Bayesian Error Based Sequences of Mutual Information Bounds

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Abstract—The inverse relation between mutual information (MI) and Bayesian error is sharpened by deriving finite sequences of upper and lower bounds on MI in terms of the minimum probability of error (MPE) and related Bayesian quantities. The well known Fano upper bound and Feder-Merhav lower bound on equivocation are tightened by including a succession of posterior probabilities starting at the largest, which directly controls the MPE, and proceeding to successively lower ones. A number of other interesting results are also derived, including a sequence of upper bounds on the MPE in terms of a previously introduced sequence of generalized posterior distributions. The tightness of the various bounds is illustrated for a simple application of joint spatial localization and spectral typing of a point source.

Index Terms—Mutual information, lower and upper bounds, equivocation, minimum probability of error, Bayesian inference, multi-hypothesis testing, Fano bound

I. INTRODUCTION

Statistical information theory [1], [2] is an essential quantitative tool for modern signal processing, computation, coding, and communication systems. Its core philosophy hinges on the notions of information potential and the ability of systems to encode, transmit and decode information about one or more input parameters.

Since information must improve with decreasing error, MI is expected to have an inverse relationship with fundamental Bayesian error metrics, such as the minimum mean squared error (MMSE) and the minimum probability of error (MPE) [8]. Two lower bounds on MI, one involving the MPE and another the MMSE, were derived over forty years ago by Fano [2] and Seidler [4], respectively. While there has been some progress made in deriving useful upper bounds [5], [6] as well as in the last twenty years, there is still need for tighter bounds than are currently available. The relationship between the MPE and MMSE for highly sensitive detectors has been clarified in a recent paper by the author [7].

The matter of MI bounds has also received attention because of the essential relation of MI to code redundancy in universal source coding [2], [9] and to Bayesian risk in multi-hypothesis testing and computational learning as elucidated by Haussler and Opper [9]. In the latter work, the authors derived a lower bound and an upper bound on MI involving double expectations of exponentiated Hellinger and Kullback-Leibler distances between two conditional data PDFs, respectively. These bounds, while tight in the asymptotic limit, are expected to be loose, however, when such a limit cannot be taken.

A related topic of bounding the MPE for multi-hypothesis testing in the Bayesian setting has received much attention for two main reasons, one being the need for computational efficiency and the other being its usefulness in developing and proving certain asymptotic results in coding theory. Bounds of this type include the Fano lower bound (FB) involving the equivocation entropy (EE) [2] and its generalization for nonuniform priors [10] and countably infinite alphabets [11], the Shannon bound [12], the Poor-Verdu bound [13], and the generalized Poor-Verdu bound [14]. Of these, only the FB and its generalizations yield bounds on the EE and thus on MI, which is the subject of main interest here.

The converse problem of bounding the EE in terms of the MPE has been elucidated by Feder and Merhav [5]. They derived rigorous convex and non-convex lower bounds as functions of the MPE alone, and showed their usefulness in formulating and proving the channel coding theorem by upper-bounding the EE, rather than MPE, as a function of the codeword length and transmission rate. Their EE bounds, while being the tightest possible when using the MPE alone, will be shown, however, to be rather loose for an application considered here. One purpose of the present paper is to tighten these lower bounds on EE by introducing secondary Bayesian measures of error that successively refine these bounds upwards while being amenable to physical interpretation. We also derive, in terms of the same secondary error measures, a finite sequence of upper bounds on EE that tighten the Fano bound as well, thus furnishing two sequences of upper and lower bounds on the EE - and thus on MI - that tighten the existing ones. We also present a different upper bound on MI, closely related to the Feder-Merhav (FM) bound, that is tighter than all others, but has no simple physical interpretation.

As part of our review and elaboration of the FM lower bound on the EE, we shall obtain a number of alternative derivations for it. We shall use one of them to also upper-bound the MPE by means of a sequence of bounds that increasingly tighten that furnished by the FM bound. These bounds, as we shall see, involve the family of generalized or tilted posterior probability mass functions (PMFs) [2], [14], of which the usual posterior PMF is a specific member and the FM bound the corresponding bound.

In Sec. VII, we describe a specific application of a proposed detector that simultaneously localizes a point source and performs its spectral characterization under daylight conditions. For this application, we shall compare all of our newly derived bounds and the existing ones with the numerically exact results for MI under varying operating conditions.
II. REVIEW

Let $\Theta$ be a discrete random input taking values in the set $\Omega_\Theta \overset{\text{def}}{=} \{\theta_1, \ldots, \theta_M\}$ according to the PMF $p_m \overset{\text{def}}{=} p_{\theta_m}$, $m = 1, \ldots, M$. Let $X$ be a random output variable, e.g., a measurement variable, that carries information about $\Theta$, and is distributed according to the conditional probability density function (PDF), $P(x|\theta_m)$, given the value $\theta_m$ of the input variable $\Theta$. The output $X$ is in general an $N$-dimensional random vector taking values in some subset of $\mathbb{R}^N$. If the $M$ different values that $\Theta$ can take may be regarded as representing $M$ different hypotheses, then the Bayesian estimation problem of determining the value of $\Theta$ becomes the Bayesian multi-hypothesis testing problem.

The MI is the difference between the input entropy, $H(\Theta)$, and EE, $H(\Theta|X)$,

$$I(\Theta; X) = H(\Theta) - H(\Theta|X),$$

where the two entropies on the right-hand side (RHS) are defined as

$$H(\Theta) = -\sum_{m=1}^{M} p_m \log p_m;$$

$$H(\Theta|X) = -\mathbb{E}_X \left[ \sum_{m=1}^{M} p(\theta_m|X) \log p(\theta_m|X) \right],$$

where the symbol $\mathbb{E}_X$ denotes averaging over the statistical fluctuations of $X$. We shall omit the subscript when a joint expectation over both the input and output variables is understood. Further, the base of the logarithm will be left unspecified throughout this paper, but whenever the logarithm is inverted, as in Sec. IIB, the base $e$ of the natural logarithm, denoted by ln, will be assumed.

A. The Fano Bound

Since $H(\Theta|X)$ may be regarded as the loss of information in the passage through the communication channel, it is expected to be related to the probability of error (PE) in estimating the input variable, $\Theta$. This is quantified by the Fano upper bound on EE in terms of the PE, namely

$$H(\Theta|X) \leq H(P_e) + P_e \log(M - 1),$$

or equivalently by the following lower bound on the successfully transmitted information:

$$I(\Theta; X) \geq H(\Theta) - [H(P_e) + P_e \log(M - 1)].$$

B. Feder-Merhav and Related Upper Bounds on the MPE

The maximum a posteriori probability (MAP) decision rule yields the maximum probability of making the correct detection among $M$ different hypotheses based on observations. The minimum probability of error (MPE) in the $M$-detection problem is one minus the former, namely

$$P_e^{(\text{min})} = 1 - \mathbb{E}_X \left[ \max_m \{ p(\theta_m|X) \} \right].$$

A tight upper bound on the MPE involving the generalized equivocation entropy (GEE) was derived in an earlier paper [7], namely

$$P_e^{(\text{min})} = 1 - \mathbb{E}_X \left[ \exp \left\{ - \int_1^{\infty} \frac{dn}{n^2} H_n(\Theta|X = x) \right\} \right] \leq 1 - \exp \left[ - \int_1^{\infty} \frac{dn}{n^2} \mathbb{E}_X H_n(\Theta|X = x) \right] = 1 - \exp \left[ - \int_1^{\infty} \frac{dn}{n^2} H_n(\Theta|X) \right],$$

where $H_n(\Theta|X)$ denotes the GEE of order $n$ defined as

$$H_n(\Theta|X) = -\mathbb{E} \ln p_n(\Theta|X), \quad p_n(\theta_m|x) \overset{\text{def}}{=} \frac{p^n(\theta_m|x)}{\sum_m p^n(\theta_m|x)}.$$

Use was made of the convexity of exponentiation to arrive at (8). Note that for a given $x$, as $n$ increases $p_n(\theta_m|x)$ approaches 1 from below for $m = m_n(x) = \arg\max_m \{ p(\theta_m|x) \}$ and 0 from above for all other $m$ values. This increasing purification of the posterior $p_n(\Theta|X)$, also known as the tilted posterior PMF of order $n$ [10], with increasing $n$ also implies a decreasing value of the GEE.

Since $H_1(\Theta|X) \geq H_n(\Theta|X)$ for all $n \geq 1$, it follows that

$$P_e^{(\text{min})} \leq 1 - \exp \left[ - \int_1^{\infty} \frac{dn}{n^2} H_1(\Theta|X) \right] \leq 1 - \exp \left[ - H(\Theta|X) \right],$$

since the GEE of order 1 is the ordinary EE, $H(\Theta|X)$. Transposing the exponential to one side and then taking the logarithm of both sides of the resulting equation yields the FM bound on $H(\Theta|X)$:

$$H(\Theta|X) \geq -\ln(1 - P_e^{(\text{min})}).$$

A tighter bound on the MPE results if we upper-bound the integral in the exponent in inequality (10) over two or more intervals, e.g.,

$$\int_1^{\infty} \frac{dn}{n^2} H_n(\Theta|X) \leq \int_1^{\lambda} \frac{dn}{n^2} H_1(\Theta|X) + \int_\lambda^{\infty} \frac{dn}{n^2} H_\lambda(\Theta|X) = \left( 1 - \frac{1}{\lambda} \right) H(\Theta|X) + \frac{1}{\lambda} H_\lambda(\Theta|X),$$

which is smaller than $H(\Theta|X)$ used in the FM bound for any $\lambda > 1$. For $\lambda = 2$, for example, the following tighter upper bound on the MPE results:

$$P_e^{(\text{min})} \leq 1 - \exp \left\{ -[H(\Theta|X) + H_2(\Theta|X)]/2 \right\}.$$

Evidently many similar but still tighter bounds on the MPE involving more and more of the higher-order GEEs may thus be derived, but the advantage of the looser FM bound [8] is its immediate relation to the more easily interpretable loss of statistical information represented by EE.
III. Other Derivations of the FM Bound and New Upper Bounds on MI and MPE

An alternative derivation of the FM bound follows immediately on noting that since the logarithm is a monotonically increasing function, \( H(\Theta | X) \), which is simply \(- \mathbb{E} \log p(\Theta | X)\), is bounded below by \(- \mathbb{E} \log \max_m p(\theta_m | X)\). But since the logarithm is also a concave function, the EE is less tightly bounded below as

\[
H(\Theta | X) \geq - \mathbb{E} \log \max_m p(\theta_m | X) = - \log (1 - P_e^{(\text{min})}),
\]

which is the FM bound.

In preparing to generalize the FM bound, we present one other derivation of it. If \( \{s_1, \ldots, s_M\} \) is a PMF, i.e., \( \sum_m s_m = 1 \), \( s_m \geq 0 \), \( \forall m \), then

\[
\max(a_1, a_2, \ldots, a_M) \geq \prod_{m=1}^{M} a_m^{s_m}.
\]

It then follows from definition (5) and the concavity of the logarithm that

\[
\log (1 - P_e^{(\text{min})}) \geq \log \prod_{m=1}^{M} p_m^{s_m}(\theta_m | X)
\]

\[
\geq \mathbb{E} \left[ \sum_m s_m(X) \log p(\theta_m | X) \right]
\]

\[
= B(s),
\]

where the bound \( B(s) \) is defined as

\[
B(s) \overset{\text{def}}{=} \mathbb{E} \left[ \sum_m s_m(X) \log p(\theta_m | X) \right].
\]

and the non-negative powers \( s_m \) have been allowed, for maximum generality, to depend on the output variable \( X \), subject to their sum being 1.

For the special choice, \( s_m(X) = p(\theta_m | X) \), the RHS of inequality (14) reduces to \(- H(\Theta | X)\), which is the FM bound. A more general choice involves the generalized posterior PMF, \( p_n(\theta_m | X) \), defined earlier in (7), that becomes sharper the larger its order \( n \),

\[
s_m(X) = p_n(\theta_m | X) = \frac{p^n(\theta_m | X)}{Z_n(X)}, \quad m = 1, \ldots, M,
\]

where the partition function \( Z_n \) is defined as

\[
Z_n(X) \overset{\text{def}}{=} \sum_{m=1}^{M} p^n(\theta_m | X).
\]

To see that for this choice of the \( s_m \), the lower bound \( B \) defined by (15) becomes tighter with increasing \( n \), we first substitute (16) into (15) and then calculate its derivative with respect to \( n \),

\[
\frac{dB_n}{dn} = (\log e) \mathbb{E}_X \left\{ \frac{1}{Z_n(X)} \sum_m p^n(\theta_m | X) \ln^2 p(\theta_m | X) \right. \\
- \frac{1}{Z^2_n(X)} \left[ \sum_m p^n(\theta_m | X) \ln p(\theta_m | X) \right]^2 \}
\]

\[
= (\log e) \mathbb{E}_X \left[ (\ln^2 p(\Theta | X))_n - (\ln p(\Theta | X))^2_n \right], \quad (18)
\]

where the triangular brackets with subscript \( n \) indicate the expectation of the quantity they enclose with respect to the generalized posterior \( p_n \) defined by (16). Since the square is a convex function, the RHS of the last expression in (18) cannot be negative, which means that \( B \) is a non-decreasing function of \( n \). Thus for \( n > 1 \), the bound \( B \) is tighter than the FM bound, and represents an increasingly tighter sequence of bounds on the MPE with increasing \( n \). For \( n \to \infty \), the generalized posterior \( p_\infty(\theta_m | X) \) takes the value 1 for that single value of index \( m \) for which \( p(\theta_m | X) \) is the largest for all \( m \) and the value 0 for all other values of \( m \). In other words, the bound \( B \) in this limit may be expressed as

\[
B_\infty = \sum \int_{R_m} \log [p(\theta_m | x)] P(x) \, dx
\]

\[
= \mathbb{E}_X \log \max_m p(\theta_m | X), \quad (19)
\]

where \( R_m \) is the \( m \)-th decision region chosen according to the MAP criterion that yields the least \( M \)-hypothesis testing error probability.

A simple improvement of the FM bound is obtained on writing

\[
- \log p(\Theta | X) = - \log \max_m p(\theta_m | X)
\]

\[
- \log \left[ p(\Theta | X) / \max_m p(\theta_m | X) \right], \quad (20)
\]

and then calculating its expectation. In the second term on the RHS above, we perform this expectation first over the posterior and then use the convexity of the negative logarithm to reverse the order of the logarithm and the posterior averaging to lower-bound that term before performing its expectation over the data \( X \). A similar reversal of the order of the logarithm and expectation in the first term on the RHS of (20) also lower-bounds it. We thus obtain the following expectation over data as a lower bound on EE:

\[
H(\Theta | X) \geq - \log (1 - P_e^{(\text{min})}) + \Delta, \quad (21)
\]

where \( \Delta \) denotes the expression

\[
\Delta \overset{\text{def}}{=} - \mathbb{E}_X \log \left[ \frac{\sum_m p^2(\theta_m | X)}{\max_m p(\theta_m | X)} \right]. \quad (22)
\]

Note that the sum in expression (22) can be bounded as

\[
\min_m p(\theta_m | X) \sum_m p(\theta_m | X) \leq \sum_m p^2(\theta_m | X)
\]

\[
\leq \max_m p(\theta_m | X) \sum_m p(\theta_m | X), \quad (23)
\]
but since \( \sum_m p_m(X) = 1 \) for any \( X \), we have the bounds
\[
\min_m p_m(X) \leq \sum_m p(m|X) \leq \max_m p_m(X). \tag{24}
\]
These bounds imply the following bounds on \( \Delta \):
\[
0 \leq \Delta \leq E_X \log \left[ \frac{\max_m p_m(X)}{\min_m p_m(X)} \right]. \tag{25}
\]
Based on these bounds, we see that the lower bound \( \sum(21) \) is tighter than the first term on its RHS, which is the FM bound.

Due to the concavity of the logarithm, \( \Delta \) as defined in \( \sum(22) \) is lower bounded by
\[
\Delta \geq -\log E_X \left[ p_m(X) \right] \geq -\log E_X \left[ p_m(X) \right] \sum_n \frac{p_m(X)}{p(n_m|X)} p_m(X) \sum_n \frac{p_m(X)}{p(n_m|X)} p_m(X)
\]
where \( m_*(X) \), defined as
\[
m_*(X) = \arg \max_m p_m(X), \tag{27}
\]
is the MAP estimator.

Since the ratio of the posterior probabilities inside the square brackets in the above bound may be recast, via Bayes rule, as the ratio of the corresponding joint PDFs while the first term inside those brackets upon taking its expectation is simply
\[
1 - P_e^{(min)} \text{ according to relation } \sum(23), \text{ we may express } \sum(26) \text{ as}
\]
\[
\Delta \geq -\log \left[ 1 - P_e^{(min)} + \int dx \sum_m \frac{p_m^2(x|\theta_m)}{p_m(x)} P(x|\theta_m) \right]
\]
In this form, the quantity \( \Delta \) is lower bounded by an expression that can be evaluated via integrals involving the conditional data PDFs alone. This is computationally efficient, particularly if such PDFs are Gaussian.

Expression \( \sum(28) \) may be recast into a simpler-looking form by splitting the integration over \( X \) into partial integrations over individual decision regions, \( R_m, m = 1, \ldots, M \), chosen according to the MAP criterion. The overall lower bound on the EE, tighter than the FM lower bound, now follows from \( \sum(21) \).

\[
H(\Theta|X) \geq -\log \left[ 1 - P_e^{(min)} \right]
- \log \left[ 1 - P_e^{(min)} + \int \sum_m \int_{R_m} dx \sum_{m \neq m} \frac{p_m^2(x|\theta_m)}{p_m(x)} P(x|\theta_m) \right], \tag{29}
\]
in which the first term on the RHS is the FM lower bound. A computationally more expedient but entirely equivalent form of the bound \( \sum(29) \) is the following:
\[
H(\Theta|X) \geq -\log \left[ 1 - P_e^{(min)} \right]
- \log \left[ \sum_m \int_{R_m} dx \sum_{m \neq m} \frac{p_m^2(x|\theta_m)}{p_m(x)} P(x|\theta_m) \right]. \tag{30}
\]
Subtracting the bound \( \sum(30) \) from \( H(\Theta) \) yields the corresponding upper bound on MI.

For the case of a nonuniform prior in the low-SNR limit, the FM lower bound on EE is not tight, since \( 1 - P_e^{(min)} \) tends in this limit to the largest of the prior probabilities, \( p^{\min} = \max_m p_m, \) and thus the FM bound tends to \(- \log p^{\min}\), while the EE tends to the sum \(- \sum_m p_m \log p_m\), which can be quite different. By contrast, the improved lower bound \( \sum(30) \) is tighter for a nonuniform prior, thanks to the second term on its RHS.

A. A Useful Form for the Uniform Prior

The concavity of the logarithm allows us to lower-bound EE as
\[
H(\Theta|X) = -E \log p(\Theta|X) \geq -\log p(\Theta|X) = -\log E_X \sum_m p_m(X). \tag{31}
\]
Denoting the difference of the posterior from the prior as \( \delta p(\Theta|X) = p(\Theta|X) - p(\Theta) \), we may write the sum in \( \sum(31) \) as
\[
\sum_m \left[ p_m + \delta p_m(X) \right]^2 = \sum_m \left[ p_m^2 + 2p_m \delta p_m(X) + 2p_m \delta p_m(X) \right] = 1 + \sum_m \delta p_m(X), \tag{32}
\]
in which we used the fact that, for the uniform prior, \( p_m = 1/M, \forall m, \) and the last term on the RHS of the second line vanishes, since the posterior, like the prior, is a probability distribution that sums to 1. In view of \( \sum(32) \), the lower bound \( \sum(31) \) may be re-expressed in terms of \( \delta p(\Theta|X) \) as
\[
H(\Theta|X) \geq \log M - \log \left[ 1 + \frac{1}{M} E \sum_m \delta p_m(X) \right], \tag{33}
\]
where the sum over \( m \) thus differs from the corresponding sum over the prior probabilities, namely \( 1/M \), by terms that are of quadratic order in the deviations \( \delta p_m(X) \). This allows us to upper-bound MI as
\[
I(\Theta; X) \leq \log \left[ 1 + M E_X \sum_m \delta p_m(X) \right]. \tag{34}
\]

The MI bound \( \sum(34) \) is expected to interpolate tightly between the \( \log M \) value of MI in the high-discrimination regime where only one of the posterior probabilities is close to 1 and all the other \( (M - 1) \) ones are close to 0, and the vanishing value of MI in the low-discrimination regime where the correction contained in the sum on the RHS in the upper bound \( \sum(34) \) tends to be small. This correction term may be interpreted in terms of an effective SNR, defined as the ratio \( \sum_m E_X \delta p_m(X)/\sum_m p_m^2 \), in a manner rather analogous to the SNR dependence of the information capacity of an additive Gaussian channel.
IV. A SEQUENCE OF TIGHTER LOWER BOUNDS ON EQUIVOCATION

From the lower bound (31), we may derive a sequence of ever tighter bounds that approach it while being interpretable in terms of a corresponding sequence of supplementary measures of Bayesian error. We first write \( p^2(\theta, X) \) as
\[
p(\theta, X)p(\theta, X) + p(\theta, X) - p(\theta, X),
\]
which, in view of the normalization of the posterior PMF, permits us to write its sum as
\[
\sum_m p^2(\theta, X) = p(\theta, X)
\]
where \( m(X) \) is defined by (27). For a given value of data \( X \), the first term is the likelihood of deciding in favor of the hypothesis satisfying the MAP criterion, while the second term is the reduction of that likelihood based on the incorrectness of the MAP based choice. That likelihood reduction may be lower-bounded, in turn, by its maximum value, namely that given by replacing \( p(\theta, X) \) inside the square brackets in (35) by its maximum value for \( \neq m(X) \), which we denote by \( p(\theta, X), \) Since from normalization the sum of \( p(\theta, X) \) over \( \neq m(X) \) simply \( 1 - p(\theta, X) \), the following upper bound on the sum (35) is obtained:
\[
\sum_m p^2(\theta, X) \leq p(\theta, X) - [1 - p(\theta, X)]
\]
where the quantity \( p(\theta, X) \) is the second largest posterior probability for the given data value \( X \).

Introducing the third largest posterior probability via a similar mathematical step tightens the bound further. Specifically, the difference between the RHSs of (35) and (36) is
\[
\sum_{m \neq m(X), m(X)} p(\theta, X) \leq p(\theta, X) - p(\theta, X),
\]
which is lower-bounded by the sum obtained by replacing \( p(\theta, X) \) inside the square brackets by \( p(\theta, X) \), the third largest posterior probability for the given value of \( X \). Since the sum of \( p(\theta, X) \) over all \( m \) except \( m(X) \) and \( m(X) \) is \( 1 - p(\theta, X) - p(\theta, X) \), this yields the following tighter bound for the sum (36):
\[
\sum_m p^2(\theta, X) \leq p(\theta, X) - [1 - p(\theta, X)] - [1 - p(\theta, X)] - [p(\theta, X) - p(\theta, X)].
\]
The successive lowering of the upper bound essentially toward the exact value can be performed by a recursive use of this mathematical strategy, but any improvement of the bound tightness is expected to decrease sharply with each such successive step.

Taking first the expectation of the sequence of bounds (36), (38),... with respect to \( X \) and then the negative logarithm of the resulting expressions yields, via (31), the corresponding sequence of lower bounds on EE,
\[
H(\Theta, X) \geq \log \left( 1 - P(\Theta, X) - \sum_{i=1}^n \delta_i \right), \quad n = 1, \ldots, M - 1,
\]
where the non-negative quantities \( \delta_i \) are defined as
\[
\delta_i \equiv \sum_{X} \left[ 1 - p(\theta, X) - \cdots - p(\theta, X) \right] 
\times [p(\theta, X) - p(\theta, X)]
\]
in which \( m(X) \) is just a shorthand for the \( \theta \) label corresponding to the \( i \)th largest posterior probability, given \( X \). One may regard the correction \( \sum_i \delta_i \) in (39) to be a bound on the increase of the probability of hypothesis-decision error beyond the MPE given by the MAP protocol.

V. GENERALIZATION OF THE FEDER-MERHAV APPROACH AND OTHER LOWER BOUNDS ON EQUIVOCATION

In their seminal paper [5], Feder and Merhav derived a different lower bound on EE as a function of the MPE, namely
\[
H(\Theta, X) \geq \varphi_*(P_e^{min}),
\]
where the function \( \varphi_* \) is the piecewise linear, convex function defined as
\[
\varphi_*(u) = \left\{ \begin{array}{ll}
  a_1 u + b_1 & 0 \leq u \leq 1/2 \\
  a_2(u - 1/2) + b_2 & 1/2 \leq u \leq 2/3 \\
  \vdots & \vdots \\
  a_n (u - n-1) + b_n & u \leq n/n+1.
\end{array} \right.
\]
where \( a_n = n(n+1) \log[(n+1)/n] \) and \( b_n = \log n \), \( n = 1, \ldots, M - 1 \). The corresponding upper bound on MI, along with the bound (12), provide the tightest available upper bounds on MI involving the MPE alone.

The Feder-Merhav approach can be refined by lower-bounding the EE more tightly, subject to the knowledge of the first two highest posterior probabilities, not just the highest one that relates directly to MPE via (41). Let \( \{p_1(x), p_2(x), p_1(x), \ldots, p_{M-2}(x)\} \) be the set of all posterior probabilities arranged in descending order, given \( x \). Here \( p_1(x) \) and \( p_2(x) \) denote, in simplified notation, what we previously called \( p(\theta, X) \) and \( p(\theta, X) \). These two are to be held fixed but the other \( (M - 2) \) posterior probabilities, \( p_1(x), \ldots, p_{M-2}(x) \), are to be varied subject only to the following constraints:
\[
\sum_{m=1}^{M-2} p_m(x) = 1 - p(x) - p_1(x),
\]

where minimizing \( H(\Theta, X) = -p(x) \log p(x) - p_2(x) \log p_2(x) + \delta H(\Theta, X) \), or equivalently \( \delta H(\Theta, X) \), where \( \delta H(\Theta, X) = \sum_{m=1}^{M-2} p_m(x) \log p_m(x) \). Since the entropy is a concave function, the constrained minimum of \( \delta H(\Theta, X) \) is
obtained at a constraint boundary, and the Kuhn-Tucker conditions for constrained minimization are active. These conditions further imply that the sum representing the minimum value of \( \delta H(\Theta|x) \) have as few equal terms containing the largest probabilities allowed by these constraints.

Because of constraints (43), \( p_\ast(x) \) is required to be bounded above both by \( \pi(x) \) and \( 1-\pi(x) \), and thus by the smaller of the two, where \( \pi(x) \) is the estimate of MPE. This leads to two possible cases and their sub-cases, depending on the value of \( p_\ast \) and \( p_\ast(x) \) (we drop the argument \( x \) of these functions whenever clarity is not affected):

A. \( \pi(x) \leq 1-\pi(x) \), i.e., \( \frac{1}{2} \leq p_\ast \leq 1 \)
   i. \( 0 \leq \pi_\ast - p_\ast \leq p_\ast \ast, \text{i.e.}, \pi_\ast/2 \leq p_\ast \leq \pi_\ast \)
      For this subcase, the minimizing posterior PMF is \( \{p_\ast,p_\ast,\pi_\ast-p_\ast,0,\ldots,0\} \), and the minimum estimate of EE is
      \[
      \min H(\Theta|x) = -p_\ast(x) \log p_\ast(x) - p_\ast(x) \log p_\ast(x) \\
      = \log(p_\ast,p_\ast). \tag{44}
      \]
      where \( h(p,q) \) is the ternary entropy for the PMF \( \{p,q,1-p-q\} \).
   ii. \( p_\ast \leq \pi_\ast - p_\ast \ast \leq 2p_\ast \ast, \text{i.e.}, \pi_\ast/3 \leq p_\ast \leq \pi_\ast/2 \)
      The minimizing posterior PMF is \( \{p_\ast,p_\ast,\pi_\ast-p_\ast,0,\ldots,0\} \), and the minimum possible estimate of EE is
      \[
      \min H(\Theta|x) = -p_\ast(x) \log p_\ast(x) - 2p_\ast(x) \log p_\ast(x) \\
      = 2p_\ast(x) \log 2 + \log(p_\ast,2p_\ast). \tag{45}
      \]

B. \( \pi(x) \geq 1-\pi(x) \), i.e., \( 0 \leq p_\ast \leq \frac{1}{2} \)
   i. \( 0 \leq \pi_\ast - p_\ast \leq p_\ast \ast, \text{i.e.}, \pi_\ast/2 \leq p_\ast \leq \pi_\ast \)
      Since \( p_\ast \ast \leq \min(\pi_\ast,1-\pi_\ast) = 1-\pi_\ast \), the bounds here can be tightened as \( \pi_\ast/2 \leq p_\ast \leq 1-\pi_\ast \), which requires for self-consistency that \( 1/2 \leq p_\ast \leq 2/3 \). The minimizing posterior PMF is \( \{p_\ast,p_\ast,\pi_\ast-p_\ast,0,\ldots,0\} \), and the minimum possible estimate of EE is given by (44).
   ii. \( p_\ast \leq \pi_\ast - p_\ast \ast \leq 2p_\ast \ast, \text{i.e.}, \pi_\ast/3 \leq p_\ast \leq \min(1-\pi_\ast,\pi_\ast/2) \)
      When \( 1-\pi_\ast \leq \pi_\ast/2 \), the allowed range of \( \pi_\ast \) is restricted to \( 3/4 \leq \pi_\ast \leq 3/4 \), but otherwise \( \pi_\ast \) need simply be bounded in \( [1/2, 2/3] \). The minimizing posterior PMF is \( \{p_\ast,p_\ast,p_\ast,\pi_\ast-2p_\ast,0,\ldots,0\} \), and the minimum possible estimate of EE is again given by (45).

iii. \( 2p_\ast \leq \pi_\ast - p_\ast \ast \leq 3p_\ast \ast, \text{i.e.}, \pi_\ast/4 \leq p_\ast \leq \min(1-\pi_\ast,\pi_\ast/3) \)

Again, if \( 1-\pi_\ast \leq \pi_\ast/3 \), the allowed range is restricted to the smaller interval \( 3/4 \leq \pi_\ast \leq 4/5 \), but otherwise to the interval \( 1/2 \leq \pi_\ast \leq 3/4 \). In either case, the the minimizing posterior PMF is \( \{p_\ast,p_\ast,p_\ast,p_\ast,\pi_\ast-3p_\ast,0,\ldots,0\} \), and the minimum possible estimate of EE is given by (46).

iv. And so on...

The results described above may be consolidated into the following lower bound on the EE estimate, given the two highest posterior probabilities \( p_\ast(x) \) and \( p_\ast(x) \):
\[
H(\Theta|x) = \min (u,v) \leq v \leq \min (u,1-u)
\]
\[
\varphi(u,v) = \begin{cases} 
\frac{u}{v} & \text{if } v \leq \frac{1-u}{u-n} \\
\frac{u}{v} & \text{if } v > \frac{1-u}{u-n} \\
\end{cases}
\tag{47}
\]

We display these different allowed sub-regions in Fig. 1. The full allowed region in the \( p_\ast - p_\ast \ast \) plane is the interior of the triangle OAB that bounds \( p_\ast \ast \) as \( 0 \leq p_\ast \ast \leq \min(\pi_\ast,1-\pi_\ast) \). Over its triangular sub-regions ABC, ACD, ADE, etc. designated by the upper-case roman numerals I, II, III, . . . the different lower bounds on the EE estimate starting from the top in (48) apply, respectively.

![Allowed Regions of the p_\ast-p_\ast plane](image)

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Fig. 1. The overall allowed triangular region, OAB, in the \( p_\ast - p_\ast \ast \) plane and its various sub-regions, ABC, ACD, ADE, etc., over each of which a separate form of the minimum value of the EE estimate, subject to the given pair of values \( p_\ast, p_\ast \ast \), applies. The text provides more detailed information.

Averaging the minimum value of the estimate of EE given by (47) and (48) over the output \( X \) yields the lower bound on EE. But since the ternary entropy is a concave function of its...
arguments, the tightest possible convex lower bound on EE, which we denote as $\Phi(u, v)$, is a piecewise linear function of $u \overset{\text{def}}{=} E_X p_*(X)$, which is $1 - P_e^{(\text{true})}$, and $v \overset{\text{def}}{=} E_X p_*(X)$, with a separate linear form for each triangular sub-region in the $p_* - p_+$ plane. For each such sub-region, if the function $\varphi$ given in (48) takes values $\varphi_1$, $\varphi_2$, and $\varphi_3$ at its three vertices whose coordinates are $(u_1, v_1)$, $(u_2, v_2)$, and $(u_3, v_3)$, respectively, then $\Phi(u, v)$ in the interior of the triangle at a point $(u, v) = \sum_{i=1}^3 (u_i, v_i) t_i$, with $t_i \geq 0$, $\sum_{i=1}^3 t_i = 1$, is equal to the value of the corresponding linear interpolant at that point, $\Phi(u, v) = \sum_{i=1}^3 t_i \varphi_i$. With the following values of $\varphi$ at the various triangular vertices in Fig. 1, as simply obtained from (48):

$$
\varphi_A = h(1, 0) = 0; \quad \varphi_B = h\left(\frac{1}{2}, \frac{1}{2}\right) = \log 2;
$$

$$
\varphi_C = h\left(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}\right) + \frac{2}{3} \log 2; \quad \varphi_D = h\left(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right) + \frac{3}{4} \log 4; \ldots
$$

$$
\varphi_n = h\left(\frac{1}{n+1}, \frac{n}{n+1}\right) + \frac{n}{n+1} \log n; \ldots, \quad (49)
$$

where $\varphi_n$ is its value at $(1/(n+1), 1/(n+1))$, the $n$th vertex point when going down the 45° diagonal line, the convex lower bound function $\Phi(u, v)$ is then fully specified in the allowed region, $v \leq \min(u, 1-u)$, $u, v \geq 0$. Since at these vertices the ternary entropy function reduces to the binary entropy function, the convex lower bound $\Phi(u, v)$ involves only the binary entropy function in all allowed sub-regions of the $p_*$ - $p_+$ plane.

The overall convexity of the so constructed piece-wise linear function $\Phi$ over the entire allowed region is easily checked numerically by verifying the convexity of the function along the main diagonal in the $uv$ plane, and is also clearly seen in Fig. 2 in which we display this function.

![Fig. 2. The piecewise linear convex bound function $\Phi(u, v)$](image)

Further refinement of the piecewise linear convex FM bound can be performed similarly as here, tightening the bound further, by including increasingly more of the posterior probabilities in the descending order of their values. We expect this procedure to improve the tightness of the bound more rapidly at the higher SNR values than at the lower ones where more, rather than fewer, of the so-ordered posterior probabilities are needed to specify the problem more accurately.

VI. An Improved Sequence of Upper Bounds on Equivocation

As in the previous section, let us fix the two highest posterior probabilities, $p_*(x)$ and $p_+(x)$, and maximize the estimator for equivocation, $H(\Theta|X = x)$, subject to the sum of the remaining $(M - 2)$ posterior probabilities being $1 - p_*(x) - p_+(x)$. The maximum is easily shown to be attained when these remaining probabilities take equal values, each being $[1 - p_*(x) - p_+(x)]/(M - 2)$, which yields the following upper bound on the equivocation estimate, given the data value $x$:

$$
H(\Theta|X = x) = -\sum_{n=1}^M \log p_*(x) - p_+(x) \log p_+(x) - [1 - p_*(x) - p_+(x)] \log \left[\frac{1 - p_*(x) - p_+(x)}{M - 2}\right].
$$

(50)

Taking the expectation of this bound with respect to $X$ and noting that $-u \log u$ is a concave function, we may obtain the following looser upper bound on equivocation in terms of the MPE and the largest contribution to it, namely $\delta P_e^{(1)} \overset{\text{def}}{=} E_X[p_*(X)]$:

$$
H(\Theta|X) \leq [1 - P_e^{(\text{true})}] \log[1 - P_e^{(\text{true})}] - \delta P_e^{(1)} \log \delta P_e^{(1)}
$$

$$
- [P_e^{(\text{true})} - P_e^{(1)}] \log[P_e^{(\text{true})} - P_e^{(1)}]
$$

$$
+ [P_e^{(\text{true})} - P_e^{(1)}] \log(M - 2).
$$

(51)

Just like the lower bounds (39) derived earlier, the upper bound (51) can be tightened further by fixing increasingly more of the posterior probabilities ordered according to decreasing values. The upper bound (51) is tighter than the original Fano bound (3), which can be regarded as the zeroth-order bound in our sequence of upper bounds, one that depends only on the expectation of the highest posterior probability, which is simply $1 - P_e^{(\text{true})}$, with the remaining $(M - 1)$ probabilities chosen to be each equal to $P_e^{(\text{true})}/(M - 1)$.

We shall now compare the tightness of the various lower and upper bounds on EE we have derived here. The specific problem for which we do so is that of jointly estimating the angular position and chemical signature of a muzzle flash using a proposed FLEM-FLASH system.

VII. Comparison of the Various Bounds for a Special Example

The Fly’s Eye Muzzle-Flash (FLEM-FLASH) detection system consists of a number of single-pixel micro-imagers, essential simple light buckets, that are arranged in a regular pattern on an opaque spherical surface. Each of the $S$ micro-imagers is capable of multi-spectral measurements, say in $B$ spectral bands, but the signal photons they record are limited both by the geometrical vignetting of the light-collection micro-tubes in which the imagers are housed and the obliquity
of illumination, which reduces the number of counts when compared to that for a head-on-illuminated imager by the factor \( \cos \theta \). The obliquity angle \( \theta \) is the angle between the imager normal and the direction from which the muzzle flash is incident. The multi-spectral counts are corrupted both by a possibly bright but fluctuating background, as for day-time observations, and the read-out noise of detection. A simple centroiding of the spatial distribution of counts on the spherical surface can provide a good estimate of the directionality of the flash, while a spectral pattern matching can reveal the chemical signature of the flash. A schematic of a one-dimensional (1D) ring version of the FLEM-FLASH system is shown in Fig. 3. Such a 1D version of the full 2D spherical system suffices for the purposes of this paper. The FLEM-FLASH system was proposed by the author as part of a DARPA funded project under its SCENICIC program in 2012 [15].

The MI between the detected multi-spectral count data and the pair of input parameters, namely flash directionality and spectral signature, yields an upper limit on the amount of statistical information about the input parameters that the count data can provide to any estimator of these parameter values. Specifically, \( \Theta \) here is a two-component vector whose possible values range over an outer product of 4 possible flash directions and 8 possible spectral signatures, the latter distinguished by their spectral traces, i.e., over 32 possible directionality-spectral signature pairs. We first take the prior over these possible pair values to be uniform, so \( H(\Theta) = \log_2(32) = 5 \) bits. The conditional fluctuations of the background and readout noise are assumed to be describable by Gaussian statistics, conditioned on the knowledge of the value of the parameter vector, i.e.,

\[
X|\Theta \sim N(\mu(\Theta), \sigma^2),
\]

where \( \sigma^2 \) is the sum of the sensor read-noise variance, set here at 25 squared electrons, and the variance of the background brightness fluctuations, considered isotropic and uniform across the different spectral channels. The latter fluctuations are taken to be a fraction, set here at 50%, of the mean background brightness level, set here at 10 electron counts. The ratio of the mean signal \( s \) for head-on illumination of a microimager and the mean background level \( b \) defines the peak signal-to-background ratio (PSBR).

In Fig. 4, we plot an exact Monte-Carlo sampling based evaluation of the exact fractional MI (fMI), which is simply the ratio of MI to \( H(\Theta) \) that is bounded between 0 and 1, by means of the dashed curve for a number of values of the PSBR. All the other curves on this plot depict bounds on the exact fMI. The upper bounds on fMI are given by subtracting the lower bounds on EE from \( H(\Theta) \), the lower bounds by subtracting the upper bounds on EE from \( H(\Theta) \), and then normalizing the difference in each case by \( H(\Theta) \) itself. Below we refer to the bounds on fMI as being related in this way to the corresponding bounds on EE derived in this paper. We use the symbol FMB to denote the Feder-Merhav bound corresponding to (12); CFMB to denote the slightly tighter, minimally convex FM bound corresponding to (41); FMB1 and FMB2 to denote the first two improved FM bounds corresponding to (29) for \( n = 1 \) and \( n = 2 \); FMp,∗ to denote the refined FM bound corresponding to (48); CFMp,∗ to denote the refined but looser FM bound obtained by piece-wise linear convexification of (48); capacity bound to denote bound (34); ∆-bound for the bound corresponding to (30); Fano to denote the Fano lower bound (42); and Fano1 and Fano2 to denote, respectively, the first and second-order corrections to the Fano bound corresponding to (51) and its next improved version involving \( P_e^{(min)} \), \( \delta P_e^{(1)} \), and the third largest posterior probability, \( \delta P_e^{(2)} \) defined \( \delta P_e^{(2)} = \mathbb{E}[p(\theta_{m+1}(X)|X)] \).

Note that the FMB and CFMB are essentially indistinguishable, but including \( \delta_1 \) and subsequently \( \delta_2 \) in (59) to yield the first two corrections to the FM bound tightens it significantly as indicated by the line segments labeled as FMB1 and FMB2. The FMp,∗ bound, which is the refined FM bound without convexification, is excellent at moderate to high PSBR values, but is no better than FMB2 at much lower PSBR. This is expected since the lower the PSBR value the more mutually comparable values all the posterior probabilities take, and

![Fig. 3. A schematic one-dimensional ring of regularly spaced single-pixel multi-spectral micro-imagers. The imagers are oriented radially outwards, so each receives maximum head-on illumination from a point source, like a muzzle flash, along the radial line on which it is located. These head-on illumination directions for the different imagers are indicated by green arrows.](image-url)
so including just the highest two posteriors is inadequate to accurately represent the exact result, but not so at the higher PSBR values. The convexified bound, $\text{CFM}_{p_1, p_2, \ldots}$, is considerably looser and virtually indistinguishable from $\text{FMB}_1$ at all PSBR values, but still tighter than $\text{FMB}$ which only includes the highest posterior probability.

The capacity bound \(\Delta\) is quite a bit tighter than these, however, since the former represents the value of \(\frac{1}{2} \log p_1 p_2\) that would be obtained were we to set \(n = M - 1 = 31\) there and thus what we would label as $\text{FMB}_31$ for the present problem. The \(\Delta\)-bound is nearly coincident with the capacity bound for the present problem over the full PSBR range. The two improved Fano lower bounds, labeled by Fano1 and Fano2, tighten the classic Fano bound considerably, but the gap between the exact results for $f\text{MI}$ and these tightened bounds is still quite significant for the present application.

VIII. Concluding Remarks

In this paper we have derived a number of useful upper and lower bounds on MI in terms of the associated MPE, which is directly related to the expectation of the maximum posterior probability, and certain secondary Bayesian metrics of error that involve the second, third, \ldots largest of the posterior probabilities. By incorporating these secondary error metrics, we are able to tighten the well known Feder-Merhav and Fano bounds on MI that are based exclusively on the MPE alone.

We have also derived an upper bound on MI that is tighter still, but it does not have a simple interpretation in terms of Bayesian error. For high-dimensional problems, however, it does provide a computationally expedient, accurate approximation to MI that can be useful when exact MI calculations would be rather prohibitive. All our bounds were compared to the numerically exact calculations of MI to assess their tightness for a specific application.

We have also derived a family of upper bounds on the MPE itself defined in terms of the generalized, or tilted, posterior PMF, which can be used, in a sequential manner, to tighten that presented by the EE in the Feder-Merhav bound. While the bound is not attained by the MPE even as the minimum of the sequence for a finite-dimensional problem, it is expected to be tight in the asymptotic limit of infinitely many data variables. These results, as well as the bounds on MI involving Bayesian error probabilities that were derived in this paper, can ultimately be useful for a study of error in channel coding and data compression when finite codewords and bit strings are involved and the asymptotic limit is not particularly meaningful.

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