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DICTATOR FUNCTIONS MAXIMIZE MUTUAL INFORMATION

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Let $(\mathbf{X}, \mathbf{Y})$ denote n independent, identically distributed copies of two arbitrarily correlated Rademacher random variables (X, Y). We prove that the inequality $\mathrm{I}(f(\mathbf{X}); g(\mathbf{Y})) \le \mathrm{I}(\mathsf{X}; \mathsf{Y})$ holds for any two Boolean functions: $f, g\colon \{-1,1\}^n \to \{-1,1\}$ [$\mathrm{I}(\cdot;\cdot)$ denotes mutual information]. We further show that equality in general is achieved only by the dictator functions $f(\boldsymbol{x}) = \pm g(\boldsymbol{x}) = \pm x_i$, $i \in \{1, 2, \ldots, n\}$.

1. Introduction and main results. Let (X, Y) be two dependent Rademacher random variables on $\{-1, 1\}$, with correlation coefficient $\rho := \mathbb{E}[\mathsf{XY}] \in [-1, 1]$. For given $n \in \mathbb{N}$, let $(\mathbf{X}, \mathbf{Y}) = (\mathsf{X}, \mathsf{Y})^n$ be n independent, identically distributed copies of (X, Y). We will use the notation from [3] for information-theoretic quantities. In particular, $\mathbb{E}[\mathsf{X}]$, $\mathrm{H}(\mathsf{X})$ and $\mathrm{I}(\mathsf{X}; \mathsf{Y})$ denote expectation, entropy and mutual information, respectively. Motivated by problems in computational biology [4], Kumar and Courtade formulated the following conjecture [5], Conjecture 1.

CONJECTURE 1. *For any Boolean function* $f\colon \{-1,1\}^n \to \{-1,1\}$,

$$\mathrm{I}\big(f(\mathbf{X}); \mathbf{Y}\big) \le \mathrm{I}(\mathsf{X}; \mathsf{Y}). \tag{1}$$

This claim—while seemingly innocent at first sight—has received significant interest and resisted several efforts to find a proof (see the discussion in [2], Section IV). Note that $f = \chi_i$ for any dictator function ([6], Definition 2.3), $\chi_i(\boldsymbol{x}) := x_i$, $i \in \{1, 2, \ldots, n\}$ achieves equality in (1).

We next state the main result of this paper, which is a relaxed version of Conjecture 1, involving two Boolean functions.

THEOREM 1. *For any two Boolean functions* $f, g\colon \{-1,1\}^n \to \{-1,1\}$,

$$\mathrm{I}\big(f(\mathbf{X}); g(\mathbf{Y})\big) \le \mathrm{I}(\mathsf{X}; \mathsf{Y}). \tag{2}$$

If (1) were true, this statement would readily follow from the data processing inequality [3], Theorem 2.8.1. Theorem 1 was stated as an open problem in [2] and

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[5], Section IV, and separately investigated in [1]. A proof of (2) was previously available only under the additional restrictive assumptions that f and g are equally biased (i.e., $\mathbb{E}[f(\mathbf{X})] = \mathbb{E}[g(\mathbf{X})]$) and satisfy the condition

$$\mathrm{P}\{f(\mathbf{X}) = 1, g(\mathbf{X}) = 1\} \geq \mathrm{P}\{f(\mathbf{X}) = 1\}\mathrm{P}\{g(\mathbf{X}) = 1\}. \tag{3}$$

The reader is invited to see [2], Section IV, for further details. In this paper, we use Fourier-analytic tools to prove Theorem 1 without any additional restrictions on f and g. We suitably bound the Fourier coefficients of f and g, and thereby reduce (2) to an elementary inequality, which is subsequently established. A more detailed discussion of our results and proofs can be found in [7].

A careful inspection of the proof of Theorem 1 reveals that in general, up to sign changes, the dictator functions χ_i, $i \in \{1, 2, \ldots, n\}$ are the unique maximizers of $\mathrm{I}(f(\mathbf{X}); g(\mathbf{Y}))$.

PROPOSITION 1. *If* $0 < |\rho| < 1$, *equality in* (2) *is achieved if and only if* $f = \pm g = \pm \chi_i$ *for some* $i \in \{1, 2, \ldots, n\}$.

2. Proof of Theorem 1. Define $[n] := \{1, 2, \ldots, n\}$ and let f, g be two Boolean functions on the Boolean hypercube, that is, $f, g\colon \{-1, 1\}^n \to \{-1, 1\}$. Denote their Fourier expansions (cf. [6], (1.6)) $f(\boldsymbol{x}) = \sum_{\mathcal{S}\subseteq[n]} \hat{f}_{\mathcal{S}} \chi_{\mathcal{S}}(\boldsymbol{x})$ and $g(\boldsymbol{x}) = \sum_{\mathcal{S}\subseteq[n]} \hat{g}_{\mathcal{S}} \chi_{\mathcal{S}}(\boldsymbol{x})$, using the basis $\chi_{\mathcal{S}}(\boldsymbol{x}) := \prod_{i\in\mathcal{S}} x_i$ for $\mathcal{S} \subseteq [n]$. Define

$$a := \frac{1 + \hat{f}_\varnothing}{2} = \mathrm{P}\{f(\mathbf{X}) = 1\},$$
$$b := \frac{1 + \hat{g}_\varnothing}{2} = \mathrm{P}\{g(\mathbf{X}) = 1\}$$

and

$$\theta_\rho := \frac{1}{4} \sum_{\mathcal{S}:|\mathcal{S}|\geq 1} \hat{f}_{\mathcal{S}} \hat{g}_{\mathcal{S}} \rho^{|\mathcal{S}|}.$$

Without loss of generality, we may assume $\frac{1}{2} \leq a \leq b \leq 1$ and $\rho \in [0, 1]$, as mutual information is symmetric and we have, with $\mathbf{Y}^* := \mathrm{sgn}(\rho)\mathbf{Y}$,

$$\mathrm{I}\big(f(\mathbf{X}); g(\mathbf{Y})\big) = \mathrm{I}\big(\mathrm{sgn}(\hat{f}_\varnothing) f(\mathbf{X}); \mathrm{sgn}(\hat{g}_\varnothing) g\big(\mathrm{sgn}(\rho)\mathbf{Y}^*\big)\big). \tag{4}$$

In analogy to [6], Proposition 1.9, the inner product satisfies

$$\langle f, T_\rho g\rangle = \mathbb{E}\big[f(\mathbf{X})g(\mathbf{Y})\big] = \hat{f}_\varnothing \hat{g}_\varnothing + 4\theta_\rho = 1 - 2\mathrm{P}\{f(\mathbf{X}) \neq g(\mathbf{Y})\}, \tag{5}$$

where T_ρ is the noise operator [6], Definition 2.46. Defining $\bar{t} := 1 - t$ for a generic t, we can express the probabilities

$$\begin{aligned} \mathrm{P}\{f(\mathbf{X}) = 1, g(\mathbf{Y}) = -1\} &= a\bar{b} - \theta_\rho, \\ \mathrm{P}\{f(\mathbf{X}) = g(\mathbf{Y}) = 1\} &= ab + \theta_\rho, \end{aligned} \tag{6}$$

$$\begin{aligned} \mathrm{P}\{f(\mathbf{X}) = -1, g(\mathbf{Y}) = 1\} &= \bar{a}b - \theta_\rho, \\ \mathrm{P}\{f(\mathbf{X}) = g(\mathbf{Y}) = -1\} &= \bar{a}\bar{b} + \theta_\rho. \end{aligned} \tag{7}$$

Using (6), (7) and fundamental properties of mutual information [3], Section 2.4, we obtain $\mathrm{I}(f(\mathbf{X}); g(\mathbf{Y})) = \xi(\theta_\rho, a, b)$ with

$$\xi(\theta, a, b) := \mathrm{H}(a) + \mathrm{H}(b) - \mathrm{H}(ab + \theta, a\bar{b} - \theta, \bar{a}b - \theta, \bar{a}\bar{b} + \theta), \tag{8}$$

where, slightly abusing notation, we defined the binary entropy function $\mathrm{H}(p) := \mathrm{H}(p, \bar{p})$ and $\mathrm{H}((p_i)_{i\in\mathcal{I}}) := -\sum_{i\in\mathcal{I}} p_i \log_2 p_i$ for $|\mathcal{I}| > 1$. By the nonnegativity of probabilities (6) and (7), for any $\rho \in [0, 1]$,

$$-\bar{a}\bar{b} \le \theta_\rho \le a\bar{b}. \tag{9}$$

With $\mathcal{P} := \{\mathcal{S} \subseteq [n] : \hat{f}_\mathcal{S}\hat{g}_\mathcal{S} > 0\} \setminus \{\varnothing\}$ and $\mathcal{N} := \{\mathcal{S} \subseteq [n] : \hat{f}_\mathcal{S}\hat{g}_\mathcal{S} < 0\}$, we define

$$\tau^+ := \frac{1}{4}\sum_{\mathcal{S}\in\mathcal{P}} \hat{f}_\mathcal{S}\hat{g}_\mathcal{S}, \qquad \tau^- := \frac{1}{4}\sum_{\mathcal{S}\in\mathcal{N}} \hat{f}_\mathcal{S}\hat{g}_\mathcal{S} \tag{10}$$

and apply the Schwarz inequality to show

$$\tau^+ - \tau^- = \frac{1}{4}\sum_{\mathcal{S}:|\mathcal{S}|\ge 1} |\hat{f}_\mathcal{S}||\hat{g}_\mathcal{S}| \tag{11}$$

$$\le \frac{1}{4}\sqrt{(1 - \hat{f}_\varnothing^2)(1 - \hat{g}_\varnothing^2)} = \sqrt{a\bar{a}b\bar{b}}. \tag{12}$$

As $\theta_1 = \tau^+ + \tau^-$, we combine (9) and (12) to obtain

$$\tau^+ \le \frac{a\bar{b} + \sqrt{a\bar{a}b\bar{b}}}{2}, \qquad \tau^- \ge -\frac{\bar{a}\bar{b} + \sqrt{a\bar{a}b\bar{b}}}{2}. \tag{13}$$

By definition, $\rho\tau^- \le \theta_\rho \le \rho\tau^+$, and hence, $\theta_\rho \in [\theta_\rho^-, \theta_\rho^+]$, where

$$\begin{aligned} \theta_\rho^- &:= \max\left\{-\bar{a}\bar{b}, -\rho\frac{\bar{a}\bar{b} + \sqrt{a\bar{a}b\bar{b}}}{2}\right\}, \\ \theta_\rho^+ &:= \min\left\{a\bar{b}, \rho\frac{a\bar{b} + \sqrt{a\bar{a}b\bar{b}}}{2}\right\}. \end{aligned} \tag{14}$$

The function $\xi(\theta, \alpha, \beta)$ is convex in θ by the concavity of entropy [3], Theorem 2.7.3, and consequently, $\mathrm{I}(f(\mathbf{X}); g(\mathbf{Y})) \le \max_{\theta\in\{\theta_\rho^+, \theta_\rho^-\}} \xi(\theta, a, b)$. Thus, Theorem 1 can be proved by establishing $1 - \mathrm{H}(\frac{\rho+1}{2}) - \xi(\theta, a, b) \ge 0$ for $\theta \in \{\theta_\rho^+, \theta_\rho^-\}$. Furthermore, it suffices to consider $\frac{1}{2} < a < b < 1$ by continuity of ξ.

Define $C_{a,b} := \frac{a\bar{b}+\sqrt{a\bar{a}b\bar{b}}}{2}$, $\rho^+ := \min\{\rho, \frac{a\bar{b}}{C_{a,b}}\}$, $\rho^- := \min\{\rho, \frac{\bar{a}\bar{b}}{C_{\bar{a},b}}\}$, and

$$\phi(\rho, a, b) := 1 - \mathrm{H}\left(\frac{\rho + 1}{2}\right) - \xi(\rho C_{a,b}, a, b). \tag{15}$$

Note that

$$\phi(\rho^+, a, b) = 1 - \mathrm{H}\left(\frac{\rho^+ + 1}{2}\right) - \xi(\theta_\rho^+, a, b) \tag{16}$$

$$\leq 1 - \mathrm{H}\left(\frac{\rho + 1}{2}\right) - \xi(\theta_\rho^+, a, b) \tag{17}$$

by the monotonicity of the binary entropy function and accordingly we also have $\phi(\rho^-, \bar{a}, b) \leq 1 - \mathrm{H}(\frac{\rho+1}{2}) - \xi(\theta_\rho^-, a, b)$. Theorem 1 thus follows from the following lemma.

LEMMA 1. *For $0 < \alpha < \beta < 1$ and $\rho \in [0, \frac{\alpha\bar{\beta}}{C_{\alpha,\beta}}]$, we have $\phi(\rho, \alpha, \beta) \geq 0$ with equality if and only if $\rho = 0$.*

Before proving Lemma 1, we note the following facts.

LEMMA 2. *For $x \in (0, 1)$, we have*

$$\frac{1}{x^{-1} - 1} + \log(1 - x) > 0. \tag{18}$$

PROOF. Using Taylor series expansion, we immediately obtain

$$-\log(1 - x) = \sum_{n=1}^{\infty} \frac{x^n}{n} < \sum_{n=1}^{\infty} x^n = \frac{x}{1 - x}. \tag{19}$$

□

The following lemma collects elementary facts about convex/concave functions and follows from elementary properties of convex functions on the real line (see, e.g., [8], Chapter I).

LEMMA 3. *Let $f : U \to \mathbb{R}$ be a continuous function, defined on the compact interval $U := [u_1, u_2] \subset \mathbb{R}$. Assuming that f is twice differentiable on V, where $(u_1, u_2) \subseteq V \subseteq U$, the following properties hold:*

1. *If $f''(u) \geq 0$ for all $u \in (u_1, u_2)$ and $f'(u^*) = 0$ for some $u^* \in V$, then $f(u) \geq f(u^*)$ for all $u \in U$. Furthermore, if additionally $f''(u) > 0$ for all $u \in (u_1, u_2)$, then $f(u) > f(u^*)$ for all $u \in U \backslash \{u^*\}$.*
2. *If $f''(u) \leq 0$ for all $u \in (u_1, u_2)$, then $f(u) \geq \min\{f(u_1), f(u_2)\}$ for all $u \in U$. Furthermore, if $f''(u) < 0$ for all $u \in (u_1, u_2)$, then $f(u) > \min\{f(u_1), f(u_2)\}$ for all $u \in (u_1, u_2)$.*

PROOF OF LEMMA 1. Let $I := \{(\alpha, \beta) \in \mathbb{R}^2 : 0 < \alpha < \beta < 1\}$, fix arbitrary $(\alpha, \beta) \in I$ and define

$$\rho_- := \frac{\max\{\alpha\beta, \bar{\alpha}\bar{\beta}\}}{C_{\alpha,\beta}}, \qquad \rho_\circ := \frac{\min\{\alpha\beta, \bar{\alpha}\bar{\beta}\}}{C_{\alpha,\beta}}, \qquad \rho_+ := \frac{\alpha\bar{\beta}}{C_{\alpha,\beta}}. \tag{20}$$

We shall adopt the simplified notation $\phi(\rho) := \phi(\rho, \alpha, \beta)$, suppressing the fixed parameters (α, β). For $\rho \in [0, \rho_+)$, we have the derivatives

$$\begin{aligned}\phi'(\rho) &= \frac{1}{2}\log_2\Bigl(\frac{1+\rho}{1-\rho}\Bigr) \\ &\quad + C_{\alpha,\beta}\log_2\Bigl(\frac{(\bar{\alpha}\beta - C_{\alpha,\beta}\rho)(\alpha\bar{\beta} - C_{\alpha,\beta}\rho)}{(\alpha\beta + C_{\alpha,\beta}\rho)(\bar{\alpha}\bar{\beta} + C_{\alpha,\beta}\rho)}\Bigr),\end{aligned} \tag{21}$$

$$\begin{aligned}\phi''(\rho) &= \frac{C_{\alpha,\beta}^2}{\log 2}\Bigl(\frac{1}{C_{\alpha,\beta}^2(1-\rho^2)} - \frac{1}{\bar{\alpha}\beta - C_{\alpha,\beta}\rho} \\ &\quad - \frac{1}{\alpha\bar{\beta} - C_{\alpha,\beta}\rho} - \frac{1}{\bar{\alpha}\bar{\beta} + C_{\alpha,\beta}\rho} - \frac{1}{\alpha\beta + C_{\alpha,\beta}\rho}\Bigr).\end{aligned} \tag{22}$$

We write $\phi''(\rho) = \frac{p(\rho)}{q(\rho)}$, where both p and q are polynomials in ρ, and choose

$$\begin{aligned}q(\rho) &= \log(2)\bigl(1-\rho^2\bigr)(\bar{\alpha}\beta - C_{\alpha,\beta}\rho) \\ &\quad \times (\alpha\bar{\beta} - C_{\alpha,\beta}\rho)(\bar{\alpha}\bar{\beta} + C_{\alpha,\beta}\rho)(\alpha\beta + C_{\alpha,\beta}\rho),\end{aligned} \tag{23}$$

such that $q(\rho) > 0$ for $\rho \in [0, \rho_+)$. By (22), $p(\rho)$ is given by

$$\begin{aligned}p(\rho) &= (\bar{\alpha}\beta - C_{\alpha,\beta}\rho)(\alpha\bar{\beta} - C_{\alpha,\beta}\rho)(\bar{\alpha}\bar{\beta} + C_{\alpha,\beta}\rho)(\alpha\beta + C_{\alpha,\beta}\rho) \\ &\quad - C_{\alpha,\beta}^2\bigl(1-\rho^2\bigr)\bigl((\alpha\bar{\beta} - C_{\alpha,\beta}\rho)(\bar{\alpha}\bar{\beta} + C_{\alpha,\beta}\rho)(\alpha\beta + C_{\alpha,\beta}\rho) \\ &\quad + (\bar{\alpha}\beta - C_{\alpha,\beta}\rho)(\bar{\alpha}\bar{\beta} + C_{\alpha,\beta}\rho)(\alpha\beta + C_{\alpha,\beta}\rho) \\ &\quad + (\bar{\alpha}\beta - C_{\alpha,\beta}\rho)(\alpha\bar{\beta} - C_{\alpha,\beta}\rho)(\alpha\beta + C_{\alpha,\beta}\rho) \\ &\quad + (\bar{\alpha}\beta - C_{\alpha,\beta}\rho)(\alpha\bar{\beta} - C_{\alpha,\beta}\rho)(\bar{\alpha}\bar{\beta} + C_{\alpha,\beta}\rho)\bigr).\end{aligned} \tag{24}$$

This entails $\deg(p) \le 5$ and a careful calculation of the coefficients reveals $\deg(p) \le 3$.

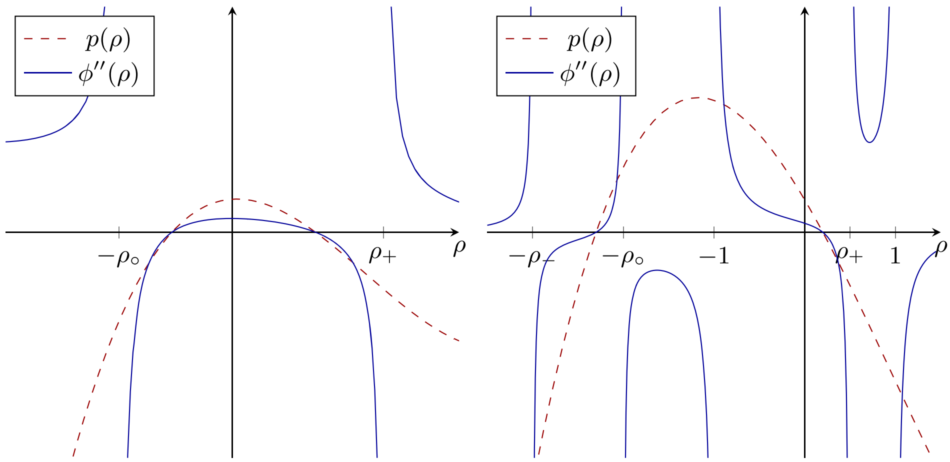
We will now demonstrate that there is a unique point $\rho^* \in (0, \rho_+)$, such that $p(\rho^*) = 0$. To this end, reinterpret $\phi''(\rho)$ as a rational function of ρ on $\mathbb{R}$. We evaluate (24) and use $\alpha < \beta$ to obtain the two inequalities

$$p(0) = \alpha\bar{\alpha}\beta\bar{\beta}\bigl(\alpha\bar{\alpha}\beta\bar{\beta} - C_{\alpha,\beta}^2\bigr) > 0 \tag{25}$$

and

$$p(\rho_+) = -\bigl(C_{\alpha,\beta}^2 - (\alpha\bar{\beta})^2\bigr)(\beta - \alpha)\bar{\beta}\alpha < 0. \tag{26}$$

The number of roots of p in $(0, \rho_+)$ is thus odd and at most equal to its degree, that is, either one or three. If we have $\rho_\circ \le 1$, then evaluation of (24) readily yields $p(-\rho_\circ) \le 0$. If, on the other hand, $\rho_\circ > 1$, we obtain $p(-\rho_-) \le 0$ from (24). Thus, p has at least one negative root and a unique root $\rho^* \in (0, \rho_+)$. Figure 1 qualitatively illustrate the behavior of $p(\rho)$ and $\phi''(\rho)$.



(a) $\rho_\circ < 1$ (b) $\rho_\circ > 1$

FIG. 1. *Sketch of $p(\rho)$ and $\phi''(\rho)$.*

Consequently, $\phi''(\rho) > 0$ for $\rho \in (0, \rho^*)$. By part 1 of Lemma 3, $\phi(\rho) > \phi(0) = 0$ for $\rho \in (0, \rho^*]$ as $\phi'(0) = 0$. Since $\phi''(\rho) < 0$ for $\rho \in (\rho^*, \rho_+)$, we have $\phi(\rho) > \min\{\phi(\rho^*), \phi(\rho_+)\}$ for all $\rho \in (\rho^*, \rho_+)$, by part 2 of Lemma 3. In total, $\phi(\rho) > \min\{0, \phi(\rho_+)\}$ for $\rho \in (0, \rho_+)$.

As $\phi(0) = 0$, it remains to show that $\phi(\rho_+, \alpha, \beta) > 0$ for $(\alpha, \beta) \in I$. To this end, we introduce the transformation

$$(\alpha, \beta) \longmapsto (c, x) := \left(\frac{\log \frac{\alpha}{\beta}}{\log \frac{\alpha\bar{\beta}}{\bar{\alpha}\beta}}, \sqrt{\frac{\alpha\bar{\beta}}{\bar{\alpha}\beta}} \right), \tag{27}$$

a bijective mapping from I to $(0,1)^2$ with the inverse

$$(c, x) \longmapsto (\alpha, \beta) = \left(\frac{x^{2c} - x^2}{1 - x^2}, \frac{1 - x^{2-2c}}{1 - x^2} \right). \tag{28}$$

In terms of c and x, we have $\phi(\rho_+, \alpha, \beta) = \psi(c, x)$, where

$$\psi(c, x) := 1 - \mathrm{H}\left(\frac{1}{2} + \frac{x}{1+x} \right) - \mathrm{H}\left(\frac{x^{2c} - x^2}{1 - x^2} \right) + \frac{1 - x^{2-2c}}{1 - x^2} \mathrm{H}(x^{2c}) \tag{29}$$

$$= 1 - \mathrm{H}\left(\frac{1 + 3x}{2 + 2x} \right) + \frac{\mathrm{H}(x^2)}{1 - x^2} + \frac{x^{2c}\mathrm{H}(x^{2-2c}) + x^{2-2c}\mathrm{H}(x^{2c})}{x^2 - 1}. \tag{30}$$

We fix a particular $x \in (0,1)$ and use the simplified notation $\psi(c) := \psi(c, x)$, obtaining the derivatives

$$\begin{aligned}\psi'(c) = {} & \frac{2\log(x)}{(x^2-1)\log(2)}\big[2x^{2c}c\log(x) \\ & + x^{2(1-c)}\log(1-x^{2c}) - x^{2c}\log(x^{2c}-x^2)\big],\end{aligned} \tag{31}$$

$$\begin{aligned}\psi''(c) = {} & \frac{4\log(x)^2x^{2c}}{(1-x^2)\log(2)}\bigg[\bigg(\frac{1}{x^{-2(1-c)}-1} + \log(1-x^{2(1-c)})\bigg) \\ & + \frac{x^2}{x^{4c}}\bigg(\log(1-x^{2c}) + \frac{1}{x^{-2c}-1}\bigg)\bigg].\end{aligned} \tag{32}$$

By applying Lemma 2 twice, we obtain $\psi''(c) > 0$. Thus, $\psi(c) > \psi(\frac{1}{2})$ by part 1 of Lemma 3 as $\psi'(\frac{1}{2}) = 0$. It remains to show that $\gamma(x) := \psi(\frac{1}{2}, x) > 0$. Note that $\gamma(0) = \gamma(1) = 0$ and

$$\gamma'(x) = \frac{1}{(1+x)^2}\log_2\big[(1+3x)(1-x)\big], \tag{33}$$

for $x \in [0,1)$. If $\gamma(x) \le 0$ for any $x \in (0,1)$ then f necessarily attains its minimum in $(0,1)$ and there exists $x^* \in (0,1)$ with $\gamma(x^*) \le 0$ and $\gamma'(x^*) = 0$. As $x^* = \frac{2}{3}$ is the only point in $(0,1)$ with $\gamma'(x^*) = 0$ and $\gamma(\frac{2}{3}) = \log_2(\frac{27}{25}) > 0$, this concludes the proof. $\square$

3. Proof of Proposition 1. We may assume $0 < \rho < 1$ and $\frac{1}{2} \le a \le b \le 1$ by virtue of (4). Clearly, $g = \pm f = \pm\chi_i$ for some $i \in [n]$ is a sufficient condition to maximize $\mathrm{I}(f(\mathbf{X}); g(\mathbf{Y}))$. A careful inspection of the proof of Theorem 1 shows that this condition is also necessary.

In the following, we will use the notation of Section 2. As $b = 1$ implies $\mathrm{I}(f(\mathbf{X}); g(\mathbf{Y})) = 0$, we assume $\frac{1}{2} \le a \le b < 1$. For equality in Theorem 1, we need either $\phi(\rho^+, a, b) = 0$ or $\phi(\rho^-, \bar{a}, b) = 0$. By Lemma 1, $\phi(\rho^-, \bar{a}, b) > 0$ unless $\bar{a} = a = \frac{1}{2}$, which in turn implies $\phi(\rho^-, \bar{a}, b) = \phi(\rho^+, a, b)$. The equality $\phi(\rho^+, a, b) = 0$ can only occur for $b = a$, implying $\rho^+ = \rho$. We want to show that $\phi(\rho, a, a) = 0$ implies $a = \frac{1}{2}$. For $a \ne \frac{1}{2}$, we have

$$\frac{\partial\phi}{\partial\rho}(\rho, a, a) = \frac{1}{2}\log_2\bigg(\frac{1+\rho}{1-\rho}\bigg) - a\bar{a}\log_2\bigg(\frac{\rho}{a\bar{a}\bar{\rho}^2} + 1\bigg), \tag{34}$$

$$\frac{\partial^2\phi}{\partial\rho^2}(\rho, a, a) = \frac{\rho(1-2a)^2}{\log(2)(a+\rho\bar{a})(1-a\bar{\rho})(1-\rho^2)} > 0. \tag{35}$$

Part (1) of Lemma 3 now yields $0 = \phi(0, a, a) < \phi(\rho, a, a)$ as $\frac{\partial\phi}{\partial\rho}(0, a, a) = 0$. By the strict convexity of $\xi(\theta, \frac{1}{2}, \frac{1}{2})$ in θ, necessarily $\theta_\rho = \frac{\langle f, T_\rho g\rangle}{4} \in \{\theta_\rho^+, \theta_\rho^-\} = \pm\frac{\rho}{4}$. The Cauchy–Schwarz inequality, together with [6], Proposition 2.50, yields $\rho^2 = \langle f, T_\rho g\rangle^2 = \langle T_{\sqrt{\rho}} f, T_{\sqrt{\rho}} g\rangle^2 \le \langle f, T_\rho f\rangle\langle g, T_\rho g\rangle \le \rho^2$. Thus, necessarily $g = \pm f = \pm\chi_i$ for some $i \in [n]$ by [6], Proposition 2.50.

4. Discussion. The key idea underlying the proof of Theorem 1 is to split $\theta_1 = \tau^+ + \tau^-$ into its positive and negative part (see Section 2). After reducing the problem to the inequality in Lemma 1, the remaining proof is routine analysis. Lemma 1 might turn out to be useful in the context of other converse proofs, in particular for the optimization of rate regions with binary random variables.

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