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Operating Characteristics for Classical and Quantum Binary Hypothesis Testing

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ABSTRACT

This monograph addresses operating characteristics for binary hypothesis testing in both classical and quantum settings and overcomplete quantum measurements for quantum binary state discrimination. We specifically explore decision and measurement operating characteristics defined as the tradeoff between probability of detection and probability of false alarm as parameters of the pre-decision operator and the binary decision rule are varied. In the classical case we consider in detail the Neyman-Pearson optimality of the operating characteristics when they are generated using threshold tests on a scalar score variable rather than threshold tests on the likelihood ratio. In the quantum setting, informationally overcomplete POVMs are explored to provide robust quantum binary state discrimination. We focus on equal trace rank one POVMs which can be specified by arrangements of points on a sphere that we refer to as an Etro sphere.
## Nomenclature

| Abbreviation | Description                                               | Page |
|--------------|------------------------------------------------------------|------|
| ROC          | Receiver operating characteristic                         | 3    |
| POVM         | Positive operator-valued measure                          | 4    |
| IC           | Informationally complete                                  | 5    |
| IOC          | Informationally overcomplete                              | 5    |
| Etro         | Equal trace rank one                                      | 5    |
| LRT          | Likelihood ratio test                                     | 7    |
| SVT          | Score variable threshold test                             | 7    |
| CDOC         | Classical decision operating characteristic               | 7    |
| CMOC         | Classical measurement operating characteristic            | 7    |
| MPE          | Minimum probability of error                              | 11   |
| MAP          | Maximum a posteriori                                      | 11   |
| AUC          | Area under an ROC                                          | 16   |
| CDF          | Cumulative distribution function                           | 18   |
| Nomenclature | Description | Page |
|--------------|-------------|------|
| QMS          | Quantum mechanical system                      | 28   |
| QDOC         | Quantum decision operating characteristic       | 29   |
| QMOC         | Quantum measurement operating characteristic    | 29   |
| ENTF         | Equal norm tight frame                          | 63   |
| Etro         | Equal trace rank one                            | 65   |
Preamble

Our intention while preparing this monograph has been for it to be readable and interesting to an audience with a wide range of backgrounds. It is written to have a strong tutorial review flavor with some perspectives that hopefully many readers will find to be interesting and somewhat novel. We anticipate that many parts of the monograph will be familiar to readers with a strong background in classical signal processing and other parts to readers with a strong background in quantum mechanics. And it is our hope that both audiences will find the perspectives on the shared issues and overlap between the two fields to be interesting. Some readers may find it helpful in acquiring a broad sense of the scope of the monograph to start by reading the summary remarks and further thoughts given in Section 7. It should be noted however, that the discussion there uses terminology and notation introduced in earlier sections. In writing a monograph intended for an audience with diverse backgrounds part of the challenge is that there are many results referred to in the presentation that will be well-known to readers with backgrounds in one of the disciplines but less so in the other. And with some of these results, we anticipate that some of the readers will want to see or be reminded of a somewhat detailed explanation while others will be very familiar with it. To accommodate these differences we identify these as exercises for the reader to be worked out or not as they choose. The details for verifying those results are contained in the appendix.
denoted as Appendix A. A second appendix denoted as Appendix B contains the details of a variety of possibly less familiar results that would be included in a traditional appendix mainly for the purpose of not interrupting the flow of the main body.
Binary decisions guide our everyday lives in situations both critical and trivial. The choices made by politicians and physicians may have consequential implications on a global or individual scale. Perhaps less consequential is whether or not we choose to carry an umbrella on a cloudy day. Any choice made inherently involves a conscious, subconscious, or formal tradeoff between benefits and detriments. The defense of a country, the prolongation of life, the ability to keep dry in a downpour, may come at the cost of soldiers’ lives, the quality of life of an individual patient, or the wasted effort of toting an umbrella on a rain-free day. In some cases our analysis of the compounding factors may be informal and the worst case outcome fairly inconsequential. But when the worst case outcome could have severe consequences as, for example, in a clinical setting or when deciding whether or not to fire a missile, it is much more desirable to have a structured analysis and process for arriving at a final decision. This may be a complicated task for many reasons, including the fact that the assignment of relative costs to the outcomes of the two possible decisions is often a judgement call itself. We may also lack a historical dataset that is large enough to allow for accurate estimation of important quantities such as the a priori probabilities, discussed further in Section 2.
In this monograph we focus on a particular set of well-studied metrics for framing the problem of binary hypothesis testing, keeping in mind that there are many alternatives, generalizations, and extensions of the viewpoints and results expressed here. We specifically consider the scenario in which one of two possible hypotheses, denoted as $H_0$ or $H_1$, is true. The objective is to make a decision as to which is true using a sample value of a random variable often referred to as the score variable, which is comprised of one or more numerical values associated with the outcome of some measurement or observation. The score variable may be a scalar or a vector and may have been constructed as a composition of multiple measurements and observations. Traditionally $H_0$ is referred to as the null hypothesis and $H_1$ as the positive hypothesis, implying that $H_1$ is the hypothesis of significance (the target is present, the patient has the disease, etc.). In this monograph we use that convention. For convenience we refer to the entire system used to distinguish between the null and positive hypotheses as the discrimination system. The components of the discrimination system are defined in Section 2. Historically a quantity considered to be of significance in binary hypothesis testing is the probability of error, denoted as $P_e$ and defined as the probability of identifying $H_0$ to be true given that $H_1$ is in fact true or vice versa. Other probabilities that may be of interest are (i) the probability of detection, denoted by $P_d$ and defined as the probability of deciding that $H_1$ is true given that it is indeed true, (ii) the probability of a miss, denoted by $P_m$ and defined as the probability of deciding that $H_0$ is true given that in fact $H_1$ is true, and (iii) the probability of false alarm, denoted by $P_f$ and defined as the probability of deciding that $H_1$ is true given that $H_0$ is in fact true. Also of importance are the a priori probabilities associated with whether $H_0$ or $H_1$ is true apart from any measurement or decision. Various of these probabilities are connected mathematically through the rules of probability. For example, the probability of error can be expressed as a combination of the probability of detection, the probability of false alarm, and the underlying a priori probabilities.

Since in many scenarios the a priori probabilities are difficult or impossible to assess, it has become common in many contexts to formulate the decision making process without explicitly requiring knowledge
of these probabilities. One approach that has become widespread for accomplishing this is to focus on the tradeoff between $P_f$ and $P_d$, often displayed using what is commonly referred to as a receiver operating characteristic (ROC). ROCs originated in the radar signal detection community, where they were used to characterize systems that detected the presence or absence of military targets during World War II [1]. The use of ROCs has become increasingly prevalent in a very broad set of application areas including biostatistics and machine learning [2]–[8]. In contrast to the problem of radar signal detection for which there are often good mathematical models for the signals and disturbances, in other contexts the score variable is typically a finely-tuned combination of many measurements and is therefore often less amenable to mathematical analysis and modeling.

More generally, the term operating characteristic is used in this monograph to refer to any characterization, such as a curve, table, or graph, of the tradeoff between $P_f$ and $P_d$ as one or more parameters of the discrimination system is varied. When displaying operating characteristics we will choose to utilize a two-dimensional graph of $P_f$ versus $P_d$. Consequently the parameter or parameters being varied are not immediately visible or explicit. This is especially important in Sections 2.5.4 and 2.5.5 when we consider multiple operating characteristics that were generated using variations of distinct parameters but have identical graphs of $P_f$ versus $P_d$. We take the viewpoint that an operating characteristic itself is essentially a trajectory in a higher-dimensional space with coordinates corresponding to all of the parameters being varied in addition to $P_f$ and $P_d$. A graph of $P_f$ versus $P_d$ is the projection of this trajectory onto the $P_f$-$P_d$ plane. Distinct trajectories including those with different numbers of variable parameters may correspond to the same $P_f$-$P_d$ projection. For the majority of our discussion we will be concerned only with the characteristics of the $P_f$-$P_d$ projection of a given operating characteristic. Thus, for the sake brevity we will only explicitly distinguish between an operating characteristic and its $P_f$-$P_d$ projection when absolutely necessary, as in Sections 2.5.4 and 2.5.5.

Sections 2 and 3 of this monograph address operating characteristics associated with binary hypothesis testing in the classical setting and the setting of quantum mechanics, respectively. By “classical” we mean in
particular that the measurement or observation processes that lead to a realized value of the score variable are not constrained by the postulates of quantum mechanics. The principles of classical binary hypothesis testing are very well-understood and as outlined above, ROCs are widely used in many classical settings. The principles of quantum binary state discrimination are also well-formulated. As we discuss in Section 3, a typical formulation of the quantum binary state discrimination problem consists of a quantum mechanical system that has been prepared in one of two quantum states by two distinct laboratory procedures or physical environments, each corresponding to one of the two hypotheses $H_0$ or $H_1$. The objective is to decide which procedure was used based on the outcome of a measurement on the system. An elegant solution to the problem of determining the measurement strategy that achieves minimum probability of error was derived by Helstrom [9].

Just as in the classical setting, the above formulation of the quantum binary hypothesis testing problem naturally involves a tradeoff between $P_f$ and $P_d$ and therefore it also involves the notion of an operating characteristic. But operating characteristics of any kind are significantly less prevalent in the quantum binary hypothesis testing literature. Perhaps one of the principal reasons for this is that although there are many similarities between the classical and quantum scenarios, there are also some fundamental differences that stem from the underlying differences between the postulates of classical versus quantum physics. Of particular importance and as described in Section 3 are the stipulations made by the postulates of quantum mechanics about the state of a quantum system and about the concept of quantum measurement. Of particular importance is the relationship between a specific quantum measurement and a set of Hermitian operators that form a positive operator-valued measure (POVM).

The theme of Sections 4 through 6 is how quantum measurements that employ redundant, or overcomplete, representations of the state of the system being measured can be used, at least in some cases, to increase the robustness of binary discrimination strategies. We start in Section 4 by describing our viewpoint on some of the basic concepts of frame theory, with the main objective of introducing the mathematical machinery and notation necessary to apply the concepts to quantum
measurement. We then describe how these concepts can be applied to an operator space consisting of all Hermitian operators on another Hilbert space. The relevant operator space $\mathcal{V}$ in quantum mechanics contains all density operators and POVM elements. This leads to a discussion in Section 5 regarding informationally complete (IC) quantum measurements, which are measurements that map every quantum state to a unique probability distribution over the possible measurement outcomes [10]–[22]. IC quantum measurements that are strictly overcomplete are sometimes referred to as informationally overcomplete (IOC) quantum measurements [19]. While the benefits of using IOC measurements have been investigated in the context of quantum state estimation [19], [20], less attention has been given to their utility in quantum binary state discrimination. We review a fundamental result stating that every IC or IOC POVM is a frame for $\mathcal{V}$. IOC POVMs with a larger number $M$ of elements correspond to frame representations of $\mathcal{V}$ that are more overcomplete.

A crucial concept in our discussion of the operator space $\mathcal{V}$ is a specific direct-sum decomposition of $\mathcal{V}$ into two orthogonal subspaces $\mathcal{U}$ and $\mathcal{U}^\perp$. All density operators have a constant component in $\mathcal{U}^\perp$ and can be distinguished from each other by their components in $\mathcal{U}$. For the density operator of a qubit the component in $\mathcal{U}^\perp$ corresponds to its Bloch vector. We define a counterpart to the Bloch ball and corresponding Bloch sphere in relation to the class of POVMs that we refer to as equal trace rank one (Etro) POVMs. An Etro POVM corresponding to a qubit measurement can be fully specified by $M$ points on what we refer to as an Etro sphere of radius $\sqrt{2}/M$. This is exactly analogous to how a pure state qubit density operator can be specified by a single point on the Bloch sphere. POVMs constructed using Platonic solids are Etro POVMs in our terminology and are used often in the literature. We provide evidence through simulation that when POVMs constructed from Platonic solids are used for qubit binary state discrimination, there is a tradeoff in probability of error between the number $L$ of identically-prepared quantum mechanical systems and the number $M$ of POVM elements. POVMs constructed from Platonic solids have been of particular interest in the quantum state estimation community because they are all either IC or IOC, and because they
all provide straightforward state reconstruction formulas. Since we are interested in state discrimination rather than estimation, we do not require the state to be reconstructed. Consequently in Section 6 we also performed an exploratory investigation into IC and IOC POVMs constructed using other arrangements of points on an Etro sphere. In particular the problem we consider is that of distinguishing between two pure state qubit density operators. It is assumed that the angle between their Bloch vectors is known but that the overall alignment of the Bloch vectors relative to the Bloch sphere is not. Equivalently, it is assumed that the two Bloch vectors are known and the relative rotational orientation of the Bloch and Etro spheres is unknown. We compare the performance of a variety of POVMs using their minimum and maximum probabilities of error over all possible orientations, as well as the difference between the two. Intuitively it is expected that higher values of $M$ and distributions of points on an Etro sphere that are maximally spread in some sense would lead to POVMs that are less sensitive to changes in the relative orientation of the Bloch and Etro spheres. Indeed, this is what we observed for values of $M$ between 4 and 12 and for distributions of points that were maximally spread with respect to numerous established criteria.
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Appendices
A

Optional Appendices

Since this monograph was intended for an audience with a diverse set of backgrounds, the purpose of the derivations contained in the following Appendices A.1 to A.10 is to provide some level of detail surrounding concepts and results that are likely familiar to some readers but perhaps not to others. Many of the derivations can also be found in some form in many classical signal processing, linear algebra, or quantum mechanics textbooks and review monographs. The title of each section contains a reference to the section in the main body of the monograph where the concept was first mentioned.

A.1 Optimal Neyman-Pearson Decision Regions

The following reasoning was adapted from [25]. Assume that the decision region $\mathcal{D}$ has been chosen to be Neyman-Pearson optimal. Then by definition it is impossible to modify it in such a way that $P_d$ is increased while $P_f$ stays the same. Mathematically we can think of modification of the decision region as taking two small portions of the real axis, one that lies in $\mathcal{D}$ and is denoted as the interval $[s, s + ds]$ and one that lies outside of $\mathcal{D}$ and is denoted as the interval $[s', s' + ds']$, and interchanging their decision region assignments. In other words, we
Optional Appendices

remove the interval \([s, s + ds]\) from \(\mathcal{D}\) and add the interval \([s', s' + ds']\). The resulting changes in \(P_f\) and \(P_d\) are

\[
\Delta P_f = f_0(s') ds' - f_0(s) ds \\
\Delta P_d = f_1(s') ds' - f_1(s) ds.
\]  

(A.1a)  

(A.1b)

If we assume that the value of \(P_f\) stays the same (\(\Delta P_f = 0\)), then since the original decision region was Neyman-Pearson optimal we know by definition that the value of \(P_d\) must have stayed the same or decreased (\(\Delta P_d \leq 0\)). Applying these conditions to Equations (A.1) and combining them together leads to the requirement that

\[
\frac{f_1(s') ds'}{f_0(s') ds'} \geq \frac{f_1(s) ds}{f_0(s) ds}.
\]  

(A.2)

After cancelling the factors of \(ds\) and \(ds'\), the right-hand side of the inequality is equal to the likelihood ratio at the point \(S = s\), which lay in the original, Neyman-Pearson optimal decision region \(\mathcal{D}\). Similarly, the left-hand side is the likelihood ratio as the point \(S = s'\), which lay outside of this region. Since the intervals \([s, s + ds]\) and \([s', s' + ds']\) were arbitrary so long as they lay inside or outside of \(\mathcal{D}\), respectively, Equation (A.2) says that for the Neyman-Pearson optimal decision region \(\mathcal{D}\), the likelihood ratio for values of the score variable lying inside \(\mathcal{D}\) is always greater than or equal to the likelihood ratio for values lying outside \(\mathcal{D}\). In other words, the Neyman-Pearson optimal decision regions represent a threshold test on the likelihood ratio.

### A.2 Orthonormality of the \(\{|w_k\}\) (Section 4.1)

We wish to show that no generality is lost by assuming that the basis vectors \(\{|w_k\}, 1 \leq k \leq M\) for \(\mathcal{W}\) are orthonormal with respect to the \(\langle \cdot | \cdot \rangle\) inner product. Assume that they are not and let \(\{|e_k\}\) be a basis for \(\mathcal{W}\) that is orthonormal with respect to the \(\langle \cdot | \cdot \rangle\) inner product. Thus

\[
\langle e_j | e_k \rangle = \delta_{jk}, \quad 1 \leq j, k \leq M,
\]  

(A.3)

where \(\delta_{jk}\) takes the value 1 if \(j = k\) and 0 otherwise. Now we define a function \(f(\cdot, \cdot)\) that takes two vectors in \(\mathcal{W}\) as input and outputs a
complex number. It is defined to satisfy the following properties,
\[
f(a u_j + b u_k, u_\ell) = a^* f(u_j, u_\ell) + b^* f(u_k, u_\ell) \tag{A.4a}
\]
\[
f(u_j, a u_k + b u_\ell) = a f(u_j, u_k) + b f(u_j, u_\ell) \tag{A.4b}
\]
\[
f(u_j, u_k) = f(u_k, u_j)^* \tag{A.4c}
\]
\[
f(w_j, w_k) = \delta_{jk}, \quad 1 \leq j, k \leq M. \tag{A.4d}
\]
In Equations (A.4), $|u_j\rangle$, $|u_k\rangle$, and $|u_\ell\rangle$ are arbitrary vectors in $W$, $a$ and $b$ are arbitrary complex numbers, and the superscript * indicates complex conjugation. Equations (A.4) imply that the function $f(\cdot, \cdot)$ is also positive definite. That is, if $|u\rangle = \sum_k c_k |w_k\rangle$ is an arbitrary nonzero vector in $W$, then $f(u, u) > 0$ since
\[
|u\rangle = \sum_{k=1}^{M} c_k |w_k\rangle \neq 0 \in W \quad \text{(arbitrary nonzero vector in W)}
\tag{A.5a}
\]
\[
f(u, u) = \left( \sum_{j=1}^{M} c_j |w_j\rangle, \sum_{k=1}^{M} c_k |w_k\rangle \right) \tag{A.5b}
\]
\[
= \sum_{j,k=1}^{M} c_j^* c_k f(w_j, w_k) \quad \text{by conjugate bilinearity} \tag{A.5c}
\]
\[
= \sum_{j=1}^{M} |c_j|^2 \quad \text{since } f(w_j, w_k) = \delta_{jk} \tag{A.5d}
\]
\[
> 0 \quad \text{since } |u\rangle \neq 0. \tag{A.5e}
\]
Thus $f(\cdot, \cdot)$ is a valid inner product function on $W$ and $\{|w_k\rangle\}$ is orthonormal with respect to this inner product. We will now show that there is an invertible linear operator $L$ on $W$ such that
\[
f(L |u_1\rangle, L |u_2\rangle) = \langle u_1 |u_2 \rangle \tag{A.6}
\]
for all $|u_1\rangle, |u_2\rangle \in W$. This implies that all calculations can be made with the $f(\cdot, \cdot)$ inner product, and then the inverse of $L$ can be used to “translate” the answers back to the $\langle \cdot | \cdot \rangle$ inner product. Note that
because the \(|w_k\rangle\) form a basis for \(\mathcal{W}\), to satisfy Equation (A.6) it is sufficient to have a linear operator \(L\) such that

\[
f(L |w_j\rangle , L |w_\ell\rangle ) = \langle w_j |w_\ell\rangle , \quad 1 \leq j, \ell \leq M. \tag{A.7}
\]

Equation (A.6) follows from Equation (A.7) by the properties of the inner product functions \(f(\cdot, \cdot)\) and \(\langle \cdot | \cdot \rangle\). To find an appropriate linear operator \(L\), let \(|w_j\rangle\) and \(|w_\ell\rangle\) be any two of the \(|w_k\rangle\) (possibly with \(j = \ell\)) and write them in terms of the \(|e_k\rangle\),

\[
|w_j\rangle = \sum_{k=1}^{M} a_k |e_k\rangle, \quad |w_\ell\rangle = \sum_{k=1}^{M} c_k |e_k\rangle. \tag{A.8}
\]

Substituting into the left- and right-hand sides of Equation (A.6) and simplifying, we find

\[
f(L |w_j\rangle , L |w_\ell\rangle ) = f \left( \sum_{k=1}^{M} a_k L |e_k\rangle , \sum_{m=1}^{M} d_m L |e_m\rangle \right)
\]

\[
= \sum_{k,m=1}^{M} a_k^* d_m f(L |e_k\rangle , L |e_m\rangle) \tag{A.9a}
\]

\[
\langle w_j |w_\ell\rangle = \left( \sum_{k=1}^{M} a_k |e_k\rangle \right) \left( \sum_{m=1}^{M} d_m |e_m\rangle \right) = \sum_{k=1}^{M} a_k^* d_k \tag{A.9b}
\]

For the two to be equal, it is sufficient to have \((L |e_k\rangle , L |e_m\rangle ) = \delta_{km}\) for all \(1 \leq k, m \leq M\). One operator that satisfies this condition is the linear operator \(L\) that is also defined to satisfy

\[
L |e_k\rangle = |w_k\rangle, \quad 1 \leq k \leq M. \tag{A.10}
\]

This operator is clearly invertible, and using it to further simplify the left-hand side of Equation (A.7) leads to

\[
(L |e_k\rangle , L |e_m\rangle ) = \sum_{k,m=1}^{M} a_k^* d_m f(w_k, w_m) = \sum_{k=1}^{M} a_k^* d_k, \tag{A.11}
\]

so Equation (A.7) is satisfied.
A.3 Expressions for a Synthesis Map (Section 4.2)

To see why $F_0$ can sometimes be written in the form $F_0 = \sum_k |f_k\rangle \langle g_k|$ where the $\{|g_k\rangle\}$ are different from the $\{|w_k\rangle\}$, note that instead of defining $F_0$ using Equation (4.5) we could equivalently define it according to the relation

$$F |w_k\rangle = |f_k\rangle, \quad 1 \leq k \leq M.$$  \hspace{1cm} (A.12)

Equation (4.5) then follows by linearity. For Equation (A.12) to be true the $\{|g_j\rangle\}$ must satisfy the relation

$$\sum_{j=1}^{M} |f_j\rangle \langle g_j| w_k\rangle = |f_k\rangle, \quad 1 \leq k \leq M.$$  \hspace{1cm} (A.13)

We can then expand the $\{|f_j\rangle\}$ and $\{|g_j\rangle\}$ as linear combinations of the $\{|w_j\rangle\}$ to arrive at a system of linear equations in which the unknowns are the basis coefficients of the $\{|g_j\rangle\}$. Depending on the frame, the equations may or may not have multiple solutions.

Another way to look at it is to note that if the $\{|f_k\rangle\}$ are linearly dependent, then there is a linear combination of them that is equal to zero. Let $\{b_k\}$ be a set of coefficients such that

$$\sum_{k=1}^{M} b_k |f_k\rangle = 0.$$  \hspace{1cm} (A.14)

Then to satisfy Equation (A.13) it is sufficient to have

$$\langle g_j| w_k\rangle = \delta_{jk} b_k, \quad 1 \leq j, k \leq M,$$  \hspace{1cm} (A.15)

where $\delta_{jk} = 1$ if $j = k$ and 0 otherwise. This is again a system of linear equations that may or may not have more than one solution depending on the frame.

A.4 The Adjoint of a Linear Transformation (Sections 4.2 and 4.3)

Assume that $\{|f_k\rangle\}$ is a given frame for $\mathcal{V}$ and that $A_0$ and $F_0$ are its analysis and synthesis maps, respectively. The adjoint of $F_0$, denoted by $F_0^\dagger$, is defined as the linear operator on $\mathcal{W}$ that satisfies

$$\langle u_1|F_0 u_2\rangle = \langle F_0^\dagger u_1| u_2\rangle \text{ for all } |u_1\rangle, |u_2\rangle \in \mathcal{W}.$$  \hspace{1cm} (A.16)
We wish to show that $F_0^\dagger = A_0$. Substituting Equation (4.6) into the left-hand side of Equation (A.16) and using the linearity of the inner product, we find
\[ \langle u_1 | F_0 u_2 \rangle = \sum_{k=1}^{M} \langle u_1 | f_k \rangle \langle w_k | u_2 \rangle. \quad (A.17) \]

On the other hand, since $\langle x | y \rangle = \langle y | x \rangle^*$ for any two vectors $|x\rangle, |y\rangle \in \mathcal{W}$, we have $\langle F_0^\dagger u_1 | u_2 \rangle = \langle u_2 | F_0^\dagger u_1 \rangle^*$. Substituting back into Equation (A.16) leads to
\[ \langle u_2 | F_0^\dagger u_1 \rangle = \left( \sum_{k=1}^{M} \langle u_1 | f_k \rangle \langle w_k | u_2 \rangle \right)^* \quad (A.18a) \]
\[ = \sum_{k=1}^{M} \langle u_2 | w_k \rangle \langle f_k | u_1 \rangle \quad (A.18b) \]
\[ = \langle u_2 | \left( \sum_{k=1}^{M} | w_k \rangle \langle f_k | \right) \langle u_1 \rangle, \quad (A.18c) \]
and since this must be true for all $|u_1\rangle, |u_2\rangle \in \mathcal{W}$, we must have
\[ F_0^\dagger = \sum_{k=1}^{M} | w_k \rangle \langle f_k | = A_0. \quad (A.19) \]

Next let $\mathcal{R}$ be an arbitrary subspace of $\mathcal{W}$ and consider the orthogonal projection operator $\mathcal{P}_\mathcal{R}$ from $\mathcal{W}$ onto $\mathcal{R}$. We wish to show that $\mathcal{P}_\mathcal{R}^\dagger = \mathcal{P}_\mathcal{R}$, i.e.,
\[ \langle u_1 | \mathcal{P}_\mathcal{R} u_2 \rangle = \langle \mathcal{P}_\mathcal{R}^\dagger u_1 | u_2 \rangle \quad \text{for all } |u_1\rangle, |u_2\rangle \in \mathcal{W}. \quad (A.20) \]
Equation (A.20) follows directly from decomposing $|u_1\rangle$ and $|u_2\rangle$ into their components in $\mathcal{R}$ and $\mathcal{R}^\perp$.

The notion of the adjoint of a linear transformation applies much more broadly beyond linear transformations acting on finite-dimensional Hilbert spaces (see, for example, [36]). We consider one extension below to linear transformations whose input and output vector spaces may be different, although we still assume that both spaces are finite-dimensional for simplicity. We will continue to use the superscript $\dagger$
to denote the adjoint. Consider two finite-dimensional Hilbert spaces $W_1$, $W_2$ and two linear transformations $T : W_1 \mapsto W_2$, $R : W_2 \mapsto W_1$ satisfying $R = T^\dagger$. We assume for simplicity that $W_1$ and $W_2$ have the same inner product denoted by $\langle \cdot | \cdot \rangle$, although this is solely for notational clarity. By definition we have

$$\langle u_2 | Tu_1 \rangle = \langle Ru_2 | u_1 \rangle \quad \text{for all} \quad |u_1\rangle \in W_1, |u_2\rangle \in W_2.$$  

(A.21)

As stated in Section 4.2, taking the complex conjugate of both sides of Equation (A.21) implies that $T = R^\dagger$. It is well-known that $T$ can always be written as a sum of rank-one operators of the form $|u_2\rangle \langle u_1|$ where $|u_1\rangle \in W_1$ and $|u_2\rangle \in W_2$. As an example, one possibility for expressing $A$ in this form would be to use its singular value decomposition. It is straightforward to show using a derivation exactly analogous to the one given above that $T^\dagger$ is the same sum of rank-one operators but with each term of the form $|u_2\rangle \langle u_1|$ replaced by $|u_1\rangle \langle u_2|$.

We will now show that $N(R) = R(T)^\perp$. It will follow by symmetry that $N(T) = R(R)^\perp$. Given an arbitrary vector $|u_2\rangle \in N(R)$, $|u_2\rangle$ must also be an element of $R(T)^\perp$. To see why this is true, let $|y\rangle$ be an arbitrary vector in $R(T)$. By definition there is some $|u_1\rangle \in W_1$ such that $|y\rangle = T|u_1\rangle$. Then $|u_2\rangle$ is orthogonal to $|y\rangle$,

$$\langle y | u_2 \rangle = \langle Tu_1 | u_2 \rangle = \langle u_1 | Ru_2 \rangle = 0.$$  

(A.22)

Since $|y\rangle$ was arbitrary, this implies that $N(R)$ is contained in $R(T)^\perp$. On the other hand, let $|u_2\rangle \in W_2$ be an arbitrary element of $R(T)^\perp$. By definition it must satisfy $\langle y | u_2 \rangle = 0$ for all $|y\rangle \in R(T)$, i.e., $\langle Tu_1 | u_2 \rangle = 0$ for all $|u_1\rangle \in W_1$. Then $R|u_2\rangle$ must equal 0,

$$\langle u_1 | Ru_2 \rangle = 0 \quad \text{for all} \quad |u_1\rangle \in W_1 \quad \text{(A.23a)}$$

$$R |u_2\rangle = 0.$$  

(A.23c)

This implies that $R(T)^\perp$ is contained in $N(R)$, and because the reverse is also true it must be that the two are identical.
A.5 The Canonical Dual Frame (Sections 4.3 and 4.6)

Let $|v\rangle$ be an arbitrary vector in $\mathcal{V}$ and let $\{|f_k\rangle\}$ be a frame for $\mathcal{V}$. We wish to find the dual frame $\{|\hat{f}_k\rangle\}$ of $\{|f_k\rangle\}$ that minimizes the squared norm of the coefficient vector $\hat{A}_0 |v\rangle = \sum_k \langle \hat{f}_k |v\rangle |w_k\rangle$. It is sufficient to solve for the analysis map $\hat{A}_0$ of the optimal dual frame. Denoting the synthesis map of $\{|f_k\rangle\}$ by $F_0$, the problem can be formulated as

\[
\begin{align*}
\text{minimize} & \quad ||\hat{A}_0 |v\rangle||^2 \\
\hat{A}_0 : \mathcal{V} \to \mathcal{W} & \quad \text{subject to} \quad F_0 \hat{A}_0 |v\rangle = |v\rangle
\end{align*}
\]

(A.24a)

(A.24b)

The optimal coefficient vector must satisfy $\hat{A}_0 |v\rangle \in R(A_0)$. To see why this is true, note that $\hat{A}_0 |v\rangle$ can always be written as the sum of a component in $R(A_0)$ and a component in $R(A_0) ^\perp = N(F_0)$,

\[
\hat{A}_0 |v\rangle = |w_1\rangle + |w_2\rangle
\]

(A.25)

where $|w_1\rangle \in R(A_0)$ and $|w_2\rangle \in N(F_0)$. We have $||\hat{A}_0 |v\rangle||^2 = ||w_1||^2 + ||w_2||^2$ and $F_0 \hat{A}_0 |v\rangle = F_0 |w_1\rangle$. Assume that Equation (A.25) holds for a given dual frame. If $|w_2\rangle$ were nonzero, then we could always find a different dual frame with analysis map $\hat{A}_0$ satisfying $\hat{A}_0 |v\rangle = |w_1\rangle$. Equation (A.24b) would still be satisfied ($F_0 \hat{A}_0 |v\rangle = F_0 |w_1\rangle = |v\rangle$) and the new coefficient vector would have smaller squared norm ($||\hat{A}_0 |v\rangle||^2 \leq ||\hat{A}_0 |v\rangle||^2$). Next note that since $|v\rangle$ was assumed to be arbitrary, Equation (A.24b) implies that $\dim R(\hat{A}_0) \geq N$. Since $\dim R(A_0) = N$ according to Section 4.2, the requirements that $\hat{A}_0 |v\rangle \in R(A_0)$ for arbitrary $|v\rangle \in \mathcal{V}$ and $\dim R(\hat{A}_0) \geq N$ together imply that the optimal analysis map satisfies $R(\hat{A}_0) = R(A_0)$. Therefore, by definition of $R(A_0)$ we must have $\hat{A}_0 |v\rangle = A_0 |x\rangle$ for some $|x\rangle \in \mathcal{V}$. Substituting into Equation (A.24b), we find that $F_0 \hat{A}_0 |v\rangle = F_0 A_0 |x\rangle$. It is straightforward to show that the operator $(F_0 A_0)$, often referred to as the frame operator of $\{|f_k\rangle\}$, is always invertible. Thus, $|x\rangle = (F_0 A_0)^{-1} |v\rangle$ and so $\hat{A}_0 |v\rangle = A_0 |x\rangle = A_0(F_0 A_0)^{-1} |v\rangle$. Again using the fact that $|v\rangle$ was assumed to be arbitrary, this implies that $\hat{A}_0 = A_0(F_0 A_0)^{-1}$, which is exactly equal to the analysis map of the canonical dual frame.

Next we wish to show that of all dual frames, the canonical dual frame minimizes the expected reconstruction error $\mathcal{E}$ as defined in
Equation (4.33). Note that the derivation given below does not assume that the analysis frame is an ENTF. The problem can be formulated as

\[
\begin{align*}
\minimize_{\tilde{F}_0 : \mathcal{W} \to \mathcal{V}} & \quad \mathbb{E} \left[ ||\tilde{F}_0 |w_e||^2 \right] \\
\text{subject to} & \quad \tilde{F}_0 A_0 |v\rangle = |v\rangle \text{ for all } |v\rangle \in \mathcal{V}
\end{align*}
\]  

(A.26a)

where the minimization is performed over all linear operators \( \tilde{F}_0 \) from \( \mathcal{W} \) to \( \mathcal{V} \). Equation (A.26b), which in effect specifies that \( \tilde{F}_0 \) must be the synthesis operator of a frame that is dual to the analysis frame, amounts to the requirement that \( \tilde{F}_0 \) is a left-inverse of \( A_0 \). A left-inverse is guaranteed to exist because as stated in Section 4.2, \( A_0 \) has rank \( N \).

Let \( \tilde{F}_0 \) be an arbitrary left-inverse of \( A_0 \) and assume that \( \{|w_k\rangle, 1 \leq k \leq M\} \) is an orthonormal basis for \( \mathcal{W} \). Further assume that the \( \{|w_k\rangle\} \) can be partitioned into an orthonormal \( \{|w_k\rangle, 1 \leq k \leq N\} \) for \( R(A_0) \) and an orthonormal \( \{|w_k\rangle, N + 1 \leq k \leq M\} \) for \( R(A_0)^\perp \). To fully specify the operator \( \tilde{F}_0 \), it is both necessary and sufficient to specify its action on each of the \( \{|w_k\rangle\} \). Its action on \( R(A_0) \) must be chosen to satisfy Equation (A.26b) while its action on \( R(A_0)^\perp \) can be chosen to minimize \( \mathbb{E} \left[ ||\tilde{F}_0 |w_e||^2 \right] \).

We first consider its action on \( R(A_0) \). For each \( \{|w_k\rangle, 1 \leq k \leq N\} \), there is a unique vector \( |v_k\rangle \in \mathcal{V} \) satisfying \( A_0 |v_k\rangle = |w_k\rangle \). Equation (A.26b) implies that \( \tilde{F}_0 |w_k\rangle = |v_k\rangle \) for all \( 1 \leq k \leq N \). The action of \( \tilde{F}_0 \) on \( R(A_0)^\perp \) can now be chosen to minimize \( ||\tilde{F}_0 |w_e||^2 \). Note that any error vector \( |w_e\rangle \in \mathcal{W} \) can be written uniquely as the sum of a component \( |w_1\rangle \in R(A_0) \) and a component \( |w_2\rangle \in R(A_0)^\perp \),

\[
|w_e\rangle = |w_1\rangle + |w_2\rangle = \sum_{k=1}^{N} c_k |w_k\rangle + \sum_{k=N+1}^{M} c_k |w_k\rangle,
\]  

(A.27)

where \( \{c_k\} \) are the coefficients of \( |w_e\rangle \) in the \( \{|w_k\rangle\} \) basis. Since the \( \{c_k\} \) are related to the \( \{e_k\} \) by an orthogonal transformation in \( \mathcal{W} \), they also have zero mean, variance \( \sigma^2 \), and are pairwise uncorrelated. The expected value of \( ||\tilde{F}_0 |w_e||^2 \) is

\[
\mathbb{E} \left[ ||\tilde{F}_0 |w_e||^2 \right] = \mathbb{E} \left[ ||\tilde{F}_0 |w_1\rangle + \tilde{F}_0 |w_2\rangle||^2 \right].
\]  

(A.28a)
As we will show below, the expected value is minimized when \( \tilde{F}_0 |w_2\) is set to zero for all possible values of \( w_2 \). The vector \( \tilde{F}_0 |w_e\) is equal to

\[
\tilde{F}_0 |w_e\rangle = \sum_{k=1}^{N} c_k \tilde{F}_0 |w_k\rangle + \sum_{k=N+1}^{M} c_k \tilde{F}_0 |w_k\rangle \tag{A.29a}
\]

\[
= \sum_{k=1}^{N} c_k |v_k\rangle + \sum_{k=N+1}^{M} c_k \tilde{F}_0 |w_k\rangle. \tag{A.29b}
\]

Its squared norm is equal to \( \langle \tilde{F}_0 |w_e\rangle |\tilde{F}_0 |w_e\rangle \rangle \), and since the \( \{c_k\} \) are pairwise uncorrelated all cross terms are equal to zero. Thus,

\[
\mathbb{E} \left[ ||\tilde{F}_0 |w_e\rangle ||^2 \right] = \mathbb{E} \left[ \sum_{k=1}^{N} c_k^2 ||v_k||^2 + \sum_{k=N+1}^{M} c_k^2 ||\tilde{F}_0 |w_k\rangle ||^2 \right] \tag{A.30a}
\]

\[
= \sum_{k=1}^{N} \mathbb{E}[c_k^2] ||v_k||^2 + \sum_{k=N+1}^{M} \mathbb{E}[c_k^2] ||\tilde{F}_0 |w_k\rangle ||^2 \tag{A.30b}
\]

\[
= \sigma^2 \sum_{k=1}^{N} ||v_k||^2 + \sigma^2 \sum_{k=N+1}^{M} ||\tilde{F}_0 |w_e\rangle ||^2. \tag{A.30c}
\]

Since the value of the first sum is fixed and since all terms in both sums must be non-negative, the minimal value is obtained when the second sum is equal to zero, which happens when \( \tilde{F}_0 |w_k\rangle = 0 \) for all \( N + 1 \leq k \leq M \). Thus, the optimal left-inverse \( \tilde{F}_0 \) inverts \( A_0 \) over its range and acts as the zero operator on \( R(A_0)^{\perp} \). The unique left-inverse with these properties is the Moore-Penrose pseudoinverse of \( A_0 \) (see, for example, Section 1 of [39]). Explicitly, the pseudoinverse is equal to

\[
A_0^* = (A_0^\dagger A_0)^{-1} A_0^\dagger = (F_0 A_0)^{-1} F_0, \tag{A.31}
\]

and this corresponds exactly to the synthesis operator of the canonical dual frame [39].

A.6 Naimark’s Theorem (Section 4.4.2)

Let \( \{|f_k\rangle\} \) be an arbitrary frame for \( \mathcal{V} \) and assume that there exists and orthonormal basis \( \{|w_k\rangle\} \) for \( \mathcal{W} \) that satisfies \( \mathcal{P}_\mathcal{V} |w_k\rangle = |f_k\rangle \) for
A.7 An Oversampling Frame in Classical Signal Processing

1 ≤ k ≤ M. As explained in Section 4.4.3, an arbitrary vector \( |v\rangle \in \mathcal{V} \) can always be written as

\[
|v\rangle = \sum_{k=1}^{M} \langle w_k |v\rangle |w_k\rangle = \sum_{k=1}^{M} b_k |w_k\rangle ,
\]

where we have defined \( b_k = \langle w_k |v\rangle \). Since the \( \{ |w_k\rangle \} \) are an orthonormal basis for \( \mathcal{W} \), the squared norm of \( |v\rangle \) is equal to the sum of the squared magnitudes of the \( \{ b_k \} \), \( ||v||^2 = \sum_k |b_k|^2 \). On the other hand and as also explained in Section 4.4.3, since the \( \{ |w_k\rangle \} \) satisfy the property \( \mathcal{P}_\mathcal{V} |w_k\rangle = |f_k\rangle \) for \( 1 ≤ k ≤ M \), we also have

\[
b_k = \langle w_k |v\rangle = \langle f_k |v\rangle , \quad 1 ≤ k ≤ M .
\]

Thus,

\[
\sum_{k=1}^{M} |\langle f_k |v\rangle|^2 = \sum_{k=1}^{M} |b_k|^2 = ||v||^2 \text{ for all } |v\rangle \in \mathcal{V},
\]

which means by definition that \( \{ |f_k\rangle \} \) is a Parseval frame.

A.7 An Oversampling Frame in Classical Signal Processing (Section 4.6.2)

It is common in many classical signal processing scenarios to sample a bandlimited continuous-time (CT) signal at an integer multiple of its Nyquist rate. This tactic is sometimes referred to as oversampling [25]. In Appendix A.7 we verify explicitly that a particular set of shifted sinc functions forms an ENTF for a space of bandlimited CT signals. Assume that \( \mathcal{V} \) is the set of all finite-energy CT signals bandlimited to \( (-\Omega_N, \Omega_N) \) and let \( T = \pi/(r \Omega_N) \) for an arbitrary positive integer \( r \). We wish to show that \( \{ f_k(t) \} \), where

\[
f_k(t) = \frac{\sin(\Omega_N(t - kT))}{\pi(t - kT)} , \quad k \text{ an integer},
\]

full text available at: http://dx.doi.org/10.1561/2000000106
is an ENTF for $\mathcal{V}$ with frame bound $C = 1/T$ and $\|f_k\| = (rT)^{-1/2}$. By definition, this means that

$$\sum_{k=-\infty}^{\infty} |\langle f_k(t), v(t) \rangle|^2 = \frac{\|v(t)\|^2}{T} \quad \text{for all } v(t) \in \mathcal{V} \quad (A.36a)$$

$$\|f_k(t)\| = \frac{1}{\sqrt{rT}} \quad \text{for all } k. \quad (A.36b)$$

Note that we are assuming the following standard inner product on $\mathcal{V}$,

$$\langle v_1(t), v_2(t) \rangle = \int_{-\infty}^{\infty} dt v_1(t) v_2(t) \quad \text{for all } v_1(t), v_2(t) \in \mathcal{V}. \quad (A.37)$$

To verify that \{f_k(t)\} satisfies Equation (A.36a), consider $f_k(t)$ for a specific value of $k$ and an arbitrary element $v(t) \in \mathcal{V}$ with CT Fourier transform (CTFT) $V(j\Omega)$. Since $v(t)$ is an element of $\mathcal{V}$, $V(j\Omega)$ is only nonzero for $|\Omega| \leq \Omega_N$. We will first show that the inner product of $f_k(t)$ with $v(t)$ is equal to $v(t)$ sampled at time $t = kT$, i.e., $\langle f_k(t), v(t) \rangle = v(kT)$. Then we will use Parseval’s theorem to show that

$$\sum_{k=-\infty}^{\infty} |\langle f_k(t), v(t) \rangle|^2 = \sum_{k=-\infty}^{\infty} |v(kT)|^2 = \frac{|v(t)|^2}{T}. \quad (A.38)$$

Let $y(t)$ be the convolution of $f_k(t)$ with $v(t)$,

$$y(t) = \int_{-\infty}^{\infty} d\tau v(\tau) f_k(t - \tau). \quad (A.39)$$

It is well-known that the CTFT of $y(t)$ is $Y(j\Omega) = F_k(j\Omega) V(j\Omega)$ where $F_k(j\Omega)$ is the CTFT of $f_k(t)$, defined by

$$F_k(j\Omega) = \begin{cases} e^{-j\Omega kT} & \text{if } |\Omega| \leq \Omega_N, \\ 0 & \text{else.} \end{cases} \quad (A.40)$$

Since $f_k(t) = f_k(-t)$, the inner product of $f_k(t)$ with $v(t)$ is equal to $y(t)$ evaluated at $t = 0$,

$$\langle f_k(t), v(t) \rangle = \int_{-\infty}^{\infty} dt f_k(t) v(t) = \int_{-\infty}^{\infty} dt f_k(-t) v(t) = y(0). \quad (A.41)$$
Using the definition of the inverse CTFT, we may express $y(0)$ as

$$y(0) = \left[ \frac{1}{2\pi} \int_{-\infty}^{\infty} d\Omega Y(j\Omega) e^{j\Omega t} \right]_{t=0} = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\Omega Y(j\Omega) \quad (A.42a)$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\Omega F_k(j\Omega) V(j\Omega). \quad (A.42b)$$

And now substituting Equation (A.40) into Equation (A.42) yields

$$\langle f_k(t), v(t) \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\Omega V(j\Omega) e^{-j\Omega kT} = v(kT), \quad (A.43)$$

where we have again used the definition of the inverse CTFT. Next we use Parseval’s theorem to show that $\sum_k |v(kT)|^2 = ||v(t)||^2/T$. The discrete time Fourier transform of the sequence $\{v(kT)\}$, denoted by $\hat{V}(e^{j\omega})$, is $2\pi$-periodic and is related to $V(j\Omega)$ via

$$\hat{V}(e^{j\omega}) = \frac{1}{T} V \left( j \frac{\omega}{T} \right), \quad -\pi < \omega \leq \pi. \quad (A.44)$$

Parseval’s theorem for discrete time sequences states that

$$\sum_{k=-\infty}^{\infty} |v(kT)|^2 = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\omega \left| \hat{V}(e^{j\omega}) \right|^2. \quad (A.45)$$

Substituting Equation (A.44) into Equation (A.45) and changing the variable of integration to $\Omega = \omega/T$, we find

$$\sum_{k=-\infty}^{\infty} |v(kT)|^2 = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\omega \frac{1}{T^2} \left| V \left( j \frac{\omega}{T} \right) \right|^2 = \frac{1}{2\pi} \int_{-\pi/T}^{\pi/T} d\Omega \frac{1}{T} \left| V(j\Omega) \right|^2$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\Omega |V(j\Omega)|^2 \quad (A.46a)$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\Omega |V(j\Omega)|^2 \quad (A.46b)$$

Note that in going from Equation (A.46a) to (A.46b), we have used the fact that $\pi/T = r \Omega_N$ and the fact that by assumption, $V(j\Omega)$ is only nonzero for $|\Omega| \leq \Omega_N$. Finally, Parseval’s theorem for CT signals states that

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} d\Omega |V(j\Omega)|^2 = \int_{-\infty}^{\infty} dt |v(t)|^2 = ||v(t)||^2 \text{ for all } v(t) \in \mathcal{V}. \quad (A.47)$$
In summary, we have
\[
\sum_{k=-\infty}^{\infty} |\langle f_k(t), v(t) \rangle|^2 = \sum_{k=-\infty}^{\infty} |v(kT)|^2 = \frac{||v(t)||^2}{T}. \tag{A.48}
\]
Since Equation (A.48) is true for any \( v(t) \in \mathcal{V} \), \( \{f_k(t)\} \) is a tight frame for \( \mathcal{V} \) with frame bound \( C = 1/T \).

To verify Equation (A.36b), we use Parseval’s theorem for CT signals to show that
\[
||f_k(t)||^2 = \int_{-\infty}^{\infty} dt \ |f_k(t)|^2 = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\Omega \ |F_k(j\Omega)|^2 \tag{A.49a}
\]
\[
= \frac{1}{2\pi} \int_{-\Omega_N}^{\Omega_N} d\Omega \ |e^{-j\Omega kT}|^2 = \frac{\Omega_N}{\pi}. \tag{A.49b}
\]
Since \( \Omega_N = \pi/(rT) \), we have
\[
||f_k(t)|| = \frac{1}{\sqrt{rT}} \text{ for all } k. \tag{A.50}
\]

A.8 Change of Basis in \( \mathcal{W} \) (Section 4.6.2)

Consider \(|e\rangle = \sum_k \Delta_k |w_k\rangle\) where the \( \{\Delta_k\} \) each have zero mean and variance \( \sigma^2 \) and are pairwise uncorrelated, as specified in Equation (4.31). Let \( \{|u_k\rangle\} \) be any orthonormal basis of \( \mathcal{W} \). We wish to show that the components of \(|e\rangle\) with respect to \( \{|u_k\rangle\} \), which we denote by \( \{\Delta'_k\} \), have these same properties. We start by expanding each of the \( \{|w_k\rangle\} \) as a linear combination of the \( \{|u_k\rangle\} \),
\[
|w_k\rangle = \sum_{\ell=1}^{M} c_{k\ell} |u_\ell\rangle, \quad 1 \leq k \leq M. \tag{A.51}
\]
Since the \( \{|w_k\rangle\} \) are orthonormal, the \( \{c_{k\ell}\} \) satisfy
\[
\sum_{\ell=1}^{M} c_{j\ell} c_{k\ell} = \delta_{jk}, \quad 1 \leq j, k \leq M, \tag{A.52}
\]
where \( \delta_{jk} \) takes the value 1 if \( j = k \) and 0 otherwise. Equation (A.52) implies that the \( \{c_{k\ell}\} \) also satisfy
\[
\sum_{k=1}^{M} c_{k\ell} c_{km} = \delta_{\ell m}, \quad 1 \leq \ell, m \leq M. \tag{A.53}
\]
A.8. Change of Basis in $\mathcal{W}$ (Section 4.6.2)

To see why this is true, consider the $M \times M$ matrix $D$ whose $k$th row and $\ell$th column contains the element $c_{k\ell}$ for $1 \leq k, \ell \leq M$. Equation (A.52) states that the columns of $D$ are orthonormal with respect to the standard inner product (often referred to as the dot product) on $\mathbb{C}^M$, the canonical $M$-dimensional complex coordinate space. A square matrix whose columns are orthonormal also has the property that its rows are orthonormal, which is exactly the meaning of Equation (A.53).

Substituting Equation (A.51) into the expression for $|e\rangle$ and rearranging, we find

$$|e\rangle = \sum_{k=1}^{M} \Delta_k \left( \sum_{\ell=1}^{M} c_{k\ell} |u_k\rangle \right) = \sum_{\ell=1}^{M} \left( \sum_{k=1}^{M} \Delta_k c_{k\ell} \right) |u_k\rangle. \quad (A.54)$$

The components $\{\Delta'\}_k$ can thus be expressed as $\Delta'_k = \sum_\ell \Delta_k c_{k\ell}$ for $1 \leq k \leq M$. We may now derive the desired result using the linearity of expectation and the properties of the $\{\Delta_k\}$,

$$E[\Delta_k] = \sum_{k=1}^{M} E[\Delta_k] c_{k\ell} = 0 \quad (A.55a)$$

$$E[\Delta'_j \Delta'_k] = \sum_{j,k=1}^{M} E[\Delta_j \Delta_k] c_{j\ell} c_{k\ell} \quad (A.55b)$$

$$= \begin{cases} \sigma^2 \sum_{k=1}^{M} c_{k\ell}^2 & \text{if } j = k \\ 0 & \text{if } j \neq k \end{cases} \quad (A.55c)$$

$$= \begin{cases} \sigma^2 & \text{if } j = k \\ 0 & \text{if } j \neq k \end{cases} \quad (A.55d)$$

Note that in Equation (A.55d) we have used Equation (A.53). Thus, we have shown that the $\{\Delta'_k\}$ have zero mean and variance $\sigma^2$ and are pairwise uncorrelated.

The fact that the $\{\Delta'_k\}$ are uncorrelated can also be interpreted in terms of the matrix $D$. This viewpoint is the one most commonly used when considering a general decorrelation transformation of a vector-valued random variable. Consider the vector-valued random variable $\tilde{\Delta}$ whose $k$th component is the random variable $\Delta_k$ for $1 \leq k \leq M$. 

Full text available at: http://dx.doi.org/10.1561/2000000106
Similarly, let \( \tilde{\Delta}' \) be the vector-valued random variable with components \( \{\Delta'_k\} \). Since \( \Delta'_k = \sum_\ell \Delta_k c_{k\ell} \) for \( 1 \leq k \leq M \), we have \( \tilde{\Delta}' = D \tilde{\Delta} \). Since the components of \( \Delta' \) clearly have zero mean, the covariance matrix of \( \tilde{\Delta}' \) can be expressed as

\[
\mathbb{E}[\tilde{\Delta}'(\tilde{\Delta}')^T] = D \mathbb{E}[\tilde{\Delta} \tilde{\Delta}^T] D^T. \tag{A.56}
\]

The \( \{\Delta_k\} \) satisfy \( \mathbb{E}[\Delta_j \Delta_k] = \sigma^2 \delta_{jk} \) by assumption, implying that \( \mathbb{E}[\tilde{\Delta} \tilde{\Delta}^T] = \sigma^2 I_M \) where \( I_M \) is the \( M \times M \) identity matrix. Thus, Equation (A.56) can be simplified to

\[
\mathbb{E}[\tilde{\Delta}'(\tilde{\Delta}')^T] = \sigma^2 D I_M D^T = \sigma^2 DD^T = \sigma^2 I_M, \tag{A.57}
\]

where in the last line we have used that fact that \( DD^T = I_M \) because the rows of \( D \) are orthonormal. The component in the \( j \)th row and \( k \)th column of the matrix \( \mathbb{E}[\tilde{\Delta}'(\tilde{\Delta}')^T] \) is \( \mathbb{E}[\Delta'_j \Delta'_k] \), and Equation (A.56) states that it is equal to \( \sigma^2 \) if \( j = k \) and 0 otherwise, as expected.

### A.9 Generalized Operator Frames (Section 4.5.2)

The definition of a special class of IC POVMs referred to as tight IC POVMs relies on the notion of a generalized operator frame with respect to (w.r.t.) a given measure, as introduced in [11]. Given a measure \( \alpha(\cdot) \) that maps each \( 1 \leq k \leq M \) to a non-negative number \( \alpha(k) \geq 0 \), a set of operators \( \{|F_k\rangle\rangle\} \) in \( \mathcal{V} \) is a generalized operator frame for \( \mathcal{V} \) w.r.t. \( \alpha(\cdot) \) if

\[
C ||V||^2 \leq \sum_{k=1}^M \alpha(k) |\langle F_k |V \rangle|^2 \leq D ||V||^2 \text{ for all } |V\rangle \in \mathcal{V}, \tag{A.58}
\]

for some \( 0 < C \leq D < \infty \).

**Example A.1.** Equation (4.26) is a special case of Equation (A.58) in which \( \alpha(\cdot) \) is the counting measure, defined by

\[
\alpha(k) = 1, \quad 1 \leq k \leq M. \tag{A.59}
\]

Thus, a set of operators satisfying Equation (4.26) is a frame for \( \mathcal{V} \) w.r.t. the counting measure.
Example A.2. The trace measure [11] is defined by

$$\alpha(k) = \text{Tr}(F_{k}), \quad 1 \leq k \leq M. \quad (A.60)$$

Note that Equation (A.60) only represents a valid measure when \(\text{Tr}(F_{k}) \geq 0\) for all values of \(k\). One instance in which this is true is when the \(\{|F_{k}\rangle\rangle\}\) are the elements of a POVM. Substituting Equation (A.60) into Equation (A.58) leads to

$$C ||V||^2 \leq \sum_{k=1}^{M} \text{Tr}(F_{k}) |\langle F_{k}|V\rangle|^2 \leq D ||V||^2 \text{ for all } |V\rangle\rangle \in \mathcal{V} \quad (A.61)$$

for some \(0 < C \leq D < \infty\). A set of operators \(\{|F_{k}\rangle\rangle\}\) in \(\mathcal{V}\) satisfying Equation (A.61) is a frame for \(\mathcal{V}\) w.r.t. the trace measure. A tight frame for \(\mathcal{V}\) w.r.t. the trace measure is one for which the upper and lower bounds in Equation (A.61) can both be set to the same value. Note that in finite dimensions, if \(\{|F_{k}\rangle\rangle\}\) is a frame for \(\mathcal{V}\) w.r.t. the trace measure, then \(\{\sqrt{\text{Tr}(F_{k})} |F_{k}\rangle\rangle\}\) is a frame for \(\mathcal{V}\) w.r.t. the counting measure.

A.10 Distribution of Relative Frequencies (Section 5.3)

While the following derivation is motivated by the quantum state estimation problem considered in Section 5.3, the concepts and conclusions rely only on the laws of probability and not on the postulates of quantum mechanics. Therefore we state the results without any reference to density operators or quantum measurement. Let \(X\) be a discrete random variable that takes values in the set \(\{1, \ldots, M\}\) with probability mass function (PMF) \(\{p(1), \ldots, p(M)\}\), i.e.,

$$X = k \text{ with probability } p(k), \quad 1 \leq k \leq M. \quad (A.62)$$

Assume that \(\{x_{i}, 1 \leq i \leq L\}\) is a set of \(L\) independent realizations of \(X\) and consider the set of relative frequencies \(\{\hat{p}(k) = \ell_{k}/L\}\), where \(\ell_{k}\) is the number of realizations \(\{x_{i}\}\) that are equal to \(k\). Defining \(d_{k} = \hat{p}(k) - p(k)\) for \(1 \leq k \leq M\), the goal is to evaluate the expected values \(E[d_{k}]\) and \(E[d_{j}d_{k}]\) for all \(1 \leq j, k \leq M\).

We first address the case where \(j = k\). Let \(k\) be a fixed integer between 1 and \(M\). To compute \(E[d_{k}]\), note that the value of \(\ell_{k}\) is
binomially distributed with parameters $p(k)$ and $L$ [ref]. Its expected value is $\mathbb{E}[\ell_k] = Lp(k)$ and its variance is $\text{var}(\ell_k) = Lp(k)(1 - p(k))$. Using linearity of expectation we find that, unsurprisingly, the expected value of $d_k$ is equal to zero,

$$\mathbb{E}[d_k] = \mathbb{E}\left[p(k) - \frac{\ell_k}{L}\right] = p(k) - \frac{Lp(k)}{L} = 0. \quad (A.63)$$

The variance of $d_k$ is

$$\text{var}(d_k) = \text{var}\left(p(k) - \frac{\ell_k}{L}\right) = \frac{\text{var}(\ell_k)}{L^2} = \frac{p(k)(1 - p(k))}{L}. \quad (A.64)$$

Furthermore, since $\mathbb{E}[d_k] = 0$ we have $\mathbb{E}[d_k^2] = \text{var}(d_k)$.

Now let $j$ and $k$ be fixed integers between 1 and $M$ with $j \neq k$. To compute $\mathbb{E}[d_j d_k]$, note that the joint distribution of $\{\ell_1, \ldots, \ell_M\}$ is given by a multinomial distribution with parameters $L$ and $\{p_1, \ldots, p_M\}$ [ref]. It can be shown using the properties of the multinomial distribution that

$$\mathbb{E}[\ell_j \ell_k] = L p(j) p(k)(L - 1). \quad (A.65)$$

Using linearity of expectation and the fact that $\mathbb{E}[\ell_j] = Lp(j)$ and $\mathbb{E}[\ell_k] = Lp(k)$, we find that the value of $\mathbb{E}[d_j d_k]$ is

$$\mathbb{E}[d_j d_k] = \mathbb{E}\left[\left(\frac{\ell_j}{L} - p(j)\right)\left(\frac{\ell_k}{L} - p(k)\right)\right] \quad (A.66a)$$

$$= \frac{\mathbb{E}[\ell_j \ell_k]}{L^2} - p(j)p(k) = -\frac{p(j) p(k)}{L}. \quad (A.66b)$$
Traditional Appendices

B.1 Generation of $P_f$-$P_d$ Projection of LRT ROC from Suboptimal SVT ROC

An explanation of the procedure is shown in Figure B.1. The graphs in Figure B.1a show $P_{f}^{SVT}$, $P_{d}^{SVT}$, and the derivative $dP_{d}^{SVT}/dP_{f}^{SVT}$ as functions of the score variable. According to Equation (2.31) the derivative is equal to the likelihood ratio function. Note that these graphs are caricatures used only for visualization, since the procedure does not require explicit knowledge of any of the aforementioned quantities as functions of the score variable. A fixed LRT threshold value $\eta_0 \geq 0$ identifies multiple disjoint regions of $s$ for which $f_1(s)/f_0(s) \geq \eta_0$, highlighted in green for $\eta_0 = 1$ in the figure. Together these regions comprise $D_{LRT}(\eta_0)$. Each individual region $j$ covers an interval $[a_j, b_j]$ with $a_j < b_j$ and corresponds to the segment in the $P_f$-$P_d$ projection of the SVT ROC with endpoints $(h_f(b_j), h_d(b_j))$ and $(h_f(a_j), h_d(a_j))$. The integrals of $f_0(\cdot)$ and $f_1(\cdot)$ over the region, shown in Figure B.1b,
can be expressed as

\[ \int_{a_j}^{b_j} ds f_0(s) = (1 - F_0(a_j)) - (1 - F_0(b_j)) = h_f(a_j) - h_f(b_j) \quad (B.1a) \]

\[ \int_{a_j}^{b_j} ds f_1(s) = (1 - F_1(a_j)) - (1 - F_1(b_j)) = h_d(a_j) - h_d(b_j) \quad (B.1b) \]

which are simply the changes in \( P^f_{SVT} \) and \( P^d_{SVT} \) between the endpoints of the segment. Summing these changes over all regions corresponds to summing the integrals of \( f_0(\cdot) \) and \( f_1(\cdot) \) over each disjoint portion of \( D_{LRT}(\eta) \). The resulting \( P_f-P_d \) projection of the LRT ROC made by varying \( \eta_0 \) over its entire range is illustrated in Figure B.1c.

### B.2 QMOCs Generated using Standard Measurements are Ellipses

We show that any QMOC generated according to the method described in Example 3.3 of Section 3.6, in which two-outcome quantum measurements with associated standard POVMs are used to distinguish between arbitrary qubit density matrices \( \rho_0 \) and \( \rho_1 \) with \( d = 2 \), is an ellipse. More specifically, it is a rotated ellipse in the \( P_f-P_d \) plane centered at the point \((1/2, 1/2)\). The derivation also applies to the case where \( \rho_0 \) and \( \rho_1 \) represent two pure states with \( d > 2 \), as long as the standard POVMs used to generate the QMOC have the following properties: The first two elements of the POVM, \( E_1 \) and \( E_2 \), should be analogous to those defined by Equation (3.19), but with the additional requirement that \( |v_1⟩ \) and \( |v_2⟩ \) should lie in the plane defined by the two pure states. The other measurement elements must therefore project onto subspaces of the orthogonal complement of that plane. Again the final decision is \( H_1 \) if the measurement outcome associated with \( E_2 \) occurs and \( H_0 \) if the measurement outcome associated with \( E_2 \) occurs. The other possible outcomes have zero probability of occurring and can be associated with either final decision. Essentially, this reduces the problem to that of distinguishing between two pure states with \( d = 2 \).
B.2. **QMOCs Generated using Standard Measurements are Ellipses**

Figure B.1: (a) Probability of false alarm, probability of detection, and derivative of SVT ROC as functions of the score variable. The highlighted regions represent regions where the derivative of the curve is greater than or equal to $\eta_0 = 1$. (b) Integrals of the conditional PDFs over the LRT decision region $D_{LRT}(\eta_0)$ for $\eta_0 = 1$. (c) $P_f$-$P_d$ projections of non-concave SVT ROC and LRT ROC generated using the procedure given in the text.
The coordinates of the QMOC in terms of the angle $\theta$ are

\[ P_f = \text{Tr}(E_1 \rho_0) = a_0 \cos^2\left(\frac{\theta}{2}\right) + a_1 \sin^2\left(\frac{\theta}{2}\right) \]  \hspace{1cm} (B.2a) 

\[ P_d = \text{Tr}(E_1 \rho_1) = b_0 \cos^2\left(\frac{\theta - \alpha}{2}\right) + b_1 \sin^2\left(\frac{\theta - \alpha}{2}\right). \]  \hspace{1cm} (B.2b) 

Assuming for the moment that this is the parametric equation of a rotated ellipse centered at $(1/2, 1/2)$, we can center the ellipse at the origin and use trigonometric identities to derive equations for the centered coordinates,

\[ P_f - \frac{1}{2} = \frac{a_0 - a_1}{2} \cos \theta \]  \hspace{1cm} (B.3a) 

\[ P_d - \frac{1}{2} = \frac{b_0 - b_1}{2} \cos(\theta - \alpha). \]  \hspace{1cm} (B.3b) 

For ease of notation we now make the substitutions

\[ x = P_f - \frac{1}{2}, \quad y = P_d - \frac{1}{2}, \quad a = \frac{a_0 - a_1}{2}, \quad b = \frac{b_0 - b_1}{2}, \]  \hspace{1cm} (B.4) 

and introduce the functions $f_x(\cdot)$ and $f_y(\cdot)$, so that the centered coordinates become

\[ x = f_x(\theta) = a \cos \theta \]  \hspace{1cm} (B.5a) 

\[ y = f_y(\theta) = b \cos(\theta - \alpha). \]  \hspace{1cm} (B.5b) 

(Note that the $x$ and $y$ above should not be confused with the $\{|x_i\}$ and $\{|y_i\}$ in Equations (3.11).) The objective now is to show that $x = f_x(\theta)$ and $y = f_y(\theta)$ represent a rotated ellipse centered at the origin. That is, the objective is to show that they can be written in the form

\[ x = g_x(t) = q \cos \beta \cos t - r \sin \beta \sin t \]  \hspace{1cm} (B.6a) 

\[ y = g_y(t) = q \sin \beta \cos t + r \cos \beta \sin t \]  \hspace{1cm} (B.6b) 

for some angle of rotation $\beta$ from the horizontal, semi-major axis $q$, semi-minor axis $r$, and parameter $t$ (which will prove inconsequential for our purposes). The functions $g_x(\cdot)$ and $g_y(\cdot)$ have been introduced for convenience. We can solve for the parameters $q, r, \beta$ in terms of the
known values of $a$, $b$, $\alpha$ by using Equations (B.5) and (B.6) to find the points on each ellipse with maximum $x$- and $y$-values and then setting their coordinates equal to one another. Taking the derivative of $f_x(\theta)$ and setting it to zero, we find that the point with maximum $x$-value occurs at $\theta_x = 0$ and has coordinates $(f_x(0), f_y(0)) = (a, b)$. The point with maximum $y$-value occurs at $\theta_y = \alpha$ and has coordinates $(f_x(\alpha), f_y(\alpha)) = (a \cos \alpha, b)$. Similarly, the point on the ellipse described by Equations (B.6) with maximum $x$-value occurs at $t_x = \tan^{-1}(-r/q \tan \beta)$ and has coordinates

$$g_x(t_x) = \sqrt{q^2 \cos^2 \beta + r^2 \sin^2 \beta}$$  

(B.7a)

$$g_y(t_x) = \frac{q^2 - r^2}{\sqrt{q^2 / \sin^2 \beta + r^2 / \cos^2 \beta}}.$$  

(B.7b)

The point with maximum $y$-value occurs at $t_y = \tan^{-1}(r/(q \tan \beta))$ and has coordinates

$$g_x(t_y) = \frac{q^2 - r^2}{\sqrt{q^2 / \cos^2 \beta + r^2 / \sin^2 \beta}}$$  

(B.8a)

$$g_y(t_y) = \sqrt{q^2 \sin^2 \beta + r^2 \cos^2 \beta}.$$  

(B.8b)

Setting $f_x(0) = g_x(t_x)$, $f_y(0) = g_y(t_x)$, $f_x(\alpha) = g_x(t_y)$, and $f_y(\alpha) = g_y(t_y)$ and solving for $q$, $r$, and $\beta$ in terms of $a$, $b$, and $\alpha$ yields

$$\beta = \frac{1}{2} \tan^{-1} \left( \frac{2ab \cos \alpha}{a^2 - b^2} \right)$$  

(B.9a)

$$q = \left[ \frac{1}{2} \left( a^2 + b^2 + \frac{a^2 - b^2}{\cos(2\beta)} \right) \right]^{1/2}$$  

(B.9b)

$$r = \left[ \frac{1}{2} \left( a^2 + b^2 - \frac{a^2 - b^2}{\cos(2\beta)} \right) \right]^{1/2}.$$  

(B.9c)

It can be verified through straightforward algebra that when $\beta$, $q$, and $r$ are given by Equations (B.9), the coordinates $x = f_x(\theta)$, $y = f_y(\theta)$ in Equation (B.5) satisfy the equation that defines an ellipse:
Ax^2 + Bxy + Cy^2 + D = 0 with B^2 - 4AC < 0, where

\[ A = q^2 \sin^2 \beta + r^2 \cos^2 \beta \]  \hspace{1cm} (B.10a)

\[ B = 2(q^2 - r^2) \sin \beta \cos \beta \]  \hspace{1cm} (B.10b)

\[ C = q^2 \cos^2 \beta + r^2 \sin^2 \beta \]  \hspace{1cm} (B.10c)

\[ D = -q^2 r^2. \]  \hspace{1cm} (B.10d)

This verifies our initial assumption that \( x = f_x(\theta) \) and \( y = f_y(\theta) \) are the coordinates of an ellipse that is centered at the origin, rotated by an angle \( \beta \) from the horizontal, and has semi-major axis \( q \) and semi-minor axis \( r \). The original QMOC is the same ellipse centered at the point \((1/2, 1/2)\).
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