about their identity. The formalism so developed should have applications to quantum cryptography on noisy channels and to error correction and stabilization in quantum computing.

4.2.1 The Model

The model we shall base our considerations on is most easily described in terms borrowed from quantum cryptography, though this problem should not be identified with the cryptographic one. Alice randomly prepares a quantum system to be in either a state $\hat{\rho}_0$ or a state $\hat{\rho}_1$. These states will be described by $N \times N$ density operators on an $N$-dimensional Hilbert space, $N$ arbitrary; there is no restriction that they be pure states or orthogonal for that matter. After the preparation, the quantum system is passed into a “black box” where it may be probed by an eavesdropper Eve in any way allowed by the laws of quantum mechanics. That is to say, Eve may first allow the system to interact with an auxiliary system, or ancilla, and then perform quantum mechanical measurements on the ancilla itself \cite{26, 156}. The outcome of such a measurement may provide Eve with some information about the quantum state and may even provide her a basis on which to make an inference as to the state’s identity. Upon this manhandling by Eve, the quantum system is passed out of the “black box” and into the possession of a third person Bob. (See related Figure 4.1 depicting Eve and Bob only.)

A crucial aspect of this model is that even if Bob knows the state actually prepared by Alice and, furthermore, the manner in which Eve operates and the exact measurement she performs, without knowledge of the answer she actually obtains, he will have to resort to a new description of the quantum system after it emerges from the “black box”—say some $\hat{\rho}'_0$ or $\hat{\rho}'_1$. This is where the detail of our work takes its start. Eve has gathered information and the state of the quantum system has changed in the process.

The ingredients required formally to pose the question of the Introduction follow from the details of the model. We shall need:

A. a convenient description of the most general kind of quantum measurement,

B. a similarly convenient description of all the possible physical interactions that could give rise to that measurement,

C. a measure of the information or inference power provided by any given measurement,

D. a good notion by which to measure the distinguishability of mixed quantum states and a measure of disturbance based on it, and finally

E. a “figure of merit” by which to compare the disturbance with the inference.
The Problem*

\[ \hat{\rho}_0 \rightarrow \rho \rightarrow \hat{\rho}_1 \]

\(-N \times N\) density operators

Inference

\[ 5 \Rightarrow \hat{\rho}_0 ? \]

\[ \hat{\rho}'_0 = \hat{\rho}_0 \]
\[ \hat{\rho}'_1 = \hat{\rho}_1 ? \]

Disturbance

* not necessarily cryptography related

Figure 4.1: Set-up for Inference–Disturbance Tradeoff
The way these ingredients are stirred together to make a good soup—very schematically—is the following. We first imagine some fixed measurement $M$ on the part of Eve and some particular physical interaction $I$ used to carry out that measurement. (Note that $I$ uniquely determines $M$, whereas in general $M$ says very little about $I$.) Using the measures from ingredients $C$ and $D$, we can then quantify the inference power

$$\text{Inf}(\hat{\rho}_0, \hat{\rho}_1; M)$$

(4.1)

accorded Eve and the necessary disturbance

$$\text{Dist}(\hat{\rho}_0, \hat{\rho}_1; I)$$

(4.2)

apparent to Bob. As the notation indicates, besides depending on $\hat{\rho}_0$ and $\hat{\rho}_1$, the inference power otherwise depends only on $M$ and the disturbance only on $I$. Using the agreed upon figure of merit $\text{FOM}$, we arrive at a number that describes the tradeoff between inference and disturbance for the fixed measurement and interaction:

$$\text{FOM}\left[\text{Inf}(\hat{\rho}_0, \hat{\rho}_1; M), \text{Dist}(\hat{\rho}_0, \hat{\rho}_1; I)\right].$$

(4.3)

Now the idea is to remove the constraint that the measurement $M$ and the interaction $I$ be fixed, to re-express $M$ in terms of $I$, and to optimize

$$\text{FOM}\left[\text{Inf}(\hat{\rho}_0, \hat{\rho}_1; M(I)), \text{Dist}(\hat{\rho}_0, \hat{\rho}_1; I)\right]$$

(4.4)

over all measurement interactions $I$. This is the whole story. With the optimal such expression in hand, one automatically arrives at a tradeoff relation between inference and disturbance: for arbitrary $M$ and $I$, expression (4.3) will be less or greater than the optimal such one, depending on its exact definition.

### 4.2.2 The Formalism

The first difficulty in our task is in finding a suitably convenient and useful formalism for describing Ingredients $A$ and $B$. The most general measurement procedure allowed by the laws of quantum mechanics is, as already stated, first to have the system of interest interact with an ancilla and then to perform a standard (von Neumann) quantum measurement on the ancilla itself. Taken at face value, this description can be transcribed into mathematical terms as follows. The system of interest, starting out in some quantum state $\hat{\rho}_s$, is placed in conjunction with an ancilla prepared in a standard state $\hat{\rho}_a$. The conjunction of these two systems is described by the initial quantum state

$$\hat{\rho}_{sa} = \hat{\rho}_s \otimes \hat{\rho}_a.$$ 

(4.5)

The interaction of the two systems leads to a unitary time evolution,

$$\hat{\rho}_{sa} \longrightarrow \hat{U}^\dagger \hat{\rho}_{sa} \hat{U}.$$ 

(4.6)

(Note that the state of the system-plus-ancilla, by way of this interaction, will generally not remain in its original tensor-product form; rather the states of the two systems will become inextricably entangled and correlated.) Finally, a reproducible measurement on the ancilla is described via a set of orthogonal projection operators $\mathbb{1} \otimes \hat{\Pi}_b$ acting on the ancilla’s Hilbert space: any particular outcome $b$ is found with probability

$$p(b) = \text{tr}\left((\mathbb{1} \otimes \hat{\Pi}_b)\hat{U}^\dagger(\hat{\rho}_s \otimes \hat{\rho}_a)\hat{U}\right),$$ 

(4.7)
and the description of the system-plus-ancilla after the finding of this outcome must be updated according to the standard rules to

\[ \hat{\rho}'_{\text{sal}|b} = \frac{1}{p(b)}(\mathbb{1} \otimes \hat{\Pi}_b)\hat{U}^\dagger(\hat{\rho}_b \otimes \hat{\rho}_a)\hat{U}(\mathbb{1} \otimes \hat{\Pi}_b) . \]  

(4.8)

Thus the quantum state describing the system alone after finding outcome \( b \) is

\[ \hat{\rho}'_{\text{sl}|b} = \text{tr}_a\left( \hat{\rho}'_{\text{sal}|b} \right) , \]

(4.9)

where \( \text{tr}_a \) denotes a partial trace over the ancilla’s Hilbert space. If one knows this measurement was performed but does not know the actual outcome, then the description given the quantum system will be rather

\[ \hat{\rho}'_s = \sum_b p(b)\hat{\rho}'_{\text{sl}|b} = \text{tr}_a\left( \hat{U}^\dagger(\hat{\rho}_s \otimes \hat{\rho}_a)\hat{U} \right) . \]

(4.10)

This face-value description of a general measurement gives—in principle—everything required of it. Namely it gives a formal description of the probabilities of the measurement outcomes and it gives a formal description of the system’s state evolution arising from this measurement. The problem with this for the purpose at hand is that it focuses attention away from the quantum system itself, placing undue emphasis on the fact that there is an ancilla in the background. Unfortunately, it is this sort of thing that can make the formulation of optimization problems over measurements and interactions more difficult than it need be. On the brighter side, there is a way of getting around this particular deficiency of notation. This is accomplished by introducing the formalism of “effects and operations” \([157, 158, 159, 160, 161, 26]\), which we shall attempt to sketch presently. (An alternative formalism that may also be of use in this context is that of Mayers \([156]\).)

Recently, more and more attention has been given to the (long known) fact that the probability formula, Eq. (4.7), can be written in a way that relies on the system Hilbert space alone with no overt reference to the ancilla \([28]\). Namely, one can write

\[ p(b) = \text{tr}_s(\hat{\rho}_s \hat{E}_b) , \]

(4.11)

where \( \text{tr}_s \) denotes a partial trace over the system’s Hilbert space, by simply taking the operator \( \hat{E}_b \) to be

\[ \hat{E}_b = \text{tr}_a\left( (\mathbb{1} \otimes \hat{\rho}_a)\hat{U}(\mathbb{1} \otimes \hat{\Pi}_b)\hat{U}^\dagger \right) . \]

(4.12)

The reason this can be viewed as making no direct reference to the ancilla is that it has been noted that any set of positive semi-definite operators \( \{\hat{E}_b\} \) satisfying

\[ \sum_b \hat{E}_b = \mathbb{1} \]

(4.13)

can be written in a form specified by Eq. (4.12). Therefore these sets of operators, known as positive operator-valued measures or POVMs, stand in one-to-one correspondence with the set of generalized quantum mechanical measurements. This correspondence gives us the freedom to exclude or to include explicitly the ancilla in our description of a measurement’s statistics, whichever is the more convenient.

A quick example illustrating why this particular representation of a measurement’s outcomes statistics can be useful is the following. Consider the problem of trying to distinguish the quantum states \( \hat{\rho}_0 \) and \( \hat{\rho}_1 \) from each other by performing some measurement whose outcome probabilities are \( p_0(b) \) if the state is actually \( \hat{\rho}_0 \) and \( p_1(b) \) if the state is actually \( \hat{\rho}_1 \). A nice measure of the
The distinguishability of the probability distributions generated by this measurement is their “statistical overlap” \[ F(p_0, p_1) = \sum_b \sqrt{p_0(b) p_1(b)}. \] (4.14)

This quantity is equal to unity whenever the probability distributions are identical and equal to zero when there is no overlap at all between them. To get a notion of how distinct \( \hat{\rho}_0 \) and \( \hat{\rho}_1 \) can be made with respect to this measure, one would like to minimize expression (4.14) over all possible quantum measurements—that is to say, over all possible measurement interactions with all possible ancilla. Without the formalism of POVMs this would be quite a difficult task to pull off. With the formalism of POVMs, however, we can pose the problem as that of finding the quantity

\[
F(\hat{\rho}_0, \hat{\rho}_1) \equiv \min_{\{\hat{E}_b\}} \sum_b \sqrt{\text{tr} \hat{\rho}_0 \hat{E}_b \text{tr} \hat{\rho}_1 \hat{E}_b}
\]
(4.15)

where the minimization is over all sets of operators \( \{\hat{E}_b\} \) satisfying \( \hat{E}_b \geq 0 \) and Eq. (4.13). This rendition of the problem makes it tractable. In fact, it can be shown \[149\] that

\[
F(\hat{\rho}_0, \hat{\rho}_1) = \text{tr} \sqrt{\hat{\rho}_1 / 2 \hat{\rho}_0 \hat{\rho}_1 / 2},
\]
(4.16)
a quantity known in other contexts as (the square root of) Uhlmann’s “transition probability” or “fidelity” for general quantum states \[7, 9\]. The key to the proof of this is in relying as heavily as one can on the defining characteristic Eq. (4.13) of all POVMs. Namely, one uses the standard Schwarz inequality to lower bound Eq. (4.15) by an expression linear in the \( \hat{E}_b \), and then uses the completeness property Eq. (4.13) to sum those operators out of this bound. Finally, checking that there is a way of satisfying equality in each step of the process, Eq. (4.16) follows.

To restate the point of this example: the tractability of our optimization problems may be greatly enhanced by the use of mathematical tools that focus on the essential formal characteristics of quantum measurements and not on their imagined implementation. (Other examples where great headway has been made by relying on the abstract defining properties of POVMs are the maximizing of Fisher information for quantum parameter estimation \[122\] and the bounding of quantum mutual information \[5, 147, 162\].) All that said, the use of POVMs only moves us partially toward our goal. This formalism in and of itself has nothing to say about the post-measurement states given by Eqs. (4.9) and (4.10); we still do not have a particularly convenient (or ancilla-independent) way of representing these state evolutions. It takes the formalism of “effects and operations” to complete the story. This fact is encapsulated by the following “representation” theorem of Kraus \[26\].

**Theorem 4.1** Let \( \{\hat{E}_b\} \) be the POVM derived from the measurement procedure described via Eqs. (4.5) through (4.10). Then there exists a set of (generally non-Hermitian) operators \( \{\hat{A}_{bi}\} \) acting on the system’s Hilbert space such that

\[
\hat{E}_b = \sum_i \hat{A}_{bi}^\dagger \hat{A}_{bi},
\]
(4.17)

and the conditional and unconditional state evolutions under this measurement can be written as

\[
\hat{\rho}'_{s|b} = \frac{1}{\text{tr}_s(\hat{\rho}_s \hat{E}_b)} \sum_i \hat{A}_{bi} \hat{\rho}_s \hat{A}_{bi}^\dagger,
\]
(4.18)

and

\[
\hat{\rho}'_s = \sum_{b,i} \hat{A}_{bi} \hat{\rho}_s \hat{A}_{bi}^\dagger.
\]
(4.19)
Moreover, for any set of operators \{\hat{A}_b\} such that
\[ \sum_{b,i} \hat{A}_b^\dagger \hat{A}_b = \hat{1} , \] (4.20)
there exists a measurement interaction whose statistics are described by the POVM in Eq. (4.17) and gives rise to the conditional and unconditional state evolutions of Eqs. (4.18) and (4.19).

(To justify the term “effects and operations” we should note that Kraus calls a POVM \{\hat{E}_b\} an effect and the state transformations described by the operators \{\hat{A}_b\} operations—the one given by Eq. (4.18) a selective operation and the one given by Eq. (4.19) a nonselective operation. In these notes we shall not make use of the term effect, but—lacking a more common term—will call the operator set \{\hat{A}_b\} an operation.)

The way this theorem comes about is seen easily enough from Eq. (4.9). Let the eigenvalues of \(\hat{\rho}_a\) be denoted by \(\lambda_\alpha\) and suppose it has an associated eigenbasis \(|a_\alpha\rangle\). Then \(\hat{\rho}_s \otimes \hat{\rho}_a\) can be written as
\[ \hat{\rho}_s \otimes \hat{\rho}_a = \sum_\alpha \sqrt{\lambda_\alpha} |a_\alpha\rangle \hat{\rho}_s |a_\alpha\rangle \sqrt{\lambda_\alpha} , \] (4.21)
and, just expanding Eq. (4.9), we have
\[ \hat{\rho}'_{sa|b} = \frac{1}{p(b)} \sum_\beta \langle a_\beta | (\hat{1} \otimes \hat{\Pi}_b) \hat{U}^\dagger (\hat{\rho}_s \otimes \hat{\rho}_a) \hat{U} (\hat{1} \otimes \hat{\Pi}_b) |a_\beta\rangle 
= \frac{1}{p(b)} \sum_{\alpha\beta} \left( \sqrt{\lambda_\alpha} \langle a_\beta | (\hat{1} \otimes \hat{\Pi}_b) \hat{U}^\dagger |a_\alpha\rangle \right) \hat{\rho}_s \left( \langle a_\alpha | \hat{U} (\hat{1} \otimes \hat{\Pi}_b) |a_\beta\rangle \sqrt{\lambda_\alpha} \right) . \] (4.22)

Equation (4.18) comes about by taking
\[ \hat{A}_{b\alpha\beta} = \sqrt{\lambda_\alpha} \langle a_\alpha | \hat{U} (\hat{1} \otimes \hat{\Pi}_b) |a_\beta\rangle \] (4.23)
and lumping \(\alpha\) and \(\beta\) into the single index \(i\). Filling in the remainder of the theorem is relatively easy once this is realized.

Kraus’s theorem is the essential new input required to define the inference–disturbance tradeoff in such a way that it may have a tractable solution. For now, in our recipe Eq. (4.3), we may replace the vague symbol \(\mathcal{M}\) (standing for a measurement) by a set of operators \{\hat{E}_b\} and we may replace the symbol \(\mathcal{I}\) (standing for a measurement interaction) by a set of operators \{\hat{A}_b\}. Moreover, we know how to connect these two sets, namely through Eq. (4.17). This reduces our problem to choosing a figure of merit FOM for the tradeoff and calculating the optimal quantity
\[ \text{optimum} \left\{ \text{FOM} \left[ \text{Inf} (\hat{\rho}_0; \hat{\rho}_1; \{\hat{A}_b\}) , \text{Dist} (\hat{\rho}_0; \hat{\rho}_1; \{\hat{A}_b\}) \right] \right\} , \] (4.24)
where, again, “optimum” means either minimum or maximum depending upon the precise definition of FOM.

### 4.2.3 Tradeoff Relations

We finally come to the point where we may attempt to build up various inference-disturbance relations. To this end we shall satisfy ourselves with the preliminary work of writing down a fairly
arbitrary relation. We do this mainly because it is somewhat easier to formulate than other more meaningful relations, but also because it appears to be useful for testing out certain simple cases.

Before going on to details, however, perhaps we should say a little more about the significance of these ideas. It is often said that it is the Heisenberg uncertainty relations that dictate that quantum mechanical measurements necessarily disturb the measured system. That, though, is really not the case. The Heisenberg relations concern the inability to get hold of two classical observables simultaneously, and thus the inability to ascribe classical states of motion to quantum mechanical systems. This is a concern that has very little to do with the ultimate limits on what can happen to the quantum states themselves when information is gathered about their identity. The foundation of this approach differs from that of the standard Heisenberg relations in that it makes no reference to conjugate or complementary variables; the only elements entering these considerations are related to the quantum states themselves. In this way one can get at a notion of state disturbance that is purely quantum mechanical, making no reference to classical considerations.

What does it really mean to say that the states are disturbed in and of themselves without reference to variables such as might appear in the Heisenberg relations? It means quite literally that Alice faces a loss of predictability about the outcomes of Bob’s measurements whenever an information gathering eavesdropper intervenes. Take as an example the case where $\hat{\rho}_0$ and $\hat{\rho}_1$ are nonorthogonal pure states. Then for each of these there exists at least one observable for which Alice can predict the outcome with complete certainty, namely the projectors parallel to $\hat{\rho}_0$ and $\hat{\rho}_1$, respectively. However, after Alice’s quantum states pass into the “black box” occupied by Eve, neither Alice nor Bob will any longer be able to predict with complete certainty the outcomes of both those measurements. This is the real content of these ideas.

A First “Trial” Relation

The tradeoff relation to be described in this subsection is literally based on a simple inference problem—that of performing a single quantum measurement on one of two unknown quantum states and then using the outcome of that measurement to guess the identity of the state. The criterion of a good inference is that its expected probability of success be as high as it can possibly be. The criterion of a small disturbance is that the expected fidelity between the initial and final quantum states be as large as it can possibly be. There are, of course, many other quantities that we might have used to gauge inference power, e.g. mutual information, just as there are many other quantities that we might have used to gauge the disturbance. We fix our attention on the ones described here to get the ball rolling. Let us set up this problem in detail.

Going back to the basic model introduced in Section 4.2.1 for this scheme, any measurement Eve performs can always be viewed as the measurement of a two-outcome POVM $\{\hat{E}_0, \hat{E}_1\}$. If the outcome corresponds to $\hat{E}_0$, she guesses the true state to be $\hat{\rho}_0$; if it corresponds to $\hat{E}_1$, she guesses the state to be $\hat{\rho}_1$.

So, first consider a fixed POVM $\{\hat{E}_0, \hat{E}_1\}$ and a fixed operation $\{\hat{A}_b\}$ ($b = 0, 1$) consistent with it in the sense of Eq. (4.17). This measurement gives rise to an expected probability of success quantified by

$$P_s = \frac{1}{2} \text{tr}(\hat{\rho}_0 \hat{E}_0) + \frac{1}{2} \text{tr}(\hat{\rho}_1 \hat{E}_1).$$

That is to say, the expected probability of success for this measurement is the probability that $\hat{\rho}_0$ is the true state times the conditional probability that the decision will be right when this is the case plus a similar term for $\hat{\rho}_1$. (Here we have assumed the prior probabilities for the two states precisely equal.) Using Eq. (4.17) and the cyclic property of the trace, the success probability can
be reexpressed as

\[ P_s = \frac{1}{2} \sum_{b,i} \text{tr} \left( \hat{A}_{bi} \hat{\rho}_0 \hat{A}_{bi}^\dagger \right). \]  

(4.26)

We shall identify this quantity as \( \text{Inf}\left(\{\hat{A}_{bi}\}\right) \), the measure of the inference power given by this measurement.

Now consider the quantum state Bob gets as the system passes out of the black box. If the original state was \( \hat{\rho}_0 \), he obtains

\[ \hat{\rho}_0' = \sum_{b,i} \hat{A}_{bi} \hat{\rho}_0 \hat{A}_{bi}^\dagger. \]  

(4.27)

If the original state was \( \hat{\rho}_1 \), he obtains

\[ \hat{\rho}_1' = \sum_{b,i} \hat{A}_{bi} \hat{\rho}_1 \hat{A}_{bi}^\dagger. \]  

(4.28)

(Eq. (4.19) is made use of rather than Eq. (4.18) because it is assumed that Bob has no knowledge of Eve’s measurement outcome.) The overall state disturbance by this interaction can be quantified in terms of any of a number of distinguishability measures for quantum states explored in Chapter 3. Here we choose to make use of Uhlmann’s “transition probability” or “fidelity”, Eq. (4.16), to define a measure of clonability,

\[ C = \frac{1}{2} \left( F(\hat{\rho}_0, \hat{\rho}_0') \right)^2 + \frac{1}{2} \left( F(\hat{\rho}_1, \hat{\rho}_1') \right)^2. \]  

(4.29)

This quantity measures the extent to which the output quantum states “clone” the input states. In particular, the quantity in Eq. (4.29)—bounded between zero and one—attains a maximum value only when both states are left completely undisturbed by the measurement interaction.

Reexpressing the clonability explicitly in terms of the operation \( \{\hat{A}_{bi}\} \), we get

\[ C = \frac{1}{2} \sum_{s=0}^{1} \left( \sum_{b,i} \hat{A}_{bi} \hat{\rho}_s \hat{A}_{bi}^\dagger \right)^{1/2}. \]  

(4.30)

(Here we have used the fact that \( F(\hat{\rho}_0, \hat{\rho}_1) \) is symmetric in its arguments.) We shall identify this quantity as \( \text{Dist}\left(\{\hat{A}_{bi}\}\right) \), the measure of (non)disturbance given by this measurement.

Now all that is left is to put the inference and disturbance into a common figure of merit by which to compare the two. There are a couple of obvious ways to do this. Since the idea is that, as the probability of success in the inference increases, the clonability decreases, and vice versa, we know that there should be nontrivial upper limits to both the sum and the products of \( P_s \) and \( C \). Indeed the same must be true for an infinite number of monotonic functions of \( P_s \) and \( C \). Here we shall be happy to focus on the sum as an appropriate figure of merit. Why? For no real reason other than that this combination looks relatively simple and is enough to demonstrate the principles involved. So, following through, we simply write down the tradeoff relation

\[ P_s + C \leq \max_{\{\hat{A}_{bi}\}} \frac{1}{2} \sum_{s=0}^{1} \left( \sum_{i} \text{tr} \left( \hat{A}_{si} \hat{\rho}_s \hat{A}_{si}^\dagger \right) + \text{tr} \left( \sum_{b,i} \hat{A}_{bi} \hat{\rho}_s \hat{A}_{bi}^\dagger \right) \right)^{1/2}. \]  

(4.31)
solved. Techniques for getting at this, however, must be a subject for future research. Presently we have no general solutions.

We should point out that, though Eq. (4.31) is the tightest bound of the form

\[ P_s + C \leq f(\hat{\rho}_0, \hat{\rho}_1), \]

(4.32)

other, looser, bounds may also be of some utility—for instance, simply because they may be easier to derive. This comes about because the right-hand side of Eq. (4.31) is the actual maximum value of \( P_s + C \); often it is easier to bound a quantity than explicitly to maximize it. The only requirement in the game is that the bound be nontrivial, i.e., smaller than the one that comes about by maximizing both \( P_s \) and \( C \) simultaneously,

\[
f(\hat{\rho}_0, \hat{\rho}_1) \leq \max_{\{A_{ib}\}} C + \max_{\{E_{ib}\}} P_s
\]

\[
= 1 + \max_{\{E_{ib}\}} P_s
\]

\[
= 1 + \frac{1}{2} \left( 1 + \sum'_j \lambda_j(\hat{\Gamma}) \right),
\]

(4.33)

where \( \lambda_j(\hat{\Gamma}) \) denotes the eigenvalues of the operator

\[
\hat{\Gamma} = \hat{\rho}_1 - \hat{\rho}_0,
\]

(4.34)

and the prime on the summation sign signifies that the sum is taken only over the positive eigenvalues. (See Section 3.2 and Refs. [76, 27].) The right-hand side of Eq. (4.33) would be the actual solution of Eq. (4.31) if and only if an inference measurement entailed no disturbance. In Eq. (4.33),

\[
\max_{\{A_{ib}\}} C = 1
\]

(4.35)

follows from the fact that there is a zero-disturbance measurement, namely the identity operation.

**An Example**

Let us work out a restricted example of this tradeoff relation, just to hint at the interesting insights it can give for concrete problems. In this example, the two initial states of interest are pure states

\[
\hat{\rho}_0 = |\psi_0\rangle\langle\psi_0| \quad \text{and} \quad \hat{\rho}_1 = |\psi_1\rangle\langle\psi_1|
\]

(4.36)

separated in Hilbert space by an angle \( \theta \). (See inset to Figure 4.1.) Eve bases her inference on the outcome of the POVM

\[
\{ \hat{\Pi}_0 = |0\rangle\langle0|, \hat{\Pi}_1 = |1\rangle\langle1| \}.
\]

(4.37)

the projection operators onto the basis vectors symmetrically straddling the states. This measurement leads to the maximal probability of success for this inference problem [76, 27]. The measurement interaction giving rise to this POVM will be assumed to be of the *restricted* class described by the operation

\[
\hat{A}_b = \hat{U}_b \hat{\Pi}_b, \quad b = 0, 1,
\]

(4.38)

A slight variation of this example is done in much greater detail and generality by Fuchs and Peres in Ref. [111].
where the $\hat{U}_b$ are arbitrary unitary operators. Note that $\hat{A}_b^\dag \hat{A}_b = \hat{1}$ for these operators, as must be the case by the definition of an operation.

With this operation, the two states evolve to post-measurement states according to
\[
|\psi\rangle \rightarrow \hat{\rho}_0' = \sum_b \hat{U}_b \hat{\Pi}_b \hat{\rho}_0 \hat{\Pi}_b \hat{U}_b^\dag
\]
\[
= |\langle 0|\psi\rangle|^2 \left( \hat{U}_0 |0\rangle \langle 0|\hat{U}_0^\dag \right) + |\langle 1|\psi\rangle|^2 \left( \hat{U}_1 |1\rangle \langle 1|\hat{U}_1^\dag \right)
\]
\[
= \cos^2 \xi \left( \hat{U}_0 |0\rangle \langle 0|\hat{U}_0^\dag \right) + \cos^2 (\xi + \theta) \left( \hat{U}_1 |1\rangle \langle 1|\hat{U}_1^\dag \right),
\]
and
\[
|\psi\rangle \rightarrow \hat{\rho}_1' = |\langle 0|\psi_1\rangle|^2 \left( \hat{U}_0 |0\rangle \langle 0|\hat{U}_0^\dag \right) + |\langle 1|\psi_1\rangle|^2 \left( \hat{U}_1 |1\rangle \langle 1|\hat{U}_1^\dag \right)
\]
\[
= \cos^2 (\xi + \theta) \left( \hat{U}_0 |0\rangle \langle 0|\hat{U}_0^\dag \right) + \cos^2 \xi \left( \hat{U}_1 |1\rangle \langle 1|\hat{U}_1^\dag \right),
\]
where $\xi$ is the angle between $|b\rangle$ and $|\psi\rangle$, $b = 0, 1$. This evolution has a simple interpretation: if Eve finds outcome $b = 0$, she sends on the quantum system in state
\[
|\phi_0\rangle \equiv \hat{U}_0 |0\rangle,
\]
if Eve finds outcome $b = 1$, she sends on the state
\[
|\phi_1\rangle \equiv \hat{U}_1 |1\rangle.
\]
The (mixed) states—according to Bob’s description—appearing in the outside world are then those given by Eqs. (4.39) and (4.40).

To calculate the disturbance given by these operations, we note a simplification to expressions for $F(\hat{\rho}_0, \hat{\rho}_0')$ and $F(\hat{\rho}_1, \hat{\rho}_1')$ due to the fact that the initial states are pure. Namely,
\[
F(\hat{\rho}_b, \hat{\rho}_b') = \text{tr} \frac{\hat{\Pi}_b \hat{\rho}_b \hat{\Pi}_b}{\text{tr} \hat{\Pi}_b} = \sqrt{\langle b|\hat{\rho}_b'|b\rangle}.
\]
If we further restrict $\hat{U}_0$ and $\hat{U}_1$ to be such that $\{|\phi_0\rangle, |\phi_1\rangle\}$ lie in the plane spanned by $\{|0\rangle, |1\rangle\}$ and determine equal angles with these basis vectors (see Figure 4.1), then the clonability under this interaction works out to be
\[
C = \frac{1}{2} \left( \langle 0|\hat{\rho}_0'|0\rangle + \langle 1|\hat{\rho}_1'|1\rangle \right)
\]
\[
= \cos^2 \xi \cos^2 \phi + \cos^2 (\xi + \theta) \cos^2 (\theta - \phi),
\]
where $\phi$ is the angle between $|\psi_0\rangle$ and $|\psi_b\rangle$.

The problem is, of course, to find the optimal tradeoff between inference and disturbance for this measurement and interaction. Since the measurement POVM is fixed, this boils down to determining the angle $\phi$ such that the clonability $C$ is maximized. Setting $dC/d\phi$ equal to zero and solving for $\phi$, we find the least disturbing final states to be specified by the angle $\phi_0$, where
\[
\phi_0 = \frac{1}{2} \arctan \left( \frac{1 + \sin \theta}{1 - \sin \theta + \cos 2\theta} \right)^{-1} \sin 2\theta.
\]
This angle ranges from 0° at θ = 0° to its maximum value 6.99° at θ = 27.73°, returning to 0° at θ = 90°. This means that, under the restrictions imposed here, the best strategy on the part of Eve for minimizing disturbance is not to send on the quantum states guessed in the inference, but rather a set of states with slightly higher overlap than the original states. This result points out that the (a priori reasonable) strategy of simply sending on the inferred states will only propagate the error in that inference; it is much smarter on Eve’s part to attempt to hide that error by decreasing the probability that a wrong guess can lead to a detection of itself outside the boundaries of the black box.

4.3 Noncommuting Quantum States Cannot Be Broadcast

The fledgling field of quantum information theory serves perhaps its most important role in delimiting wholly new classes of what is and is not physically possible. A particularly elegant example of this is the theorem that there are no physical means with which an unknown pure quantum state can be reproduced or copied. This situation is often summarized with the phrase, “quantum states cannot be cloned.” Here, we demonstrate an impossibility theorem that extends and generalizes the pure-state no-cloning theorem to mixed quantum states. This theorem strikes very close to the heart of the distinction between the classical and quantum theories, because it provides a nontrivial physical classification of commuting versus noncommuting states.

In this Section we ask whether there are any physical means—fixed independently of the identity of a quantum state—for broadcasting that quantum state onto two separate quantum systems. By broadcasting we mean that the marginal density operator of each of the separate systems is the same as the state to be broadcast.

The pure-state “no-cloning” theorem prohibits broadcasting pure states. This is because the only way to broadcast a pure state |ψ⟩ is to put the two systems in the product state |ψ⟩ ⊗ |ψ⟩, i.e., to clone |ψ⟩. Things are more complicated when the states are mixed. A mixed-state no-cloning theorem is not sufficient to demonstrate no-broadcasting, for there are many conceivable ways to broadcast a mixed state ρ without the joint state being in the product form ρ ⊗ ρ, the mixed-state analog of cloning; the systems might be correlated or entangled in such a way as to give the right marginal density operators. For instance, if the density operator has the spectral decomposition

\[ ρ = \sum_b \lambda_b |b⟩⟨b| , \tag{4.46} \]

a potential broadcasting state is the highly correlated joint state

\[ \tilde{ρ} = \sum_b \lambda_b |b⟩|b⟩⟨b| , \tag{4.47} \]

which, though not of the product form ρ ⊗ ρ, reproduces the correct marginal density operators.

The general problem, posed formally, is this. A quantum system AB is composed of two parts, A and B, each having an N-dimensional Hilbert space. System A is secretly prepared in one state from a set \( A = \{ \rho_0, \rho_1 \} \) of two quantum states. System B, slated to receive the unknown state, is in a standard quantum state Σ. The initial state of the composite system AB is the product state \( ρ_s ⊗ Σ \), where s = 0 or 1 specifies which state is to be broadcast. We ask whether there is any

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3This Section represents a collaboration with Howard Barnum, Carlton M. Caves, Richard Jozsa, and Benjamin Schumacher. The presentation here is based largely on a manuscript submitted to Physical Review Letters; as such, it contains a small redundancy with the previous Chapters. Also note that this Section breaks from the notation of the rest of the dissertation in that operators are not distinguished by hats; for instance we now write ρ instead of \( \hat{ρ} \).
physical process \( \mathcal{E} \), consistent with the laws of quantum theory, that leads to an evolution of the form
\[
\rho_s \otimes \Sigma \rightarrow \mathcal{E}(\rho_s \otimes \Sigma) = \tilde{\rho}_s ,
\] (4.48)
where \( \tilde{\rho}_s \) is any state on the \( N^2 \)-dimensional Hilbert space \( AB \) such that
\[
\text{tr}_A(\tilde{\rho}_s) = \rho_s \quad \text{and} \quad \text{tr}_B(\tilde{\rho}_s) = \rho_s .
\] (4.49)

Here \( \text{tr}_A \) and \( \text{tr}_B \) denote partial traces over \( A \) and \( B \). If there is an \( \mathcal{E} \) that satisfies Eq. (4.49) for both \( \rho_0 \) and \( \rho_1 \), then the set \( \mathcal{A} \) can be broadcast. A special case of broadcasting is the evolution specified by
\[
\mathcal{E}(\rho_s \otimes \Sigma) = \rho_s \otimes \rho_s .
\] (4.50)
We reserve the word cloning for this strong form of broadcasting.

The most general action \( \mathcal{E} \) on \( AB \) consistent with quantum theory is to allow \( AB \) to interact unitarily with an auxiliary quantum system \( C \) in some standard state and thereafter to ignore the auxiliary system [26]; that is,
\[
\mathcal{E}(\rho_s \otimes \Sigma) = \text{tr}_C(U(\rho_s \otimes \Sigma \otimes \Upsilon)U^\dagger),
\] (4.51)
for some auxiliary system \( C \), some standard state \( \Upsilon \) on \( C \), and some unitary operator \( U \) on \( ABC \). We show that such an evolution can lead to broadcasting if and only if \( \rho_0 \) and \( \rho_1 \) commute. (In this way the concept of broadcasting makes a communication theoretic cut between commuting and noncommuting density operators, and thus between classical and quantum state descriptions.) We further show that \( \mathcal{A} \) is clonable if and only if \( \rho_0 \) and \( \rho_1 \) are identical or orthogonal, i.e.,
\[
\rho_0 \rho_1 = 0 .
\] (4.52)

To see that the set \( \mathcal{A} \) can be broadcast when the states commute, we do not have to go to the extra trouble of attaching an auxiliary system. Since orthogonal pure states can be cloned, broadcasting can be obtained by cloning the simultaneous eigenstates of \( \rho_0 \) and \( \rho_1 \). Let \( |b\rangle, \ b = 1, \ldots, N \), be an orthonormal basis for \( A \) in which both \( \rho_0 \) and \( \rho_1 \) are diagonal, and let their spectral decompositions be
\[
\rho_s = \sum_b \lambda_{sb}|b\rangle\langle b| .
\] (4.53)
Consider any unitary operator \( U \) on \( AB \) consistent with
\[
U|b\rangle|1\rangle = |b\rangle|b\rangle .
\] (4.54)
If we choose \( \Sigma = |1\rangle\langle 1| \) and let
\[
\tilde{\rho}_s = U(\rho_s \otimes \Sigma)U^\dagger = \sum_b \lambda_{sb}|b\rangle\langle b| ,
\] (4.55)
we immediately have that \( \tilde{\rho}_0 \) and \( \tilde{\rho}_1 \) satisfy Eq. (4.49).

The converse of this statement—that if \( \mathcal{A} \) can be broadcast, \( \rho_0 \) and \( \rho_1 \) commute—is more difficult to prove. Our proof is couched in terms of the concept of fidelity between two density operators. The fidelity \( F(\rho_0, \rho_1) \) is defined by
\[
F(\rho_0, \rho_1) = \text{tr} \left( \sqrt{\rho_0^{1/2} \rho_1 \rho_0^{1/2}} \right) ,
\] (4.56)
where for any positive operator $O$, i.e., any Hermitian operator with nonnegative eigenvalues, $O^{1/2}$ denotes its unique positive square root. (Note that Ref. [9] defines fidelity to be the square of the present quantity.) Fidelity is an analogue of the modulus of the inner product for pure states [7, 9] and can be interpreted as a measure of distinguishability for quantum states: it ranges between 0 and 1, reaching 0 if and only if the states are orthogonal and reaching 1 if and only if $\rho_0 = \rho_1$. It is invariant under the interchange $0 \leftrightarrow 1$ and under the transformation

$$\rho_0 \rightarrow U\rho_0 U^\dagger \quad \text{and} \quad \rho_1 \rightarrow U\rho_1 U^\dagger$$  \hspace{1cm} (4.57)

for any unitary operator $U$ [9, 149]. Also, from the properties of the direct product, one has that

$$F(\rho_0 \otimes \sigma_0, \rho_1 \otimes \sigma_1) = F(\rho_0, \rho_1)F(\sigma_0, \sigma_1) . \hspace{1cm} (4.58)$$

Another reason $F(\rho_0, \rho_1)$ defines a good notion of distinguishability [8] is that it equals the minimal overlap between the probability distributions $p_0 (b) = \text{tr}(\rho_0 E_b)$ and $p_1 (b) = \text{tr}(\rho_1 E_b)$ generated by a generalized measurement or positive operator-valued measure (POVM) $\{E_b\}$ [26]. That is [149],

$$F(\rho_0, \rho_1) = \min_{\{E_b\}} \sum_b \sqrt{\text{tr}(\rho_0 E_b)} \sqrt{\text{tr}(\rho_1 E_b)} , \hspace{1cm} (4.59)$$

where the minimum is taken over all sets of positive operators $\{E_b\}$ such that

$$\sum_b E_b = 1 . \hspace{1cm} (4.60)$$

This representation of fidelity has the advantage of being defined operationally in terms of measurements. We call a POVM that achieves the minimum in Eq. (4.59) an optimal POVM.

One way to see the equivalence of Eqs. (4.59) and (4.56) is through the Schwarz inequality for the operator inner product $\text{tr}(AB^\dagger)$:

$$\text{tr}(AA^\dagger) \text{tr}(BB^\dagger) \geq |\text{tr}(AB^\dagger)|^2 , \hspace{1cm} (4.61)$$

with equality if and only if

$$A = \alpha B \hspace{1cm} (4.62)$$

for some constant $\alpha$. Going through this exercise is useful because it leads directly to the proof of the no-broadcasting theorem. Let $\{E_b\}$ be any POVM and let $U$ be any unitary operator. Using the cyclic property of the trace and the Schwarz inequality, we have that

$$\sum_b \sqrt{\text{tr}(\rho_0 E_b)} \sqrt{\text{tr}(\rho_1 E_b)} = \sum_b \sqrt{\text{tr}(U^{1/2} E_b \rho_0^{1/2} U^\dagger)} \sqrt{\text{tr}(\rho_1^{1/2} E_b \rho_1^{1/2})} \geq \sum_b \left| \text{tr}(U^{1/2} E_b \rho_0^{1/2} E_b^{1/2} \rho_1^{1/2}) \right| \geq \sum_b \left| \text{tr}(U^{1/2} E_b \rho_1^{1/2}) \right| = \left| \text{tr}(U^{1/2} \rho_1^{1/2}) \right| . \hspace{1cm} (4.63)$$

We can use the freedom in $U$ to make the inequality as tight as possible. To do this, we recall [8, 72] that

$$\max_V |\text{tr}(VO)| = \text{tr} \sqrt{O^2} \hspace{1cm} (4.65)$$

115
where $O$ is any operator and the maximum is taken over all unitary operators $V$. The maximum is achieved only by those $V$ such that

$$VO = \sqrt{OV} e^{-i\phi}, \quad (4.66)$$

where $\phi$ is an arbitrary phase. That there exists at least one such $V$ is insured by the operator polar decomposition theorem [75]. Therefore, by choosing

$$e^{i\phi} U_{0}^{1/2} \rho_{1}^{1/2} = \sqrt{\rho_{1}} \rho_{0}^{1/2} \rho_{1}^{1/2}, \quad (4.67)$$

we get that

$$\sum_{b} \sqrt{\text{tr}(\rho_{0} E_{b})} \sqrt{\text{tr}(\rho_{1} E_{b})} \geq F(\rho_{0}, \rho_{1}). \quad (4.68)$$

To find optimal POVMs, we consult the conditions for equality in Eq. (4.64). These arise from Step (4.63) and the one following it: a POVM $\{E_{b}\}$ is optimal if and only if

$$U_{0}^{1/2} \rho_{1}^{1/2} E_{b} = \mu_{b} \rho_{1}^{1/2} E_{b}, \quad (4.69)$$

and $U$ is rephased such that

$$\text{tr}(U_{0}^{1/2} \rho_{1}^{1/2} E_{b}) = \mu_{b} \text{tr}(\rho_{1} E_{b}) \geq 0 \iff \mu_{b} \geq 0. \quad (4.70)$$

When $\rho_{1}$ is invertible, Eq. (4.69) becomes

$$M E_{b}^{1/2} = \mu_{b} E_{b}^{1/2}, \quad (4.71)$$

where

$$M = \rho_{1}^{-1/2} U_{0}^{1/2} \rho_{1}^{-1/2} \rho_{1}^{-1/2} \rho_{1}^{-1/2} \rho_{1}^{-1/2} \quad (4.72)$$

is a positive operator. Therefore one way to satisfy Eq. (4.69) with $\mu_{b} \geq 0$ is to take $E_{b} = |b\rangle\langle b|$, where the vectors $|b\rangle$ are an orthonormal eigenbasis for $M$, with $\mu_{b}$ chosen to be the eigenvalue of $|b\rangle$. When $\rho_{1}$ is noninvertible, there are still optimal POVMs. One can choose the first $E_{b}$ to be the projector onto the null subspace of $\rho_{1}$; in the support of $\rho_{1}$, i.e., the orthocomplement of the null subspace, $\rho_{1}$ is invertible, so one can construct the analogue of $M$ and proceed as for an invertible $\rho_{1}$. Note that if both $\rho_{0}$ and $\rho_{1}$ are invertible, $M$ is invertible.

We begin the proof of the no-broadcasting theorem by using Eq. (4.59) to show that fidelity cannot decrease under the operation of partial trace; this gives rise to an elementary constraint on all potential broadcasting processes $E$. Suppose Eq. (4.49) is satisfied for the process $E$ of Eq. (4.51), and let $\{E_{b}\}$ denote an optimal POVM for distinguishing $\rho_{0}$ and $\rho_{1}$. Then, for each $s$,

$$\text{tr}(\tilde{\rho}_{s}(E_{b} \otimes 1)) = \text{tr}_{\lambda}(\text{tr}_{b}(\tilde{\rho}_{s}) E_{b}) = \text{tr}_{\lambda}(\rho_{s} E_{b}); \quad (4.73)$$

it follows that

$$F_{\lambda}(\rho_{0}, \rho_{1}) = \sum_{b} \sqrt{\text{tr}(\tilde{\rho}_{0}(E_{b} \otimes 1))} \sqrt{\text{tr}(\tilde{\rho}_{1}(E_{b} \otimes 1))} \geq \min_{\{E_{c}\}} \sum_{c} \sqrt{\text{tr}(\tilde{\rho}_{0} E_{c})} \sqrt{\text{tr}(\tilde{\rho}_{1} E_{c})} = F(\tilde{\rho}_{0}, \tilde{\rho}_{1}). \quad (4.74)$$
Here \( F_A(\rho_0, \rho_1) \) denotes simply the fidelity \( F(\rho_0, \rho_1) \), but the subscript \( A \) emphasizes that \( F_A(\rho_0, \rho_1) \) stands for the particular representation on the first line. The inequality in Eq. (4.74) comes from the fact that \( \{E_b \otimes 1\} \) might not be an optimal POVM for distinguishing \( \tilde{\rho}_0 \) and \( \tilde{\rho}_1 \); this demonstrates the said partial trace property. Similarly since

\[
\text{tr}(\tilde{\rho}_s(1 \otimes E_b)) = \text{tr}_B(\text{tr}_A(\tilde{\rho}_s(1 \otimes E_b))) = \text{tr}_B(\rho_s E_b),
\]

it follows that

\[
F_B(\rho_0, \rho_1) \equiv \sum_b \sqrt{\text{tr}(\tilde{\rho}_0(1 \otimes E_b))} \sqrt{\text{tr}(\tilde{\rho}_1(1 \otimes E_b))} \geq F(\tilde{\rho}_0, \tilde{\rho}_1),
\]

where the subscript \( B \) emphasizes that \( F_B(\rho_0, \rho_1) \) stands for the representation on the first line.

On the other hand, we can just as easily derive an inequality that is opposite to Eqs. (4.74) and (4.76). By the direct product formula and the invariance of fidelity under unitary transformations,

\[
F(\rho_0, \rho_1) = F(\rho_0 \otimes \Sigma \otimes \Upsilon, \rho_1 \otimes \Sigma \otimes \Upsilon) = F(U(\rho_0 \otimes \Sigma \otimes \Upsilon)U^\dagger, U(\rho_1 \otimes \Sigma \otimes \Upsilon)U^\dagger).
\]

(4.77)

Therefore, by the partial-trace property,

\[
F(\rho_0, \rho_1) \leq F\left(\text{tr}_C\left(U(\rho_0 \otimes \Sigma \otimes \Upsilon)U^\dagger\right), \text{tr}_C\left(U(\rho_1 \otimes \Sigma \otimes \Upsilon)U^\dagger\right)\right),
\]

(4.78)

or, more succinctly,

\[
F(\rho_0, \rho_1) \leq F(\mathcal{E}(\rho_0 \otimes \Sigma), \mathcal{E}(\rho_1 \otimes \Sigma)) = F(\tilde{\rho}_0, \tilde{\rho}_1).
\]

(4.79)

The elementary constraint now follows: the only way to maintain Eqs. (4.74), (4.76), and (4.79) is with strict equality. In other words, we have that if the set \( \mathcal{A} \) can be broadcast, then there are density operators \( \tilde{\rho}_0 \) and \( \tilde{\rho}_1 \) on \( AB \) satisfying Eq. (4.49) and

\[
F_A(\rho_0, \rho_1) = F(\tilde{\rho}_0, \tilde{\rho}_1) = F_B(\rho_0, \rho_1).
\]

(4.80)

Let us pause at this point to consider the restricted question of cloning. If \( \mathcal{A} \) is to be clonable, there must exist a process \( \mathcal{E} \) such that \( \tilde{\rho}_s = \rho_s \otimes \rho_s \) for \( s = 0, 1 \). But then, by Eq. (4.80), we must have

\[
F(\rho_0, \rho_1) = F(\rho_0 \otimes \rho_0, \rho_1 \otimes \rho_1) = \left(\frac{1}{2} F(\rho_0, \rho_1)\right)^2,
\]

(4.81)

which means that \( F(\rho_0, \rho_1) = 1 \) or 0, i.e., \( \rho_0 \) and \( \rho_1 \) are identical or orthogonal. There can be no cloning for density operators with nontrivial fidelity. The converse, that orthogonal and identical density operators can be cloned, follows, in the first case, from the fact that they can be distinguished by measurement and, in the second case, because they need not be distinguished at all.

Like the pure-state no-cloning theorem [3, 4], this no-cloning result for mixed states is a consistency requirement for the axiom that quantum measurements cannot distinguish nonorthogonal
states with perfect reliability. If nonorthogonal quantum states could be cloned, there would exist a measurement procedure for distinguishing those states with arbitrarily high reliability: one could make measurements on enough copies of the quantum state to make the probability of a correct inference of its identity arbitrarily high. That this consistency requirement, as expressed in Eq. (4.80), should also exclude more general kinds of broadcasting problems is not immediately obvious. Nevertheless, this is the content of our claim that Eq. (4.80) generally cannot be satisfied; any broadcasting process can be viewed as creating distinguishability \textit{ex nihilo} with respect to measurements on the larger Hilbert space AB. Only for the case of commuting density operators does broadcasting not create any extra distinguishability.

We now show that Eq. (4.80) implies that \( \rho_0 \) and \( \rho_1 \) commute. To simplify the exposition, we assume that \( \rho_0 \) and \( \rho_1 \) are invertible. We proceed by studying the conditions necessary for the representations \( F_A(\rho_0, \rho_1) \) and \( F_B(\rho_0, \rho_1) \) in Eqs. (4.74) and (4.76) to equal \( F(\tilde{\rho}_0, \tilde{\rho}_1) \). Recall that the optimal POVM \( \{E_b\} \) for distinguishing \( \rho_0 \) and \( \rho_1 \) can be chosen so that the POVM elements \( E_b = |b\rangle\langle b| \) are a complete set of orthogonal one-dimensional projectors onto orthonormal eigenstates of \( M \). Then, repeating the steps leading from Eqs. (4.64) to (4.70), one finds that the necessary conditions for equality in Eq. (4.80) are that each

\[
E_b \otimes \mathbb{1} = (E_b \otimes \mathbb{1})^{1/2}
\]

and each

\[
\mathbb{1} \otimes E_b = (\mathbb{1} \otimes E_b)^{1/2}
\]

satisfy

\[
\tilde{U} \tilde{\rho}_0^{1/2} (\mathbb{1} \otimes E_b) = \alpha_b \tilde{\rho}_1^{1/2} (\mathbb{1} \otimes E_b),
\]

and

\[
\tilde{V} \tilde{\rho}_0^{1/2} (E_b \otimes \mathbb{1}) = \beta_b \tilde{\rho}_1^{1/2} (E_b \otimes \mathbb{1}),
\]

where \( \alpha_b \) and \( \beta_b \) are nonnegative numbers and \( \tilde{U} \) and \( \tilde{V} \) are unitary operators satisfying

\[
\tilde{U} \tilde{\rho}_0^{1/2} \tilde{\rho}_1^{1/2} = \tilde{V} \tilde{\rho}_0^{1/2} \tilde{\rho}_1^{1/2} = \sqrt{\tilde{\rho}_0^{1/2} \tilde{\rho}_1^{1/2} \tilde{\rho}_0^{1/2} \tilde{\rho}_1^{1/2}}.
\]

Although \( \rho_0 \) and \( \rho_1 \) are assumed invertible, one cannot demand that \( \tilde{\rho}_0 \) and \( \tilde{\rho}_1 \) be invertible—a glance at Eq. (4.55) shows that to be too restrictive. This means that \( \tilde{U} \) and \( \tilde{V} \) need not be the same. Also we cannot assume that there is any relation between \( \alpha_b \) and \( \beta_b \).

The remainder of the proof consists in showing that Eqs. (4.84) through (4.86), which are necessary (though perhaps not sufficient) for broadcasting, are nevertheless restrictive enough to imply that \( \rho_0 \) and \( \rho_1 \) commute. The first step is to sum over \( b \) in Eqs. (4.84) and (4.85). Defining the positive operators

\[
G = \sum_b \alpha_b |b\rangle\langle b|
\]

and

\[
H = \sum_b \beta_b |b\rangle\langle b|
\]

we obtain

\[
\tilde{U} \tilde{\rho}_0^{1/2} = \tilde{\rho}_1^{1/2} (\mathbb{1} \otimes G)
\]

and

\[
\tilde{V} \tilde{\rho}_0^{1/2} = \tilde{\rho}_1^{1/2} (H \otimes \mathbb{1})
\]
The next step is to demonstrate that $G$ and $H$ are invertible and, in fact, equal to each other. Multiplying the two equations in Eq. (4.90) from the left by $\tilde{\rho}_0^{1/2} \tilde{U}^\dagger$ and $\tilde{\rho}_0^{1/2} \tilde{V}^\dagger$, respectively, and partial tracing the first over $A$ and the second over $B$, we get

$$\rho_0 = \text{tr}_A \left( \tilde{\rho}_0^{1/2} \tilde{U}^\dagger \tilde{\rho}_1^{1/2} \right) G \quad (4.91)$$

and

$$\rho_0 = \text{tr}_B \left( \tilde{\rho}_0^{1/2} \tilde{V}^\dagger \tilde{\rho}_1^{1/2} \right) H \quad (4.92)$$

Since, by assumption, $\rho_0$ is invertible, it follows that $G$ and $H$ are invertible. Returning to Eq. (4.90), multiplying both parts from the left by $\tilde{\rho}_1^{1/2}$ and tracing over $A$ and $B$, respectively, we obtain

$$\text{tr}_A \left( \tilde{\rho}_1^{1/2} \tilde{U} \rho_0^{1/2} \right) = \rho_1 G \quad (4.93)$$

and

$$\text{tr}_B \left( \tilde{\rho}_1^{1/2} \tilde{V} \rho_0^{1/2} \right) = \rho_1 H \quad (4.94)$$

Conjugating Eqs. (4.93) and (4.94) and inserting the results into the two parts of Eq. (4.92) yields

$$\rho_0 = G \rho_1 G \quad \text{and} \quad \rho_0 = H \rho_1 H \quad (4.95)$$

This shows that $G = H$, because these equations have a unique positive solution, namely the operator $M$ of Eq. (4.72). This can be seen by multiplying Eq. (4.95) from the left and right by $\tilde{\rho}_1^{1/2}$ to get

$$\rho_1^{1/2} \rho_0 \rho_1^{1/2} = \left( \rho_1^{1/2} G \rho_1^{1/2} \right)^2 \quad (4.96)$$

The positive operator $\rho_1^{1/2} G \rho_1^{1/2}$ is thus the unique positive square root of $\rho_1^{1/2} \rho_0 \rho_1^{1/2}$.

Knowing that

$$G = H = M \quad (4.97)$$

we return to Eqs. (4.89) and (4.90). The two, taken together, imply that

$$\tilde{V}^\dagger \tilde{U} \rho_0^{1/2} = \tilde{\rho}_0^{1/2} \left( M^{-1} \otimes M \right) \quad (4.98)$$

If $|b\rangle$ and $|c\rangle$ are eigenvectors of $M$, with eigenvalues $\mu_b$ and $\mu_c$, Eq. (4.98) implies that

$$\tilde{V}^\dagger \tilde{U} \left( \tilde{\rho}_0^{1/2} |b\rangle |c\rangle \right) = \frac{\mu_c}{\mu_b} \left( \tilde{\rho}_0^{1/2} |b\rangle |c\rangle \right) \quad (4.99)$$

This means that $\tilde{\rho}_0^{1/2} |b\rangle |c\rangle$ is zero or it is an eigenvector of the unitary operator $\tilde{V}^\dagger \tilde{U}$. In the latter case, since the eigenvalues of a unitary operator have modulus 1, it must be true that $\mu_b = \mu_c$. Hence we can conclude that

$$\tilde{\rho}_0^{1/2} |b\rangle |c\rangle = 0 \quad \text{when} \quad \mu_b \neq \mu_c \quad (4.100)$$

This is enough to show that $M$ and $\rho_0$ commute and hence

$$[\rho_0, \rho_1] = 0 \quad (4.101)$$
To see this, consider the matrix element
\[
\langle b' | (M \rho_0 - \rho_0 M) | b \rangle = (\mu_{b'} - \mu_b) \langle b' | \rho_0 | b \rangle
\]
\[
= (\mu_{b'} - \mu_b) \langle b' | [\text{tr}_A(\tilde{\rho}_0)] | b \rangle
\]
\[
= (\mu_{b'} - \mu_b) \sum_c \langle b' | (c \tilde{\rho}_0 | c) | b \rangle .
\]
(4.102)

If \( \mu_b = \mu_{b'} \), this is automatically zero. If, on the other hand, \( \mu_b \neq \mu_{b'} \), then the sum over \( c \) must vanish by Eq. (4.100). It follows that \( \rho_0 \) and \( M \) commute. Hence, using Eq. (4.95),
\[
\rho_1 \rho_0 = M^{-1} \rho_0 M^{-1} \rho_0
\]
\[
= \rho_0 M^{-1} \rho_0 M^{-1}
\]
\[
= \rho_0 \rho_1 .
\]
(4.103)
This completes the proof that noncommuting quantum states cannot be broadcast.

Note that, by the same method as above,
\[
\tilde{\rho}_1^{1/2} | b \rangle | c \rangle = 0 \quad \text{when} \quad \mu_b \neq \mu_c .
\]
(4.104)

This condition, along with Eq. (4.100), determines the conceivable broadcasting states, in which the correlations between the systems A and B range from purely classical to purely quantum. For example, since \( \rho_0 \) and \( \rho_1 \) commute, the states of Eq. (4.55) satisfy these conditions, but so do the perfectly entangled pure states
\[
| \tilde{\psi}_s \rangle = \sum_b \sqrt{\lambda_{sb}} | b \rangle | b \rangle .
\]
(4.105)

However, not all such potential broadcasting states can be realized by a physical process \( E \). The reason for this is quite intuitive: since the states \( \rho_0 \) and \( \rho_1 \) commute, the eigenvalues \( \lambda_{0b} \) and \( \lambda_{1b} \) correspond to two different probability distributions for the eigenvectors. Any device that could produce the states in Eq. (4.105) would have to essentially read the mind of the person who set the (subjective) probability assignments—clearly this cannot be done.

Nevertheless, this can be seen in a more formal way with a simple example. Suppose \( S(\rho_0) \neq S(\rho_1) \), where
\[
S(\rho) = -\text{tr}(\rho \ln \rho)
\]
(4.106)
denotes the von Neumann entropy. In order for the states in Eq. (4.105) to come about, the unitary operator in Eq. (4.51) must be such that
\[
U(\rho_s \otimes \Sigma \otimes \Upsilon) U^\dagger = | \tilde{\psi}_s \rangle \langle \tilde{\psi}_s | \otimes \Upsilon_s .
\]
(4.107)

It then follows, by the unitary invariance of the von Neumann entropy and the fact that entropies add across independent subsystems, that
\[
S(\rho_0) - S(\rho_1) = S(\Upsilon_0) - S(\Upsilon_1) .
\]
(4.108)

However,
\[
F(\rho_0, \rho_1) = | \langle \tilde{\psi}_0 | \tilde{\psi}_1 \rangle |
\]
by construction. Therefore, by Eq. (4.107), \( F(\Upsilon_0, \Upsilon_1) = 1 \). Hence \( \Upsilon_0 = \Upsilon_1 \) and it follows that Eq. (4.108) cannot be satisfied.
In closing, we mention an application of this result. In some versions of quantum cryptography, the legitimate users of a communication channel encode the bits 0 and 1 into nonorthogonal pure states. This is done to ensure that any eavesdropping is detectable, since eavesdropping necessarily disturbs the states sent to the legitimate receiver. If the channel is noisy, however, causing the bits to evolve to noncommuting mixed states, the detectability of eavesdropping is no longer a given. The result presented here shows that there are no means available for an eavesdropper to obtain the signal, noise and all, intended for the legitimate receiver without in some way changing the states sent to the receiver. Because the dimensionality of the density operators in the no-broadcasting theorem are completely arbitrary, this conclusion holds for all possible eavesdropping attacks. This includes those schemes where measurements are made on whole strings of quantum systems rather than the individual ones.
Chapter 5

References for Research in Quantum Distinguishability and State Disturbance

“Of course, serendipity played its role—some of the liveliest specimens . . . were found while looking for something else.”

—Nicolas Slonimsky
Lexicon of Musical Invective

This Chapter contains 528 references that may be useful in answering the following questions in all their varied contexts: “How statistically distinguishable are quantum states?” and “What is the best tradeoff between disturbance and inference in quantum measurement?” References are grouped under three major headings: Progress Toward the Quantum Problem; Information Theory and Classical Distinguishability; and Matrix Inequalities, Operator Relations, and Mathematical Techniques.

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129


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145


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159


