TWO DICTATOR FUNCTIONS MAXIMIZE MUTUAL INFORMATION

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For two arbitrarily correlated Rademacher random variables $X$ and $Y$ on $\{-1,1\}$, i.e., $E[X] = E[Y] = 0$, let $(X^n, Y^n)$ be $n$ independent, identically distributed copies of $(X, Y)$. It is shown that the inequality $I(f(X^n); g(Y^n)) \leq I(X; Y)$ holds for any two functions $f, g : \{-1,1\}^n \to \{-1,1\}$, where $I(\cdot; \cdot)$ denotes mutual information. Furthermore, a necessary and sufficient condition for equality is obtained. This positively resolves a conjecture published by Kumar and Courtade in 2013.

1. Introduction and Main Results. Boolean functions play a role in questions of complexity theory, the design of digital circuits and cryptography as well as to implicitly represent massive data based upon an efficient data structure called the zero-suppressed binary decision diagram.

Let $(X, Y)$ be two dependent Rademacher random variables on $\{-1,1\}$, i.e., their expectation is $E[X] = E[Y] = 0$. By defining $\rho := E[XY] \in [-1,1]$, the mutual information of $X$ and $Y$ (in bits) [4, Section 2.3] equals $I(X; Y) = 1 - h_0(1 + \rho^2)$, where $h_0(r) := -r \log_2(r) - (1 - r) \log_2(1 - r)$ is the binary entropy function. Fix $n \in \mathbb{N}$ and let $(X^n, Y^n)$ be $n$ independent, identically distributed copies of $(X, Y)$. Motivated by problems in computational biology [9], Kumar and Courtade formulated the following conjecture [10].

Conjecture 1. For any function $f : \{-1,1\}^n \to \{-1,1\}$,

$$I(f(X^n); Y^n) \leq 1 - h_0\left(\frac{1 + \rho}{2}\right).$$

(1)

The dictator functions [11, Definition 2.3] $f(x) = x_i$, $i \in \{1,2,\ldots,n\}$ achieve equality in eq. (1).

As mentioned in the original publication [10], Conjecture 1 appears easy at first sight, but it turns out to be much deeper. Standard information-theoretic manipulations fail at establishing eq. (1), as does induction over $n$. Primary 94A15; secondary 94C10

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Furthermore, Conjecture 1 seems to be special for doubly symmetric binary sources [5, Example 10.1], as was shown in [2, Section I.A], its generalization to arbitrary binary sources fails. After the original publication, significant interest was generated and several efforts were made to solve this problem. A summary can be found in [3, Section IV]. More recently, Ordentlich et al. [12] used Fourier-analytic techniques and leveraged hypercontractivity to improve upon previously known bounds on $I(f(X^n);Y^n)$ and Kindler et al. [8] studied an analogous problem in Gaussian spaces.

We next state the main result of this paper.

**Theorem 1.** For any two functions $f, g: \{-1,1\}^n \to \{-1,1\}$,

$$I(f(X^n);g(Y^n)) \leq I(X;Y) = 1 - h_0\left(\frac{1 + \rho}{2}\right).$$

(2)

This statement involving two Boolean functions is weaker than Conjecture 1 (in fact, eq. (2) would readily follow from eq. (1) via the data processing inequality [4, Theorem 2.8.1]). Despite its simplicity, standard information-theoretic tools seem to be insufficient for establishing eq. (2).

Theorem 1 was mentioned as an open problem in the original publication [10, Section IV] as well as [3]. A proof was previously only available under the additional restrictive assumptions that $f$ and $g$ are equally biased (i.e., $E[g(X)] = E[f(X)]$) and satisfy the condition

$$P \{f(X^n) = 1, g(X^n) = 1\} \geq P \{f(X^n) = 1\} P \{g(X^n) = 1\}.$$  

(3)

Refer to [3, Section IV] for further details.

In this paper, we prove Theorem 1 without any restrictions using Fourier-analytic tools. By suitably bounding the Fourier coefficients of $f$ and $g$, we reduce eq. (2) to elementary inequalities, which are subsequently proved. Anantharam et al. [2] had a different approach towards Theorem 1. They conjectured a result concerning the hypercontractivity ribbon of two binary random variables, which would imply Theorem 1. This stronger result still remains open, as our proof does not invoke hypercontractivity but purely relies on Fourier-analytic arguments.

**Remark 1.** Like Conjecture 1, Theorem 1 also generally fails if $(X,Y)$ are binary asymmetric sources. In particular, the counterexample given in [2, Section I.A] shows that our Fourier analytic proof of Theorem 2 will not carry over to $p$-biased Fourier analysis [15, 16].

Clearly, the dictator functions $f(x) = x_i, g(y) = y_i$ for any $i \in \{1,2,\ldots,n\}$ achieve equality in eq. (2). By carefully analyzing the proof of Theorem 1,
we will show that this solution is in fact unique, up to multiplications by $-1$:

**Proposition 1.** Depending on $\rho$, we have the following necessary and sufficient conditions for equality in eq. (2):

- If $\rho = 0$, any pair of functions $f, g : \{-1,1\}^n \to \{-1,1\}$ achieves $I(f(X^n); g(Y^n)) = 0$.
- If $\rho = 1$, equality in eq. (2) holds if and only if $f : \{-1,1\}^n \to \{-1,1\}$ is unbiased (i.e., $E[f(X)] = 0$) and $g = \pm f$.
- If $\rho = -1$, equality in eq. (2) holds if and only if $f : \{-1,1\}^n \to \{-1,1\}$ is unbiased and $g(x) = \pm f(-x)$ for all $x \in \{-1,1\}^n$.
- If $\rho \in (-1,0) \cup (0,1)$, we have equality in eq. (2) if and only if $f(x) = \pm x_i$ and $g(y) = \pm y_i$, for some $i \in \{1,2,\ldots,n\}$.

2. Notation and Definitions. We use $E[\cdot]$ as the expectation operator and $P\{\cdot\}$ to denote the probability of an event. For brevity define $\Omega := \{-1,1\}$ and let $(X, Y)$ be two Rademacher random variables on $\Omega$, i.e., $E[X] = E[Y] = 0$. Defining $\rho := E[XY] \in [-1,1]$ and $r := P\{X = Y\} = \frac{1}{2}(1 + \rho) \in [0,1]$, we say that $X$ and $Y$ are $\rho$-correlated. Fix $n \in \mathbb{N}$ and let $(X, Y) := (X, Y)^n$ be $n$ independent, identically distributed copies of $(X, Y)$.

For convenience we define $\bar{t} := 1 - t$ for $t \in \mathbb{R}$ and use $\log_2(\cdot)$ and $\log(\cdot)$ to denote the binary and the natural logarithm, respectively. We will require some basic concepts from information theory, in particular mutual information and entropy [4, Section 2.3], given here for the sake of completeness. As customary we will adopt the convention $0 \cdot \log_2(0) := 0$.

**Definition 1.** Given two random variables $X, Y$ on the finite probability space $\mathcal{X} \times \mathcal{Y}$, with probability mass function $p$, the mutual information (in bit) of $X$ and $Y$ is given by

\[
I(X; Y) := \sum_{(x,y) \in \mathcal{X} \times \mathcal{Y}} p(x,y) \log_2 \left( \frac{p(x,y)}{p(x)p(y)} \right),
\]

where $p(x) := \sum_{y \in \mathcal{Y}} p(x,y)$ (and $p(y)$ accordingly) denotes the marginal. The entropy of $X$ is defined as

\[
H(X) := -\sum_{x \in \mathcal{X}} p(x) \log_2 (p(x)).
\]

Note that mutual information and entropy only depend on the probability mass function $p$ and are therefore unaffected by one-to-one mappings. In
the special case of a binary random variable \( X \), e.g., \( \mathcal{X} = \Omega \) eq. (5) becomes \( H(X) = h_0(P\{X = 1\}) \), where \( h_0(t) := -t \log_2(t) - \bar{t} \log(\bar{t}) \), \( t \in [0, 1] \) is the binary entropy function. The binary entropy function is symmetric around \( \frac{1}{2} \) (i.e., \( h_0(t) = h_0(\bar{t}) \), \( t \in [0, 1] \)), its unique maximum is \( h_0(\frac{1}{2}) = 1 \), and it is strictly decreasing on \( [\frac{1}{2}, 1] \). Several fundamental properties of mutual information [4, Theorem 2.4.1] will also be used.

We will need several Fourier-analytic properties of Boolean functions. In particular, we need the inner product of two functions \( f, g : \Omega^n \rightarrow \mathbb{R} \), defined as

\[
\langle f, g \rangle := E[f(X)g(X)] = 2^{-n} \sum_{x \in \Omega^n} f(x)g(x)
\]

and the norm, defined as the nonnegative square root \( \|f\| := \sqrt{\langle f, f \rangle} \). This gives rise to the Fourier-Walsh expansion \( \hat{f} \) of \( f : \Omega^n \rightarrow \mathbb{R} \), which is [11, Proposition 1.8]

\[
\hat{f}(S) := \langle f, \chi_S \rangle = 2^{-n} \sum_{x \in \Omega^n} f(x)\chi_S(x)
\]

for each \( S \subseteq [n] := \{1, 2, \ldots, n\} \), where \( \chi_S(x) := \prod_{i \in S} x_i \) is the canonical base. We also write \( \chi_i := \chi_{\{i\}} \), \( i \in [n] \) for the dictator functions [11, Definition 2.3]. Let \( T_\rho \) denote the noise operator [11, Definition 2.46], i.e.,

\[
T_\rho f : \Omega^n \rightarrow \mathbb{R}
\]

\[
x \mapsto E[f(Y)|X = x],
\]

defined for any function \( f : \Omega^n \rightarrow \mathbb{R} \). Whenever \( f, g : \Omega^n \rightarrow \Omega \), we use the following abbreviations:

- \( \alpha := E[f(X)] = \hat{f}(\emptyset) \),
- \( \beta := E[g(X)] = \hat{g}(\emptyset) \),
- \( a := \frac{1}{2}(1 + \alpha) = P\{f(X) = 1\} \),
- \( b := \frac{1}{2}(1 + \beta) = P\{g(X) = 1\} \).

We call \( \alpha \) the bias of \( f \) and say that \( f \) is unbiased if \( \alpha = 0 \).

**Lemma 1.** For two functions \( f, g : \Omega^n \rightarrow \Omega \), the following properties hold for all \( S \subseteq [n] \) and \( x \in \Omega^n \):

1. \( f(x) = \sum_{S \subseteq [n]} \hat{f}(S)\chi_S(x) \);
2. \( \sum_{S \subseteq [n]} \hat{f}(S)^2 = 1 \);
3. \( T_\rho \hat{f}(S) = \rho^{|S|} \hat{f}(S) \);
4. \( \langle f, g \rangle := \mathbb{E}[f(X)g(X)] = \sum_{S \subseteq [n]} \hat{f}(S)\hat{g}(S) = 1 - 2\mathbb{P}\{f(X) \neq g(X)\} \).

The proofs of these well known properties of Boolean functions can be found, e.g., in [11, Sections 1, 2].

We use the convention that the sign of zero equals one and denote (higher-order) derivatives by (multiple) superscript primes. The symbol “±” is used to denote “either + or −”, that is, the statement (in logical notation)

\[(a = \pm x \land b = \pm x) \implies A \tag{10} \]

should be interpreted as

\[
\left[(a = x \land b = x) \lor (a = -x \land b = x) \lor (a = x \land b = -x) \lor (a = -x \land b = -x)\right] \implies A \tag{11}
\]

and \( A \implies a = \pm x \) means \( A \implies (a = x \lor a = -x) \).

3. Proof of the Main Result. We first show that Theorem 1 is equivalent to the next theorem, which is the restriction of Theorem 1 to the special case of nonnegative values of \( \rho, \alpha, \) and \( \beta \).

**Theorem 2.** Assuming \( \rho \geq 0 \), for any two functions \( f, g : \Omega^n \to \Omega \) with \( \hat{g}(\varnothing) \geq \hat{f}(\varnothing) \geq 0 \), it holds that

\[ I(f(X); g(Y)) \leq 1 - h_0(r). \tag{12} \]

Similarly, Proposition 1 is also equivalent to the following restriction:

**Proposition 2.** Necessary and sufficient conditions for equality in eq. (12) are provided by the following properties:

- If \( \rho = 0 \), any pair of functions \( f, g : \Omega^n \to \Omega \) achieves \( I(f(X); g(Y)) = 0 \).
- If \( \rho = 1 \), equality in eq. (2) holds if and only if \( \hat{f}(\varnothing) = 0 \) and \( g = \pm f \).
- If \( \rho \in (0, 1) \), we have equality in eq. (2) if and only if \( f(x) = \pm x_i \) and \( g(y) = \pm y_i \), for any \( i \in [n] \).

3.1. Proof of Equivalence of Theorems 1 and 2. Theorem 2 follows from Theorem 1 since the later holds for any correlation and any two Boolean functions and thus necessarily for \( \rho \geq 0 \) and \( \beta \geq \alpha \geq 0 \) (recall that \( \alpha = \hat{f}(\varnothing), \beta = \hat{g}(\varnothing) \)). In order to show that Theorem 2 implies Theorem 1, we need to prove that Theorem 2 remains true for arbitrary values of \( \alpha, \beta, \rho \).
For \( n \) i.i.d. random variables \((X, Y)\) with arbitrary \( \rho = 2r - 1 \), define \( \tilde{Y} := \text{sgn}(\rho)Y \) such that the components of \( X \) and \( \tilde{Y} \) are i.i.d. and \(|\rho|\)-correlated \((\tilde{r} := (1 + |\rho|)/2)\). Furthermore, for arbitrary Boolean functions \( f(x) \) and \( g(y) \) define:

\[
\begin{align*}
    f^{(0)}(x) &:= \text{sgn}(\alpha)f(x); \\
    g^{(0)}(y) &:= \text{sgn}(\beta)g(y); \\
    g^{(1)}(\tilde{y}) &:= g^{(0)}(\text{sgn}(\rho)\tilde{y}) = g^{(0)}(y);
\end{align*}
\]

we have \( \hat{f}^{(0)}(\emptyset) = |\alpha| \geq 0 \) and \( \hat{g}^{(0)}(\emptyset) = \hat{g}^{(1)}(\emptyset) = |\beta| \geq 0 \). Since mutual information is not affected by applying one-to-one functions, it follows that \( I(f(X); g(Y)) = I(f^{(0)}(X); g^{(0)}(Y)) \). We may assume without loss of generality that \(|\alpha| \leq |\beta|\); otherwise, we swap \( f^{(0)} \) and \( g^{(0)} \) without affecting \( I(f^{(0)}(X); g^{(0)}(Y)) \).

In total, we have

\[
\begin{align*}
    I(f(X); g(Y)) &= I\left(f^{(0)}(X); g^{(0)}(Y)\right) \\
    &= I\left(f^{(0)}(X); g^{(1)}(\tilde{Y})\right) \\
    &\leq 1 - h_0(\tilde{r}) \\
    &= 1 - h_0(r),
\end{align*}
\]

where eq. (18) follows from Theorem 2 and we used that the binary entropy is symmetric around \( \frac{1}{2} \) in eq. (19).

### 3.2. Proof of Equivalence of Propositions 1 and 2

Clearly Proposition 2 follows immediately from Proposition 1.

To show the converse, first assume \( \rho = -1 \). Sufficiency of the given conditions is clear, as

\[
\begin{align*}
    I(f(X); g(Y)) &= I(f(X); g(-X)) \\
    &= I(f(X); \pm f(X)) \\
    &= H(f(X)) \\
    &= 1,
\end{align*}
\]

where eq. (22) follows from [4, Theorem 2.4.1] and the fact that mutual information is not affected by one-to-one mappings. Assuming equality in eq. (2) we have by Proposition 2, with the notation of Section 3.1, that \( \mathbb{E}\left[f^{(0)}(X)\right] = 0 \) and \( g^{(1)} = \pm f^{(0)} \). By the definition of \( f^{(0)} \) this entails
the second-order derivative $\phi$ where
\begin{equation}
(24) \quad I(\hat{f}(X); \hat{g}(Y)) = I(\pm \chi_i(X); \pm \chi_i(Y)) = I(X; Y) = 1 - h_0(r),
\end{equation}

where $i \in [n]$. Assuming equality in eq. (2) we have by Proposition 2, with the notation of Section 3.1, that $f^{(0)} = \pm \chi_i$ and $g^{(1)} = \pm \chi_i$ for some $i \in [n]$. Clearly this entails $f = f^{(0)} = \pm \chi_i$ and $g(y) = \text{sgn}(\beta)g^{(1)}(-y) = \pm \chi_i$.

3.3. Auxiliary Results. Before proving Theorem 2, we need to show several auxiliary results. The following lemma formalizes the minimization and maximization of a convex real, twice differentiable function on a compact interval. It is stated in a way, facilitating its use in subsequent proofs. A proof can, e.g., be obtained from Taylor’s Theorem [13, Theorem 5.15] and [13, Theorem 5.8].

**Lemma 2.** Consider a function $\phi : I \rightarrow \mathbb{R}$ defined on the interval $I := [t_1, t_2]$ with $t_1 < t_2$. If the first-order derivative $\phi'$ is continuous on $I$ and the second-order derivative $\phi''(t)$ exists for every $t \in I^0 := (t_1, t_2)$, then the following two properties hold:

1. If $\phi''(t) \geq 0$, $t \in I^0$, and $\phi'(t^*) = 0$ for some $t^* \in I$, then $\phi(t) \geq \phi(t^*)$ for all $t \in I$. Furthermore, if $\phi''(t) > 0$, $t \in I^0$, and $f'(t^*) = 0$ for some $t^* \in I$, then $f(t) > f(t^*)$ for all $t \in I \setminus \{t^*\}$.

2. If $\phi''(t) \leq 0$, $t \in I^0$, then $\phi(t) \geq \min\{\phi(t_1), \phi(t_2)\}$ for all $t \in I$. Furthermore, if $\phi''(t) < 0$, $t \in I^0$, then $f(t) > \min\{f(t_1), f(t_2)\}$ for all $t \in I^0$.

We will furthermore need the following powerful lemma, which allows us to obtain the necessary bounds on the parameters of the joint distribution of $f(X)$ and $g(Y)$.

**Lemma 3.** Let $f, g : \Omega^n \rightarrow \Omega$ with $0 \leq \alpha \leq \beta \leq 1$ and define $\mathcal{P} := \{S \subseteq [n] : \hat{f}(S)\hat{g}(S) > 0\} \setminus \emptyset$, $\mathcal{N} := \{S \subseteq [n] : \hat{f}(S)\hat{g}(S) < 0\}$. Then the following inequalities hold:
\begin{align}
(25) \quad & \sum_{S \in \mathcal{P}} \hat{f}(S)\hat{g}(S) \leq 2 \left( \bar{a}b + \sqrt{a\bar{a}bb} \right), \\
(26) \quad & \sum_{S \in \mathcal{N}} \hat{f}(S)\hat{g}(S) \geq -2 \left( \bar{a}b + \sqrt{a\bar{a}bb} \right).
\end{align}

If $\alpha = \beta = 0$, equality holds in eq. (25) if and only if $f = g$, and equality in eq. (26) is equivalent to $g = -f$. 

$|\alpha| = 0$ and thus $f = f^{(0)}$. By the definition of $g^{(1)}$, it follows that $g(x) = \text{sgn}(\beta)g^{(1)}(-x) = \pm f(-x)$, for all $x \in \Omega^n$.

Now assume $\rho \in (-1, 0)$. Again, sufficiency follows immediately from
Proof. We will show the inequalities:

\begin{align}
\sum_{S \in P} \hat{f}(S)\hat{g}(S) - \sum_{S \in N} \hat{f}(S)\hat{g}(S) & \leq 4\sqrt{a\bar{a}b\bar{b}}, \\
\sum_{S \in P} \hat{f}(S)\hat{g}(S) + \sum_{S \in N} \hat{f}(S)\hat{g}(S) & \geq -4\bar{a}b, \\
\sum_{S \in P} \hat{f}(S)\hat{g}(S) + \sum_{S \in N} \hat{f}(S)\hat{g}(S) & \leq 4\bar{a}b.
\end{align}

(27) \hspace{1cm} (28) \hspace{1cm} (29)

It is easy to see that eq. (25) can be obtained by adding eq. (27) to eq. (29) while eq. (26) follows by subtracting eq. (27) from eq. (28).

Subtracting the means of \( f \) and \( g \) yields the unbiased functions \( f_0 := f - \alpha \), \( g_0 := g - \beta \). We then define \( f_1 \) and \( g_1 \) in terms of their Fourier transforms \( \hat{f}_1(S) := |\hat{f}_0(S)| \) and \( \hat{g}_1(S) := |\hat{g}_0(S)| \). We obtain eq. (27) as

\begin{align}
\sum_{S \in P} \hat{f}(S)\hat{g}(S) - \sum_{S \in N} \hat{f}(S)\hat{g}(S) &= \sum_{S \subseteq [n]} |\hat{f}_0(S)||\hat{g}_0(S)| \\
&= \langle \hat{f}_0, \hat{g}_0 \rangle \\
&\leq ||\hat{f}_0|| ||\hat{g}_0|| \\
&= \sqrt{(1 - \alpha^2)(1 - \beta^2)} \\
&= 4\sqrt{a\bar{a}b\bar{b}},
\end{align}

(30) \hspace{1cm} (31) \hspace{1cm} (32) \hspace{1cm} (33) \hspace{1cm} (34)

where we used the Cauchy-Schwarz inequality \([14, 4.2]\) in eq. (32). To show eqs. (28) and (29), we use

\begin{align}
\sum_{S \in P} \hat{f}(S)\hat{g}(S) + \sum_{S \in N} \hat{f}(S)\hat{g}(S) &= \sum_{S \subseteq [n]} \hat{f}_0(S)\hat{g}_0(S) \\
&= \langle f_0, g_0 \rangle \\
&= \langle f, g \rangle - \alpha\beta \\
&= 1 - 2P \{ f(X) \neq g(X) \} - \alpha\beta,
\end{align}

(35) \hspace{1cm} (36) \hspace{1cm} (37) \hspace{1cm} (38)

where eq. (38) follows from part 4 of Lemma 1. Let \( \mathcal{A} := f^{-1}(1) \) and \( \mathcal{B} := g^{-1}(1) \) denote the corresponding inverse images. From \( \alpha, \beta \geq 0 \) obtain

\begin{align}
P \{ f(X) \neq g(X) \} &= 2^{-n}(|\mathcal{A} \cap \mathcal{B}^c| + |\mathcal{A}^c \cap \mathcal{B}|) \\
&\leq 2^{-n}(|\mathcal{B}^c| + |\mathcal{A}^c|) \\
&= \bar{a} + \bar{b}
\end{align}

(39) \hspace{1cm} (40) \hspace{1cm} (41)
and since also $\alpha \leq \beta$,

\[(42) \quad P\{f(X) = g(X)\} = 2^{-n}(|A \cap B| \cup |A^c \cap B^c|) \leq 2^{-n}(|A| + |B^c|) = a + \bar{b}.\]

In total we have $1 - (a + \bar{b}) = b - a \leq P\{f(X) \neq g(X)\} \leq \bar{a} + \bar{b}$ and obtain eq. (28) by substituting in eq. (38),

\[(45) \quad \langle f_0, g_0 \rangle = 1 - 2P\{f(X) \neq g(X)\} - \alpha \beta \geq 1 - 2(a + \bar{b}) - \alpha \beta = -(1 - \alpha)(1 - \beta)\]

\[(46) \quad = -4\bar{a}\bar{b}.\]

Similarly we obtain eq. (29) by

\[(47) \quad \langle f_0, g_0 \rangle \leq 1 - 2(b - a) - \alpha \beta = (1 + \alpha)(1 - \beta)\]

\[(48) \quad = 4\bar{a}\bar{b}.\]

To show the necessary condition for equality in eq. (26), assume $\alpha = \beta = 0$ and define $W_P := \sum_{S \in P} \hat{f}(S)^2$ and $W_N := \sum_{S \in N} \hat{f}(S)^2$, where clearly $W_P + W_N = 1$ by part 2 of Lemma 1. Apparently, equality in either eq. (26) or eq. (25) necessitates equality in eq. (32). The Cauchy-Schwarz inequality is satisfied with equality if $g'_0 = \lambda f'_0$ for some $\lambda \in \mathbb{R}$. We have

\[(52) \quad 1 = \|g'_0\| = \|\lambda f'_0\| = |\lambda| \|f'_0\| = |\lambda|\]

and consequently $\lambda = 1$ as $f'_0(S)$ and $g'_0(S)$ are both nonnegative for all $S \subseteq [n]$. Noticing that $f = f_0$ and $g = g_0$, we write

\[(53) \quad g(x) = \sum_{S \subseteq [n]} \hat{g}(S) \chi_S(x)\]

\[(54) \quad = \sum_{S \in P \cup N} \text{sgn}(\hat{g}(S)) \hat{g}'_0(S) \chi_S(x)\]

\[(55) \quad = \sum_{S \in P \cup N} \text{sgn}(\hat{g}(S)) \hat{f}'_0(S) \chi_S(x)\]

\[(56) \quad = \sum_{S \in P \cup N} \text{sgn}(\hat{g}(S)) \hat{f}(S) \chi_S(x)\]

\[(57) \quad = \sum_{S \in P} \hat{f}(S) \chi_S(x) - \sum_{S \in N} \hat{f}(S) \chi_S(x),\]
which leads to
\[(f, g) = W_P - W_N.\]

For equality in eq. (26) we also need equality in eq. (46), i.e., \[(f, g) = -1.\]
Together with eq. (58) and considering that \(W_P + W_N = 1\), we obtain \(W_N = 1\) and consequently \(g = -f\) by eq. (57). When requiring equality in eq. (25), one obtains the necessary condition \(g = f\) in the same manner, using equality in eq. (49).

**Definition 2.** For \(1/2 \leq a \leq b < 1\) and \(t \in [1 - 2(b + \bar{a}), 1 - 2(b - a)]\) define the function
\[
\phi_{a,b}(t) := b h_0 \left( \frac{1}{2} \left( 1 + \frac{a}{b} - \frac{1-t}{2b} \right) \right) + \bar{b} h_0 \left( \frac{1}{2} \left( 1 + \frac{\bar{a}}{\bar{b}} - \frac{1-t}{2\bar{b}} \right) \right).
\]

We next show that \(\phi_{a,b}(t)\) is strictly concave.

**Lemma 4.** For \(1/2 \leq a \leq b < 1\) and \(1 - 2(b + \bar{a}) < t < 1 - 2(b - a)\), we have \(\phi''_{a,b}(t) < 0\).

**Proof.** We calculate the first-order derivative
\[
\phi'_{a,b}(t) = \frac{1}{4} \log_2 \left( \frac{(2(b-a) + t)(2(b - a) + \bar{t})}{(2(b+a) - t)(2(b + a) - \bar{t})} \right)
\]
and the second-order derivative
\[
\phi''_{a,b}(t) = -\frac{1}{4 \log(2)} \left( \frac{1}{2(b-a) + \bar{t}} + \frac{1}{2(b - a) + t} + \frac{1}{2(b+a) - t} + \frac{1}{2(b + a) - \bar{t}} \right).
\]
The proof is concluded by observing that each term in eq. (61) is nonnegative if \(1/2 \leq a \leq b < 1\) and \(2(b - a) < \bar{t} < 2(b + \bar{a})\).

The following result on \(\phi_{a,b}(t)\) follows from elementary results in real analysis. Although conceptually simple, the proof is rather lengthy and therefore deferred to Section 4.

**Lemma 5.** For \(1/2 \leq a \leq b < 1\) and \(0 \leq \rho \leq 1\), let
\[
t_0 := \max \left\{ 1 - 2(\bar{a} + \bar{b}), 1 - 2 \left( ab + b\bar{a} + \rho \left( \bar{a}b + \sqrt{a\bar{a}bb} \right) \right) \right\},
\]
\[
t_1 := \min \left\{ 1 - 2(b - a), 1 - 2 \left( \bar{a}b + \bar{a} \right) - \rho \left( ab + \sqrt{a\bar{a}bb} \right) \right\}.
\]
Then,

\begin{align}
(64) & \quad h_0(a) - \phi_{a,b}(t_0) \leq 1 - h_0(r) \\
(65) & \quad h_0(a) - \phi_{a,b}(t_1) \leq 1 - h_0(r)
\end{align}

with equality if and only if either \( \rho = 0 \) or \( a = b = \frac{1}{2} \).

3.4. **Proof of Theorem 2.** It is easy to see, that \( b = 1 \) entails \( g \equiv 1 \) and therefore \( I(f(X);g(Y)) = 0 \leq 1 - h_0(r) \). Thus, we assume in the following \( \frac{1}{2} \leq a \leq b < 1 \). We can then write \( I(f(X);g(Y)) \) as

\begin{equation}
I(f(X);g(Y)) = h_0(a) - bh_0(P \{ f(X) = 1|g(Y) = 1 \})
- \bar{b}h_0(P \{ f(X) = -1|g(Y) = -1 \}).
\end{equation}

This identity can be verified using the connection between mutual information and entropy [4, Theorem 2.4.1]

\begin{align}
(67) & \quad I(f(X);g(Y)) = H(f(X)) - H(f(X)|g(Y)) \\
(68) & \quad = H(f(X)) - \sum_{t \in \Omega} P \{ g(Y) = t \} H(f(X)|g(Y) = t) \\
(69) & \quad = h_0(a) - bH(f(X)|g(Y) = 1) - \bar{b}H(f(X)|g(Y) = -1).
\end{align}

We will obtain bounds for \( P \{ f(X) = \pm 1|g(Y) = \pm 1 \} \) and reduce eq. (12) to elementary inequalities by way of eq. (66).

In analogy to [11, Proposition 1.9] we have

\begin{equation}
\langle f, T_\rho g \rangle = 2P \{ f(X) = g(Y) \} - 1
\end{equation}

and write

\begin{align}
(70) & \quad P \{ f(X) = 1|g(Y) = 1 \} \\
(71) & \quad = \frac{P \{ f(X) = 1, g(Y) = 1 \}}{P \{ g(Y) = 1 \}} \\
(72) & \quad = \frac{1}{2b} \left( P \{ f(X) = 1 \} + P \{ g(Y) = 1 \} + P \{ f(X) = g(Y) \} - 1 \right) \\
(73) & \quad = \frac{1}{2b} \left( a + b + \frac{1}{2} \langle f, T_\rho g \rangle + 1 - 1 \right) \\
(74) & \quad = \frac{1}{2} \left( 1 + \frac{a}{b} - \frac{1 - \langle f, T_\rho g \rangle}{2b} \right).
\end{align}

Similarly we obtain

\begin{equation}
P \{ f(X) = -1|g(Y) = -1 \} = \frac{1}{2} \left( 1 + \frac{a}{b} - \frac{1 - \langle f, T_\rho g \rangle}{2b} \right)
\end{equation}
and it follows from \( 0 \leq P \{ f = -1 | g = -1 \} \leq 1 \) that

\[
1 - 2(\bar{a} + \bar{b}) \leq \langle f, T_\rho g \rangle \leq 1 - 2(b - a).
\]

We may thus write eq. (66) as

\[
I(f(X); g(Y)) = h_0(a) - \phi_{a,b}(\langle f, T_\rho g \rangle).
\]

In addition to eq. (77) the following lower bound holds:

\[
\langle f, T_\rho g \rangle = \sum_{S \subseteq [n]} \rho^{|S|} \hat{f}(S) \hat{g}(S)
\]

\[
= \alpha \beta + \sum_{S \in \mathcal{P}} \rho^{|S|} \hat{f}(S) \hat{g}(S) + \sum_{S \in \mathcal{N}} \rho^{|S|} \hat{f}(S) \hat{g}(S)
\]

\[
\geq \alpha \beta + \sum_{S \in \mathcal{N}} \rho^{|S|-1} \hat{f}(S) \hat{g}(S)
\]

\[
= \alpha \beta + \rho \sum_{S \in \mathcal{N}} \check{f}(S) \check{g}(S)
\]

\[
\geq \alpha \beta - 2\rho \left( \bar{a}\bar{b} + \sqrt{a\bar{a}b\bar{b}} \right)
\]

\[
= (2a - 1)(2b - 1) - 2\rho \left( \bar{a}\bar{b} + \sqrt{a\bar{a}b\bar{b}} \right)
\]

\[
= 1 - 2 \left( ab + \bar{b}a + \rho \left( \bar{a}\bar{b} + \sqrt{a\bar{a}b\bar{b}} \right) \right).
\]

The steps are justified as follows. Equation (79) follows from parts 3 and 4 of Lemma 1. Equation (81) is a consequence of \( \rho \geq 0 \) and \( \hat{f}(S) \hat{g}(S) \geq 0 \) for \( S \in \mathcal{P} \). Equation (83) holds as \( \emptyset \notin \mathcal{N} \), \( \rho \in [0,1] \), and \( \hat{f}(S) \hat{g}(S) \leq 0 \) for \( S \in \mathcal{N} \). In eq. (84), we applied Lemma 3. Using Lemma 3, we also obtain the upper bound

\[
\langle f, T_\rho g \rangle = \alpha \beta + \sum_{S \in \mathcal{P}} \rho^{|S|} \hat{f}(S) \hat{g}(S) + \sum_{S \in \mathcal{N}} \rho^{|S|} \hat{f}(S) \hat{g}(S)
\]

\[
\leq \alpha \beta + 2\rho \left( \bar{a}\bar{b} + \sqrt{a\bar{a}b\bar{b}} \right)
\]

\[
= 1 - 2 \left( ab + \bar{b}a - \rho \left( \bar{a}\bar{b} + \sqrt{a\bar{a}b\bar{b}} \right) \right).
\]

In total, eqs. (77), (86) and (89) yield \( t_0 \leq \langle f, T_\rho g \rangle \leq t_1 \) with \( t_0 \) and \( t_1 \) as
defined in Lemma 5. This implies

\begin{align}
I(f(X); g(Y)) & = h_0(a) - \phi_{a,b}(\langle f, T_\rho g \rangle) \\
& \leq h_0(a) - \min_{t \in \{t_0, t_1\}} \phi_{a,b}(t) \\
& \leq 1 - h_0(r),
\end{align}

where eq. (91) follows from Lemma 4 and part 2 of Lemma 2, and eq. (92) simply follows from Lemma 5.

**Remark 2.** There is a rich literature on the noise sensitivity of Boolean functions (see [6] for an introduction). Hypercontractivity theorems are an important tool in this area, which have also found applications in information theory [1]. Among other important results, a Small-Set Expansion Theorem was proved by Kahn, Kalai, and Linial in the landmark paper [7], using hypercontractivity. A two-set generalization of their Small-Set Expansion Theorem [11, Section 10.1] can be used directly to obtain bounds on \( \langle f, T_\rho g \rangle \) in the context of Theorem 2. Although these bounds are essentially sharp [11, Exercise 10.5], they are not sufficient for proving Theorem 2. This is due to the fact that the Small-Set Expansion Theorem is sharp only asymptotically for very biased functions. However, the critical regime for showing eq. (12) is around unbiased functions.

3.5. **Proof of Proposition 2.** Clearly the given conditions are sufficient. We will perform careful analysis of the proof of Theorem 2 to show that they are also necessary.

The statement for \( \rho = 0 \) is trivial, thus assume \( \rho \in (0, 1] \). For equality in eq. (12) it is necessary to obtain equality in eq. (92), which implies \( a = b = \frac{1}{2} \) by Lemma 5. This entails \( t_0 = -\rho \) and \( t_1 = \rho \). For equality in eq. (12) we also need equality in eq. (91), which can only hold if \( \langle f, T_\rho g \rangle = \pm \rho \) by Lemma 4 and part 2 of Lemma 2. Furthermore, \( \langle f, T_\rho g \rangle \in \{t_0, t_1\} \) implies equality in either eq. (84) or eq. (88). Together with \( \alpha = \beta = 0 \), this means by Lemma 3 that \( g = \pm f \), which implies \( \langle f, T_\rho f \rangle = \rho \). If \( \rho \in (0, 1) \) we have by [11, Proposition 2.50] that \( f = \pm \chi_i \) for some \( i \in [n] \).

4. **Proof of Lemma 5.** The proof of Lemma 5 consists of a series of lemmas, all of which follow from elementary results in real analysis.

4.1. **Auxiliary Results.**

**Lemma 6.** For \( x \in (0, 1) \), \( y \in [0, 1] \) and \( z > 0 \),

\[ f(x, y, z) = (1 - 2x)(1 - 2y)(1 - 2z) \]
1. 
\[ \psi_1(x, z) := \frac{1}{x^{-z} - 1} + \log(1 - x^z) \geq 0. \]

2. 
\[ \psi_2(x, y) := 1 - h_0\left(\frac{1+y}{2}\right) - h_0(x) + x h_0(x \bar{y}) + \bar{x} h_0(x \bar{y}) \geq 0, \]
with equality if and only if either \( x = \frac{1}{2} \) or \( y = 0 \).

3. 
\[ \psi_3(y) := 1 - h_0\left(\frac{1}{2} + \frac{y}{1+y}\right) - h_0\left(\frac{y}{1+y}\right) + \frac{1}{1+y} h_0(y) \geq 0, \]
with equality if and only if \( y \in \{0, 1\} \).

**Proof.** To show part 1, fix \( z > 0 \) and observe that \( \lim_{x \to 0} \psi_1(x, z) = 0 \).

We conclude by showing that \( \psi_1(x, z) \) increases in \( x \), as

\[
\begin{align*}
\frac{\partial}{\partial x} \psi_1(x, z) &= -\frac{1}{(x^{-z} - 1)^2}(-z)x^{-z-1} + \frac{1}{1-x^z}(-z)x^{z-1} \\
&= \frac{z}{x} \left( \frac{1}{(x^{-z} - 1)^2}x^{-z} - \frac{1}{1-x^z}x^z \right) \\
&= \frac{z}{x} \left( \frac{1}{(x^{-z} - 1)^2}x^{-z} - \frac{1}{x^{-z} - 1} \right) \\
&= \frac{z}{x(x^{-z} - 1)} \left( \frac{1}{x^{-z} - 1} \right) \\
&= \frac{z}{x(x^{-z} - 1)} \left( 1 \right) \\
&\geq 0.
\end{align*}
\]

Moving to part 2, it is easily verified, that \( \psi_2(\frac{1}{2}, y) = \psi_2(x, 0) = 0 \) for any \( y \in [0, 1] \) and \( x \in (0, 1) \). Thus, assume \( x \neq \frac{1}{2} \) in the following. We obtain for \( y \in [0, 1] \),

\[
\begin{align*}
\frac{\partial}{\partial y} \psi_2(x, y) &= \frac{1}{2} \log_2 \left( \frac{1+y}{1-y} \right) - x \bar{x} \log_2 \left( \frac{y}{x \bar{x} y^2} + 1 \right) \\
\end{align*}
\]

and

\[
\begin{align*}
\frac{\partial^2}{\partial y^2} \psi_2(x, y) &= \frac{y(1-2x)^2}{\log(2)(x+y)(1-xy)(1-y^2)}.
\end{align*}
\]
Clearly, \( \frac{\partial^2}{\partial y^2} \psi_2(x, y) > 0 \) for \( y \in (0, 1) \) as every factor occurring in eq. (100) is positive. By inspection of eq. (99), \( \frac{\partial}{\partial y} \psi_2(x, 0) = 0 \). We apply part 1 of Lemma 2 to intervals \([0, 1 - \epsilon]\) for arbitrarily small \( \epsilon > 0 \) and have \( 0 = \psi_2(x, 0) < \psi_2(x, y) \) for all \( y \in (0, 1) \). For \( y = 1 \), we have \( \psi_2(x, 1) = 1 - h_0(x) > 0 \).

Regarding part 3, note \( \psi_3(0) = \psi_3(1) = 0 \) and

\[ \psi'_3(y) = \frac{1}{(1 + y)^2} \log_2 \left( (1 + 3y)(1 - y) \right) \quad (101) \]

for \( y \in [0, 1) \). If \( \psi_3(y) \leq 0 \) for any \( y \in (0, 1) \) then \( f \) necessarily attains its minimum on \((0, 1)\) and there exists \( y^* \in (0, 1) \) with \( \psi_3(y^*) \leq 0 \) and \( \psi'_3(y^*) = 0 \) [13, Theorem 5.8]. Clearly \( y^* = \frac{2}{3} \) is the only point in \((0, 1)\) with \( \psi'_3(y^*) = 0 \) and there we have

\[ \psi_3 \left( \frac{2}{3} \right) = 1 - h_0 \left( \frac{1}{2} + \frac{2}{1 + \frac{2}{3}} \right) - h_0 \left( \frac{2}{3} \right) - h_0 \left( \frac{2}{3} \right) + \frac{1}{1 + \frac{2}{3}} h_0 \left( \frac{2}{3} \right) \geq 0 \quad (102) \]

\[ = 1 - h_0 \left( \frac{1}{2} + \frac{2}{3 + 2} \right) - h_0 \left( \frac{2}{5} \right) + \frac{3}{5} h_0 \left( \frac{2}{3} \right) \quad (103) \]

\[ = 1 - h_0 \left( \frac{9}{10} \right) - h_0 \left( \frac{2}{5} \right) + \frac{3}{5} h_0 \left( \frac{2}{3} \right) \quad (104) \]

\[ = 3 \log_2(3) - 2 \log_2(5) \quad (105) \]

\[ = \log_2 \left( \frac{27}{25} \right) \quad (106) \]

\[ > 0. \quad (107) \]

Based on Lemma 6 we show the following two lemmas, which capture the main portion of the proof of Lemma 5.

**Lemma 7.** For \( 0 < a \leq b < 1 \),

\[ \psi(a, b) := 1 - h_0 \left( \frac{1}{2} + \frac{\sqrt{ab}}{\sqrt{ab} + \sqrt{ab}} \right) - h_0(a) + bh_0 \left( \frac{a}{b} \right) \geq 0 \quad (108) \]

with equality if and only if \( a = b = \frac{1}{2} \).

**Proof.** First we consider the case \( b = a \) where we have \( \psi(a, a) = 1 - h_0(a) \geq 0 \), with equality if and only if \( b = a = \frac{1}{2} \). Define the open set
\[ J := \{(a, b) \in \mathbb{R}^2 : 0 < a < b < 1\}. \] We will show \( \psi(a, b) > 0 \) for \((a, b) \in J\).

To this end, introduce the variable transformation

\[(a, b) \mapsto (x, y) := \left(\sqrt{\frac{ab}{\bar{a} \bar{b}}}, \frac{a}{b}\right), \tag{109}\]

and its inverse for \((a, b) \in J\),

\[(x, y) \mapsto (a, b) := \left(\frac{y - x^2}{1 - x^2}, \frac{y - x^2}{y - x^2 y}\right). \tag{110}\]

Also note that \(y \in (0, 1)\) and

\[0 < x^2 = \frac{ab}{\bar{a} \bar{b}} = \frac{\bar{b}}{\bar{a}} < y, \tag{111}\]

thus \((x^2, y) \in J\). We introduce the additional transformation \(c := \frac{\log(y)}{2 \log(x)}\), yielding \(y = x^{2c}\) and

\[0 < c = \frac{\log(y)}{2 \log(x)} < \frac{\log(x^2)}{2 \log(x)} = 1, \tag{112}\]

i.e., \((x, c) \in (0, 1)^2\). Now we redefine \(\psi(a, b)\) in terms of \(x\) and \(c\) as

\[\tilde{\psi}(x, c) = 1 - h_0 \left(\frac{1}{2} + \frac{x}{1 + x}\right) - h_0 \left(\frac{x^{2c} - x^2}{1 - x^2}\right) + \frac{1 - x^{2-2c}}{1 - x^2} h_0(x^{2c}). \tag{113}\]

Fix a particular \(x \in (0, 1)\) and define \(\gamma_x(c) := \tilde{\psi}(x, c)\) for \(c \in (0, 1)\). We obtain

\[\gamma_x'(c) = \frac{2 \log(x)}{(x^2 - 1) \log(2)} \left(2x^{2c} c \log(x) \right. \right.
\left. + x^{2-2c} \log(1 - x^{2c}) - x^{2c} \log(x^{2c} - x^2)\right), \tag{114}\]

where clearly \(\gamma_x'(\frac{1}{2}) = 0\). The second-order derivative is

\[\gamma_x''(c) = \frac{4 \log(x)^2 x^{2c}}{(1 - x^2) \log(2)} \tilde{\gamma}_x(c), \tag{115}\]
with

\[ \tilde{\gamma}_x(c) := \log(x^{2c} - x^2) - 2c \log(x) + \frac{x^2}{x^{4c}} \log(1 - x^{2c}) \]
\[ + \frac{x^2}{x^{2c} - x^2} + \frac{x^2}{(1 - x^{2c})x^{4c}} \]
\[ = \log(1 - x^{2-2c}) + \frac{x^2}{x^{4c}} \log(1 - x^{2c}) \]
\[ + \frac{x^2}{x^{2c} - x^2} + \frac{x^2}{(1 - x^{2c})x^{4c}} \]
\[ = \left( \frac{1}{x^{-2+2c} - 1} + \log(1 - x^{2-2c}) \right) \]
\[ + \frac{x^2}{x^{4c}} \left( \log(1 - x^{2c}) + \frac{1}{x^{-2c} - 1} \right) \]
\[ \geq 0 \]  

where the inequality in eq. (119) follows by applying part 1 of Lemma 6 to each term in eq. (118). Since \( \tilde{\gamma}_x \) determines the sign of \( \gamma''_x \), we have \( \gamma''_x(c) \geq 0 \) for \( c \in (0,1) \). Choose \( 0 < \varepsilon < 1 \) and apply part 1 of Lemma 2 to \( \gamma_x \) with \( I = [\varepsilon, 1 - \varepsilon] \). This entails \( \gamma_x(c) \geq \gamma_x(\frac{1}{2}) \) for \( c \in (0,1) \) as we already established \( \gamma'_x(\frac{1}{2}) = 0 \) and \( \varepsilon \) was arbitrary. We conclude the proof by remarking that \( \gamma_x(\frac{1}{2}) = \tilde{\psi}(x, \frac{1}{2}) > 0 \) for \( x \in (0,1) \) by part 3 of Lemma 6. \[ \square \]

**Lemma 8.** For \( 0 < a \leq b < 1 \) and \( 0 \leq \rho \leq \frac{2\sqrt{ab}}{\sqrt{ab} + \sqrt{ab}} \),

\[ 0 \leq 1 - h_0 \left( \frac{1 + \rho}{2} \right) - h_0(a) + bh_0 \left( a + \rho \frac{ab + \sqrt{ab^2}}{2b} \right) \]
\[ + \tilde{b}h_0 \left( a - \rho \frac{ab + \sqrt{ab^2}}{2b} \right) \]

with equality if and only if either \( a = b = \frac{1}{2} \) or \( \rho = 0 \).
**Proof.** Fix \(0 < a \leq b < 1\) and define

\[
A := \frac{\bar{a}b + \sqrt{a\bar{a}ab}}{2},
\]

(121)

\[
\rho_1 := \frac{2\sqrt{ab}}{\sqrt{a\bar{a}} + \sqrt{\bar{a}b}} = \frac{ab}{A},
\]

(122)

\[
\rho_0 := \min\{ab, \bar{a}\bar{b}\} \frac{A}{\bar{a}b},
\]

(123)

\[
\rho_{-1} := \max\{ab, \bar{a}\bar{b}\} \frac{A}{\bar{a}b}.
\]

(124)

We can write eq. (120) as \(\phi(\rho) \geq 0\) for \(\rho \in [0, \rho_1]\) with

\[
\phi(\rho) := 1 - \log_2 \left( \frac{1 + \rho}{2} \right) - \log_2 \left( a + \rho \frac{A}{b} \right) + \log_2 \left( a - \rho \frac{A}{b} \right).
\]

(125)

If \(\rho = 0\), then clearly \(\phi(0) = 0\). Therefore, assume in the following \(\rho \in (0, \rho_1]\). Next, consider the case \(b = a\). We then have \(A = a\bar{a}\) and

\[
\phi(\rho) = 1 - \log_2 \left( \frac{1 + \rho}{2} \right) - \log_2 \left( a + \rho \frac{a\bar{a}}{a} \right) + \log_2 \left( a - \rho \frac{a\bar{a}}{a} \right)
\]

(126)

\[
= 1 - \log_2 \left( \frac{1 + \rho}{2} \right) - \log_2 \left( a + \rho \bar{a} \right) + \log_2 \left( a - \rho \bar{a} \right)
\]

(127)

\[
\geq 0,
\]

(128)

by part 2 of Lemma 6 with equality if and only if \(a = \frac{1}{2}\).

Assuming \(0 < a < b < 1\), we will now show \(\phi(\rho) < 0\) for \(\rho \in (0, \rho_1]\). We obtain for \(\rho \in [0, \rho_1]\)

\[
\phi'(\rho) = \frac{1}{2} \log_2 \left( \frac{1 + \rho}{1 - \rho} \right) + A \log_2 \left( \frac{(\bar{a}b - A\rho)(\bar{a}b - A\rho)}{(ab + A\rho)(\bar{a}b + A\rho)} \right)
\]

(129)

and

\[
\phi''(\rho) = \frac{A^2}{\log_2 2} \left( \frac{1}{A^2(1 - \rho^2)} - \frac{1}{\bar{a}b - A\rho} \right)
\]

(130)

\[\quad - \frac{1}{ab - A\rho} - \frac{1}{\bar{a}b + A\rho} - \frac{1}{ab + A\rho} \right).\]

Note, that \(\phi'(\rho_1)\) and \(\phi''(\rho_1)\) are undefined, but

\[
\lim_{\rho \uparrow \rho_1} \phi'(\rho) = \lim_{\rho \uparrow \rho_1} \phi''(\rho) = -\infty.
\]

(131)
Moreover, we have

\[
\phi''(0) = \frac{A^2}{\log 2} \left( \frac{1}{A^2 - \frac{1}{ab}} - \frac{1}{ab} - \frac{1}{\bar{ab}} - \frac{1}{\bar{a} \bar{b}} \right)
\]

\[
= \frac{1}{\log 2} \left( 1 - \frac{A^2}{a \bar{a} \bar{b} b} \right)
\]

\[
= \frac{1}{\log 2} \left( 1 - \left( \frac{\sqrt{ab} + \sqrt{\bar{a} \bar{b}}}{\sqrt{ab} + \sqrt{\bar{a} \bar{b}}} \right)^2 \right)
\]

\[
> 0
\]

as \(ab < \bar{a} \bar{b}\). We can write \(\phi''(\rho) = \frac{p(\rho)}{q(\rho)}\), where both \(p\) and \(q\) are polynomials in \(\rho\). We choose

\[
q(\rho) = \log(2)(1 - \rho^2)(\bar{a}b - A\rho)(\bar{a}b - A\rho)(\bar{a}b + A\rho)(ab + A\rho)
\]

and notice that

\[
q(\rho) > 0 \quad \forall \rho \in [0, \rho_1).
\]

And from eq. (130),

\[
p(\rho) = (\bar{a}b - A\rho)(\bar{a}b - A\rho)(\bar{a}b + A\rho)(ab + A\rho)
\]

\[
- A^2(1 - \rho^2) \left( (\bar{a}b - A\rho)(\bar{a}b + A\rho)(ab + A\rho) + (\bar{a}b - A\rho)(\bar{a}b + A\rho)(ab + A\rho) + (\bar{a}b - A\rho)(\bar{a}b - A\rho)(ab + A\rho) + (\bar{a}b - A\rho)(ab - A\rho)(\bar{a}b + A\rho) \right).
\]

This entails \(\deg(p) \leq 5\), i.e., \(p(\rho) = c_5\rho^5 + c_4\rho^4 + c_3\rho^3 + c_2\rho^2 + c_1\rho + c_0\). Calculation of the coefficients reveals \(c_5 = c_4 = 0\), implying \(\deg(p) \leq 3\).

We will now demonstrate that there is one unique point \(\rho^* \in (0, \rho_1)\) with \(p(\rho^*) = 0\). To this end, reinterpret \(\phi''(\rho)\) as a rational function in \(\rho\) on \(\mathbb{R}\). By eqs. (131), (135) and (137), we know that the number of zeros of \(p\) in \((0, \rho_1)\) is odd and less than its degree, i.e., either one or three. We next show that \(p\) has at least one zero in \((-\infty, 0)\), ensuring that there is only one zero in \((0, \rho_1)\). Distinguish the following cases:

1. \(\rho_0 < 1\): We have \(q(\rho) > 0\) for \(\rho \in (-\rho_0, 0)\), \(\phi''(0) > 0\) and \(\lim_{\rho \to -\rho_0} \phi''(\rho) = -\infty\). Thus, there is an odd number of zeros in \((-\rho_0, 0)\).
2. \(\rho_0 = 1\): Note that \(p(-1) = 0\).
3. $\rho_0 = \rho_{-1}$: Observe that $p(-\rho_0) = 0$.
4. $\rho_{-1} > \rho_0 > 1$: Let $I := (-\rho_{-1}, -\rho_0)$ and observe that $q(\rho) > 0$ for $\rho \in I$. Thus, there needs to be an odd number of zeros in $I$ as $\lim_{\rho \to -\rho_{-1}} \phi''(\rho) = -\infty$ and $\lim_{\rho \to -\rho_0} \phi''(\rho) = \infty$.

For illustration, Fig. 1 shows a qualitative sketch of $p(\rho)$ and $\phi''(\rho)$ for the case $\rho_0 < 1$ and Fig. 2 depicts the case $\rho_{-1} > \rho_0 > 1$.

Consequently $\phi''(\rho) > 0$ for $\rho \in (0, \rho^*)$ and by inspection of eq. (129) we have $\phi'(0) = 0$. Thus, by part 1 of Lemma 2, $\phi(\rho) > \phi(0) = 0$ for $\rho \in (0, \rho^*)$. In particular, $\phi(\rho^*) > 0$. Choose any $\varepsilon \in (0, \rho_1 - \rho^*)$. Since
\( \phi''(\rho) < 0 \) for \( \rho \in (\rho^*, \rho_1) \) we have \( \phi(\rho) > \min\{\phi(\rho^*), \phi(\rho_1 - \varepsilon)\} \) for all \( \rho \in (\rho^*, \rho_1 - \varepsilon) \), by part 2 of Lemma 2. From eq. (131) we obtain by the mean value Theorem [13, Theorem 5.10], \( \phi(\rho_1 - \varepsilon) \geq \phi(\rho_1) \) for all \( \varepsilon \in (0, \varepsilon_0) \) for some suitably small \( \varepsilon_0 > 0 \). This implies that \( \phi(\rho) > \min\{\phi(\rho^*), \phi(\rho_1)\} \) for \( \rho \in (\rho^*, \rho_1) \) as \( \varepsilon \) was arbitrary. In summary, we have \( \phi(\rho) > \min\{0, \phi(\rho_1)\} \) for \( \rho \in (0, \rho_1) \) and finish the proof by remarking that \( \phi(\rho_1) \geq 0 \) was shown in Lemma 7.

4.2. Proof of Lemma 5. We will show eqs. (64) and (65) by distinguishing four cases. Starting with eq. (64), first assume

\[
1 - 2(\bar{a} + \bar{b}) \geq 1 - 2\left( a\bar{b} + b\bar{a} + \rho (\bar{a}\bar{b} + \sqrt{a\bar{a}b\bar{b}}) \right),
\]

which is equivalent to

\[
\rho \geq \frac{2\sqrt{ab}}{\sqrt{a\bar{a}b\bar{b}}}.
\]

Now \( t_0 = 1 - 2(\bar{a} + \bar{b}) \) by eq. (62) and

\[
1 - h_0(r) - h_0(a) + \phi_{a,b}(t_0) = 1 - h_0(r) - h_0(a) + \phi_{a,b}(1 - 2(\bar{a} + \bar{b}))
\]

\[
= 1 - h_0(r) - h_0(a) + bh_0\left( \frac{\bar{a}}{\bar{b}} \right)
\]

\[
\geq 1 - h_0\left( \frac{1}{2} + \frac{\sqrt{ab}}{\sqrt{a\bar{a}b\bar{b}}} \right) - h_0(a) + bh_0\left( \frac{\bar{a}}{\bar{b}} \right)
\]

\[
\geq 0,
\]

where eq. (144) follows from eq. (140) and the monotonicity of \( h_0(\cdot) \) on \([\frac{1}{2}, 1]\), and eq. (145) follows from Lemma 7 using the substitution \( a \mapsto \bar{a} \). Note that equality holds in eq. (145) if and only if \( a = b = \frac{1}{2} \).

Conversely, for \( \rho < \frac{2\sqrt{ab}}{\sqrt{a\bar{a}b\bar{b}}} \), we have \( t_0 = 1 - 2\left( a\bar{b} + b\bar{a} + \rho (\bar{a}\bar{b} + \sqrt{a\bar{a}b\bar{b}}) \right) \).
by eq. (62) and obtain

\begin{equation}
1 - h_0(r) - h_0(a) + \phi_{a,b}(t_0) \\
= 1 - h_0(r) - h_0(a) \\
+ \phi_{a,b} \left(1 - 2 \left(\bar{a}b + \bar{b}a + \rho \left(\bar{a}b + \sqrt{a\bar{a}b}\right)\right)\right)
\end{equation}

\begin{equation}
= 1 - h_0(r) - h_0(a) + b h_0 \left(a - \rho \frac{\bar{a}b + \sqrt{a\bar{a}b}}{2b}\right)
\end{equation}

\begin{equation}
+ \tilde{b} h_0 \left(a + \rho \frac{\bar{a}b + \sqrt{a\bar{a}b}}{2b}\right)
\end{equation}

\begin{equation}
\geq 0,
\end{equation}

where eq. (148) follows from Lemma 8 with the substitution \(a \mapsto \bar{a}\). Note that equality holds in eq. (148) if and only if either \(\rho = 0\) or \(a = b = \frac{1}{2}\). This finishes the proof of eq. (64).

To show eq. (65), we first assume

\begin{equation}
1 + \alpha - \beta \leq 1 - 2 \left(\bar{a}b + \bar{b}a - \rho \left(\bar{a}b + \sqrt{a\bar{a}b}\right)\right),
\end{equation}

which is equivalent to

\begin{equation}
\rho \geq \frac{2\sqrt{ab}}{\sqrt{a\bar{a}b} + \sqrt{a\bar{a}b}}
\end{equation}

and implies \(t_1 = 1 - 2(b - a)\) by eq. (63). We obtain

\begin{equation}
1 - h_0(r) - h_0(a) + \phi_{a,b}(t_1) \\
= 1 - h_0(r) - h_0(a) + b h_0 \left(\frac{a}{b}\right)
\end{equation}

\begin{equation}
\geq 1 - h_0 \left(\frac{1}{2} + \frac{\sqrt{ab}}{\sqrt{a\bar{a}b} + \sqrt{a\bar{a}b}}\right) - h_0(a) + b h_0 \left(\frac{a}{b}\right)
\end{equation}

\begin{equation}
\geq 0,
\end{equation}

where eq. (152) holds by eq. (150) and the monotonicity of \(h_0(\cdot)\) on \([\frac{1}{2}, 1]\), and eq. (153) is a consequence of Lemma 7. Note that equality holds in eq. (153) if and only if \(a = b = \frac{1}{2}\).

Conversely, assume \(\rho < \frac{2\sqrt{ab}}{\sqrt{a\bar{a}b} + \sqrt{a\bar{a}b}}\), which entails \(t_1 = 1 - 2 \left(\bar{a}b + \bar{b}a - \rho \left(\bar{a}b + \sqrt{a\bar{a}b}\right)\right)\).
by eq. (63) and we obtain
\begin{equation}
1 - h_0(r) - h_0(a) + \phi_{a,b}(t_1)
\end{equation}
\begin{equation}
= 1 - h_0(r) - h_0(a) + b h_0 \left( a + \frac{\rho}{2b} \left( a\bar{b} + \sqrt{a\bar{a}b\bar{b}} \right) \right)
\end{equation}
\begin{equation}
+ \bar{b} h_0 \left( a - \frac{\rho}{2b} \left( a\bar{b} + \sqrt{a\bar{a}b\bar{b}} \right) \right)
\end{equation}
where eq. (156) follows from Lemma 8. Note that equality holds in eq. (156) if and only if either \( \rho = 0 \) or \( a = b = \frac{1}{2} \).

5. Discussion. The key idea underlying the proof of Theorem 1 is expressed using Fourier-analytic tools in Lemma 3. Based upon this result, we were able to reduce the statement of Theorem 1 to elementary inequalities, which were subsequently proved. These inequalities—in particular Lemma 8, which contains Lemmas 6 and 7 as special cases—required considerable effort. They might turn out to be useful in the context of other converse proofs concerning the optimization of rate regions with binary random variables.

Although we provided a conclusive and complete proof for the tight upper bound on the mutual information of two Boolean functions, Conjecture 1 remains open. Our proof might provide some insight into the general problem. However, it seems unlikely that the idea behind Lemma 3 can be applied to fully resolve Conjecture 1 affirmatively.

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