Gray–Wyner and Mutual Information Regions for Doubly Symmetric Binary Sources and Gaussian Sources

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Abstract-Nonconvex optimization plays a key role in multiuser information theory and related fields, but it is usually difficult to solve. The rate region of the Gray-Wyner source coding system (or almost equivalently, the mutual information region) is a typical example in nonconvex optimization, whose single-letter expression was given by Gray and Wyner. However, due to the nonconvexity of the optimization involved in this expression, previously, there was none nontrivial discrete source for which the analytic expression is known. In this paper, we propose a new strategy to solve nonconvex optimization problems. By this strategy, we provide the analytic expression for the doubly symmetric binary source (DSBS), which confirms positively a conjecture of Gray and Wyner in 1974. We also provide the analytic expression of the mutual information region for the Gaussian source, and provide (or recover) the analytic expressions of the lossy Grav-Wyner region for both the DSBS and Gaussian source. Our proof strategy relies on an auxiliary measure technique and the analytical expression of the optimaltransport divergence region.

Index Terms—Nonconvex optimization, Gray–Wyner rate region, mutual information region, conditional entropy region, auxiliary measure method.

I. INTRODUCTION

The Gray-Wyner coding system illustrated in Fig. 1 was initially investigated by Gray and Wyner in a seminal work [1], and then widely investigated in the literature; see, e.g., [2]–[8]. In this system, two correlated memoryless sources X^n, Y^n are respectively required to be transmitted almost losslessly from one sender to two receivers. The joint distribution of these sources is denoted by P_{XY} which is assumed to be defined on finite alphabets. Both the decoders are connected to the encoder by a common channel, and each decoder is also connected to the encoder by its own private channel. All these channels are noiseless. The common rate is denoted by R_0 and the private rates are respectively denoted by R_1 and R_2 . The (lossless) Gray–Wyner rate region is the set of (R_0, R_1, R_2) such that the sources X^n, Y^n can be transmitted almost losslessly by using some code with rates (R_0, R_1, R_2) . Gray and Wyner showed that the Gray-Wyner rate region is equal to the set

$$\mathcal{R} := \{ (R_0, R_1, R_2) : \exists P_{W|XY}, R_0 \ge I(X, Y; W), \\ R_1 \ge H(X|W), R_2 \ge H(Y|W) \}.$$

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Figure 1. Gray-Wyner coding system.

The cardinality of the alphabet of W can be assumed no larger than $|\mathcal{X}| |\mathcal{Y}| + 2$. This is a single-letter characterization which means the expression is independent of the dimension (or blocklength). The region \mathcal{R} is obviously determined by its lower envelope which is given by

$$R_0(R_1, R_2) := \inf \{ R_0 : (R_0, R_1, R_2) \in \mathcal{R} \}$$

=
$$\inf_{\substack{P_{W|XY}: H(X|W) \le R_1, \\ H(Y|W) < R_2}} I(X, Y; W). \quad (1)$$

Solving this optimization is in fact a difficult open question, due to its nonconvexity. In fact, previously, there was even none nontrivial case for which the analytic expression is known. Gray and Wyner [1] tried to provide an analytic expression for the doubly symmetric binary source (DSBS), and made a conjecture. Consider a DSBS with disagree probability $p \in (0, 1/2)$, whose distribution, denoted by DSBS(p), is given in Table I. In other words, for $(X, Y) \sim DSBS(p)$, X is a Bernoulli random variable with parameter 1/2, and Y is the output distribution of a binary symmetric channel BSC(p) with crossover probability p when the input is X. For such a DSBS, its rate distortion function under the Hamming distortion $d_{\rm H}$ is given by [1], [9]

$$R(D_{1}, D_{2}) := \inf_{\substack{P_{UV|XY}: \mathbb{E}d_{H}(X,U) \le D_{1}, \\ \mathbb{E}d_{H}(Y,U) \le D_{2}}} I(X,Y;U,V) \\ = \begin{cases} 1 - (1-p)h\left(\frac{a+b-p}{2(1-p)}\right) \\ -ph\left(\frac{a-b+p}{2p}\right), & a * p \ge b, a * b \ge p \\ 1 + h(p) - h(a) - h(b), & a * b \le p \\ 1 - h(a), & a * p \le b \end{cases}$$
(2)

Table I The distribution of a DSBS with parameter $p \in (0, 1/2)$, which is denoted by DSBS(p).

$X \backslash Y$	0	1
0	$\frac{1-p}{2}$	$\frac{p}{2}$
1	$\frac{p}{2}$	$\frac{1-p}{2}$

with $b = D_1 \vee D_2$, $a = D_1 \wedge D_2$, where $h: t \mapsto -t \log t - (1 - t) \log(1-t)$ denotes the binary entropy function, and h^{-1} is the inverse of the restriction of h to the set $[0, \frac{1}{2}]$. Here, $x \vee y := \max\{x, y\}, x \wedge y = \min\{x, y\}$, and a * b = a(1-b) + b(1-a) is the binary convolution operation. Throughout this paper, for the DSBS, we always use the logarithm with base 2, denoted by log, and for Gaussian sources, always use the one with natural base, denoted by ln. For the DSBS, Gray and Wyner [1] made the following conjecture.

Conjecture 1. [1], [10] For the source DSBS(p), it holds that for $(R_1, R_2) \in [0, 1]^2$,

$$R_0(R_1, R_2) = R(h^{-1}(R_1), h^{-1}(R_2)).$$

This conjecture has been open for nearly 50 years since 1974. Although there are now a vast number of works existing in the literature on the Gray–Wyner coding system, surprisingly, there seems no progress on this conjecture until now. The intuition behind this conjecture is that the sender first encodes the source into W = (U, V) by using an optimal pointto-point lossy compression code with distortions (D_1, D_2) and rate $R(D_1, D_2)$, and then compress $X \oplus U$ and $Y \oplus V$ losslessly using rate $h(D_1)$ and $h(D_2)$ respectively. Here we choose $(D_1, D_2) = (h^{-1}(R_1), h^{-1}(R_2))$. In other words, the Gray–Wyner conjecture above states that this layered coding scheme is optimal for the Gray–Wyner system for the DSBS.

The Gray–Wyner region can be also expressed by the mutual information region. Given an arbitrary (not necessarily discrete) joint distribution P_{XY} , define the mutual information region as

$$\mathcal{I} := \mathcal{I}(P_{XY}) := \{ (I(X; W), I(Y; W), I(X, Y; W)) \}_{P_{W|XY}} .$$

Its projection region on the plane of the first two coordinates is

$$\mathcal{I}_0 := \{(I(X; W), I(Y; W))\}_{P_{W|XY}}$$

The mutual information region is determined by its lower and upper envelopes which are respectively defined as for $(\alpha, \beta) \in \mathcal{I}_0$,

$$\underline{\Upsilon}(\alpha,\beta) := \inf \left\{ \gamma : (\alpha,\beta,\gamma) \in \mathcal{I} \right\}$$
$$= \inf_{\substack{P_{W|XY}: I(X;W) = \alpha, I(Y;W) = \beta}} I(X,Y;W),$$

and

$$\Upsilon(\alpha,\beta) := \sup \left\{ \gamma : (\alpha,\beta,\gamma) \in \mathcal{I} \right\}$$
$$= \sup_{P_{W|XY}: I(X;W) = \alpha, I(Y;W) = \beta} I(X,Y;W)$$

We also define the lower increasing envelope as

$$\Upsilon(\alpha,\beta) := \inf \left\{ \gamma : (\alpha,\beta,\gamma) \in \mathcal{I} \right\}$$

=
$$\inf_{P_{W|XY}: I(X;W) \ge \alpha, I(Y;W) \ge \beta} I(X,Y;W). \quad (3)$$

Observe that $R_0(R_1, R_2) = \Upsilon(H(X) - R_1, H(Y) - R_2)$, and hence, characterizing $R_0(R_1, R_2)$ is equivalent to characterizing $\Upsilon(\alpha, \beta)$. In this paper we only focus on $\Upsilon(\alpha, \beta)$ and also $\Upsilon(\alpha, \beta)$ and $\overline{\Upsilon}(\alpha, \beta)$. In fact, the function $\Upsilon(\alpha, \beta)$ is determined by $\Upsilon(\alpha, \beta)$. It should be also noted that the function $\Upsilon(\alpha, \beta)$ for Gaussian distributions was already expressed in terms of optimizations over Gaussian random variables by using the doubling trick [11], [12]. Furthermore, the mutual information region can be also expressed in terms of the conditional entropy region $\mathcal{H} := \{(H(X|W), H(Y|W), H(X, Y|W))\}_{P_{W|XY}}$.

A. Our Contributions

The main difficulty in proving Conjecture 1 is that the optimization problem in (1) (or (3)) is nonconvex. One routine strategy to solve nonconvex optimization is to apply Karush–Kuhn–Tucker (KKT) conditions to obtain several necessary optimality equations, and then solve these equations to find the optimal solution. However, it is a challenge to solve these optimality equations in this setting, since logarithmic functions are involved in them. Therefore, new techniques are required to resolve Conjecture 1.

In fact, nonconvex optimization is very common in today's information theory, which originated with accompanied by multi-user information theory; e.g., Mrs. Gerber's lemma [13]–[15] and Wyner's common information [16] which both involves nonconvex optimization. Although this kind of problems exist in the literature for a long time, nowadays relatively little is known about them. In other words, finding new ideas to solve nonconvex optimization is a very difficult task. During the last decade, Nair and his collaborators have made some significant contributions in this field; see e.g., [11], [17]-[19]. For example, the change of variables technique was exploited by them to convert a nonconvex optimization problem to a convex one. However, such a technique seems failed to be applied directly to the optimization problem in (1) (or (3)). Readers can refer to [20] for recent advances in this field, especially for optimizations for discrete distributions.

In this paper, we propose a new strategy to solve nonconvex optimization problems. By this strategy, we confirm Conjecture 1 positively, which yields the first explicit expression for the Gray–Wyner region of a certain source. We also prove the analytic expression of the mutual information region for the Gaussian source, and also prove (or recover) the analytic expressions of the lossy Gray–Wyner region for both the DSBS and Gaussian source. Our proof strategy integrates an auxiliary measure technique with the convexity of the envelopes of the optimal-transport divergence region [21] for the DSBS, and integrates the same auxiliary measure technique with hypercontractivity inequalities for the Gaussian source. For the Gaussian Gray–Wyner system, the lossy Gray–Wyner region was previously presented in [22] and partially in [7] by using methods different from ours. It is worth noting that our convexity result derived in [21] turns out to be important, since it is not only used in [21] as a key ingredient in the proof of the Ordentlich–Polyanskiy–Shayevitz conjecture [23] (which is a conjecture on the strong version of the small-set expansion theorem), but also used in this paper to resolve the Gray–Wyner conjecture. Both the auxiliary measure technique and the convexity result in [21] are indispensable in our proofs, which makes our proofs nontrivial.

B. Notations

We use $X \xrightarrow{P_{Y|X}} Y$ to denote that the random variable Y is the output of the channel $P_{Y|X}$ when the input is X. We denote BSC(a) as a binary symmetric channel with crossover probability a. We denote DSBS(p) as the DSBS with disagree probability p, and Bern(a) as the Bernoulli distribution with parameter a. For a real-valued function f, we denote convf and concf respectively as the lower convex envelope and the upper concave envelope of f.

II. MAIN RESULTS

A. Mutual Information Region for DSBS

In this subsection and in the corresponding proofs of results stated in this subsection, we use the logarithm with base 2, which is denoted by log.

For $(\alpha, \beta) \in [0, 1]^2$, denote $a = h^{-1}(1-\alpha), b = h^{-1}(1-\beta)$. Define several disjoint sets

$$\begin{aligned} \mathcal{D}_1 &:= \{ (\alpha, \beta) \in [0, 1]^2 : a * p \ge b, \\ b * p \ge a, \ a * b \ge p \}, \\ \mathcal{D}_2 &:= \{ (\alpha, \beta) \in [0, 1]^2 : a * b$$

For $(\alpha, \beta) \in [0, 1]^2$, define

$$\Upsilon^*(\alpha,\beta) := \begin{cases} 1 - (1-p)h\left(\frac{a+b-p}{2(1-p)}\right) \\ -ph\left(\frac{a-b+p}{2p}\right), & (\alpha,\beta) \in \mathcal{D}_1 \\ 1 + h(p) - h(a) - h(b), & (\alpha,\beta) \in \mathcal{D}_2 \\ 1 - h(a), & (\alpha,\beta) \in \mathcal{D}_3 \\ 1 - h(b), & (\alpha,\beta) \in \mathcal{D}_4 \end{cases}$$

$$(4)$$

In fact, $\Upsilon^*(\alpha, \beta)$ is nothing but $R(h^{-1}(1-\alpha), h^{-1}(1-\beta))$, where $R(\cdot, \cdot)$ is the rate-distortion function for DSBS(p) given in (2). The following is one of our main results, whose proof is given in Section IV.

Theorem 1 (Gray–Wyner Region for DSBS). For the source DSBS(p) with $p \in (0, 1/2)$, it holds that for $(\alpha, \beta) \in [0, 1]^2$,

$$\Upsilon(\alpha,\beta) = \Upsilon^*(\alpha,\beta)$$

Observe that by definitions, $R_0(R_1, R_2) = \Upsilon(1 - R_1, 1 - R_2)$ and $\Upsilon^*(1 - R_1, 1 - R_2) = R(h^{-1}(R_1), h^{-1}(R_2))$, where $R_0(\cdot, \cdot)$ and $R(\cdot, \cdot)$ are respectively given in (1) and (2). So, Theorem 1 implies $R_0(R_1, R_2) = R(h^{-1}(R_1), h^{-1}(R_2))$, which confirms Conjecture 1 positively. The function Υ^* is plotted in Fig. 2.

As mentioned in Section I-A, the main difficulty to prove Theorem 1 is the nonconvexity of the optimization involved in the definition of Υ (see (3)). One might plan to use Karush– Kuhn–Tucker (KKT) conditions to obtain several necessary optimality equations, and then solve these equations to find the optimal solution. However, solving these equations is a challenge, due to the fact that logarithmic functions are involved. Instead, we propose the following strategy to prove Theorem 1, which consists of two steps.

- 1) Note that the optimization in (3) can be written as the one over Q_{WXY} with the marginal constraint $Q_{XY} = P_{XY}$. In this step, we introduce an auxiliary probability measure R_{XY} , and by the formula $D(Q_{Z|W}||R_Z|Q_W) - D(P_Z||R_Z)$ with Z = X, Y, or (X,Y), rewrite all the mutual informations in the objective function or the constraints as relative entropies (since the latter are easier to deal with). Then, relax the optimization problem by discarding the marginal constraint $Q_{XY} = P_{XY}$. That is, we obtain a new optimization problem which only involves relative entropies (with fixed distribution R as the second arguments).
- 2) The new optimization problem obtained above is in fact an optimization over the time-sharing variable (or convex-combination variable) W. In other words, the value of this new optimization problem is determined by the lower convex envelope of the relative entropy region $\{(D(Q_X || R_X), D(Q_Y || R_Y), D(Q_{XY} || R_{XY}))\}_{Q_{XY}}$.

Hence, to solve this new optimization problem, more specifically, to remove the time-sharing variables, it suffices to prove the convexity of this lower convex envelope. This part has been done in our another work [21], or see Lemma 3 in Section III. The proof therein relies on a new technique, called the first-order method, which is based on the equivalence between the convexity of a function and the convexity of the set of minimizers of its Lagrangian dual. Denote the optimal solution to the new optimization by Q_{XY}^* .

In Step 1, to make the optimization problem simpler, we would like to discard the marginal constraint $Q_{XY} = P_{XY}$. Although we can discard it directly without introducing the auxiliary measure R_{XY} , the resultant bound would be far from optimal. In other words, the role of the auxiliary measure is that by properly choosing this measure, it enables us not to lose too much when we discard the marginal constraint. To ensure that the bound derived by the method above is tight, we need choose the R_{XY} as an optimal distribution (called shadow measure), which can be specified in the following way.

For the DSBS, denote $P_{W|XY}^*$ as an optimal distribution attaining the infimum in (3) (i.e., the one in the Gray–Wyner conjecture). In fact, the distribution $P_{XY|W}^*$ induced by $P_{WXY}^* := P_{W|XY}^* P_{XY}$ satisfies certain symmetry so that given any DSBS S_{XY} , $D(P_{XY|W}^* || S_{XY} |P_W^*) = D(P_{XY|W=w}^* || S_{XY})$ holds for any w. In our proof, we choose R_{XY} as a DSBS for which the optimal solution Q_{XY}^* in Step 2 is exactly $P_{XY|W=w}^*$ for some w. Hence, the final bound obtained in Step 2 is

$$D(Q_{XY}^* || R_{XY}) - D(P_{XY} || R_{XY})$$

= $D(P_{XY|W=w}^* || R_{XY}) - D(P_{XY} || R_{XY})$
= $D(P_{XY|W}^* || R_{XY} |P_W^*) - D(P_{XY} || R_{XY})$
= $I_{P^*}(X, Y; W),$

where the last line follows since the (X, Y)-marginal of P_{WXY}^* is exactly P_{XY} . Therefore, the bound induced by such R_{XY} is tight. In other words, such a choice of R_{XY} is optimal.

As mentioned in Section I-A, our convexity result in [21] was previously used as a key ingredient in the proof of the Ordentlich-Polyanskiy-Shayevitz conjecture [23]; refer to [21] for more details. Interestingly, it also can be used as a key tool to resolve the Grav–Wyner conjecture (in Step 2) in this paper. This forces us to re-examine the importance of the convexity result in [21]. At the technical level, our proof strategy in present paper integrates two techniques: the auxiliary measure method (in Step 1) and the first-order method (in Step 2). These two indispensable techniques are nontrivial on their own, which hence in turn makes our proof nontrivial. Furthermore, although we only consider the optimization with marginal distributions fixed, we believe that our strategy above can be also applied to many other similar optimization problems, e.g., optimizations in which a channel is fixed and the input of this channel is to be optimized.

As a consequence of Theorem 1, the rate-distortion region of the lossy Gray–Wyner system can be obtained. In the Gray–Wyner system, consider a distortion measure d. If the reconstructions of the sources at two receivers are allowed to be within distortion levels D_1 and D_2 respectively, then the rate-distortion region is defined as the set of tuples $(R_0, R_1, R_2, D_1, D_2)$. Such a region was shown by Gray and Wyner [1] to be

$$\begin{aligned} \mathcal{R}_{\text{lossy}} &:= \left\{ (R_0, R_1, R_2, D_1, D_2) : \\ & \exists P_{W|XY}, P_{\hat{X}|WX}, P_{\hat{Y}|WY}, \\ & R_0 \ge I(X, Y; W), \\ & R_1 \ge I(X; \hat{X}|W), R_2 \ge I(Y; \hat{Y}|W), \\ & \mathbb{E}d(X, \hat{X}) \le D_1, \mathbb{E}d(Y, \hat{Y}) \le D_2 \right\}. \end{aligned}$$

Computing this region is equivalent to computing the following function

$$R_{0}(R_{1}, R_{2}, D_{1}, D_{2}) \\ := \inf_{\substack{P_{W|XY}, P_{\hat{X}|WX}, P_{\hat{Y}|WY}:\\I(X; \hat{X}|W) \le R_{1}, I(Y; \hat{Y}|W) \le R_{2},\\\mathbb{E}d(X, \hat{X}) \le D_{1}, \mathbb{E}d(Y, \hat{Y}) \le D_{2}}} I(X, Y; W).$$
(5)

Using Theorem 1, we obtain the analytical expression for this function.

Corollary 1 (Lossy Gray–Wyner Rate Region for DSBS). For the source DSBS(p) with $p \in (0, 1/2)$, under the Hamming distortion measure, it holds that for $R_1, R_2, D_1, D_2 \ge 0$,

$$R_0(R_1, R_2, D_1, D_2) = \Upsilon^*([R(D_1) - R_1]^+, [R(D_2) - R_2]^+)$$

where Υ^* is defined in (4), $[x]^+ := \max\{x, 0\}$, and R(D) := 1 - h(D) is the rate-distribution function of Bernoulli source Bern $(\frac{1}{2})$.

Proof: For a feasible tuple $(P_{W|XY}, P_{\hat{X}|WX}, P_{\hat{Y}|WY})$ satisfying the constraints in (5), it holds that

$$I(X;W) \ge \left[I(X;\hat{X}W) - R_1\right]^+$$
$$\ge \left[I(X;\hat{X}) - R_1\right]^+$$
$$\ge \left[R(D_1) - R_1\right]^+,$$

and similarly,

$$I(Y;W) \ge [R(D_2) - R_2]^+$$

Therefore,

$$R_0(R_1, R_2, D_1, D_2) \geq \inf_{\substack{P_{W|XY}: I(X;W) \ge [R(D_1) - R_1]^+ \\ I(Y;W) \ge [R(D_2) - R_2]^+}} I(X, Y; W) \\ = \Upsilon([R(D_1) - R_1]^+, [R(D_2) - R_2]^+).$$

We now prove the other direction. From the proof of Theorem 1, there is a conditional distribution $P_{W|XY}$ attaining $\Upsilon([R(D_1) - R_1]^+, [R(D_2) - R_2]^+)$ (i.e., the infimum in (3)) such that¹ both (W, X) and (W, Y) are DSBSes. It is well known that for a DSBS (W, X), we can write $X \xrightarrow{BSC(\theta_1)} \hat{X} \xrightarrow{BSC(\theta_2)} W$ for any parameters $\theta_1, \theta_2 \in [0, 1]$ such that $\theta_1 * \theta_2 = \mathbb{E}d_H(X, W)$ where $d_H(x, y) = \mathbbm{I}\{x \neq y\}$ denotes the Hamming distance. If $\mathbb{E}d_H(X, W) > D_1$, then we choose \hat{Y} in a similar way. This set of induced distributions $(P_{W|XY}, P_{\hat{X}|WX}, P_{\hat{Y}|WY})$ obviously satisfies the distortion constraints in (5). Moreover, if $R_1 \geq R(D_1)$, then

$$I(X; X|W) = H(X|W) - H(X|X)$$
$$\leq I(X; \hat{X}) = R(D_1) \leq R_1$$

If $R_1 < R(D_1)$, then $I(X;W) \ge R(D_1) - R_1$ (since $P_{W|XY}$ attains $\Upsilon([R(D_1) - R_1]^+, [R(D_2) - R_2]^+)$). So, for this case,

$$I(X; X|W) = I(X; X) - I(X; W)$$

= $R(D_1) - I(X; W) \le R_1.$

So, it always holds that $I(X; \hat{X}|W) \leq R_1$ for any cases. By symmetry, $I(Y; \hat{Y}|W) \leq R_2$ also holds. So, $(P_{W|XY}, P_{\hat{X}|WX}, P_{\hat{Y}|WY})$ also satisfies the rate constraints in

¹Rigorously speaking, (W, X) and (W, Y) are not always DSBSes, since in some case of our proof, W = (U, V) such that $X \xrightarrow{BSC(a)} U \xrightarrow{BSC(c)} V \xrightarrow{BSC(b)} Y$, and hence (U, X) and (V, Y) are DSBSes. However, for this case, the argument given here with slight modification still works.

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Figure 2. Illustration of Υ^* , $\underline{\Upsilon}^*$, and $\overline{\Upsilon}^*$ for p = 0.05 (equivalently, the correlation coefficient $\rho = 0.9$). The boundaries of the graphs of $\underline{\Upsilon}^*$ and $\overline{\Upsilon}^*$ coincide except at (α, β) belonging to a neighborhood of the origin.

(5). This implies that $(P_{W|XY}, P_{\hat{X}|WX}, P_{\hat{Y}|WY})$ is a feasible and $h(D'_2) - h(D_2)$ respectively. Note that here solution to (5), and hence,

$$R_0(R_1, R_2, D_1, D_2) \le I(X, Y; W) = \Upsilon([R(D_1) - R_1]^+, [R(D_2) - R_2]^+).$$
(6)

$$h(D'_1) - h(D_1) = R(D_1) - R(D'_1)$$

= $R(D_1) - [R(D_1) - R_1]^+$
= $\min\{R_1, R(D_1)\}$
< R_1 ,

This completes the proof.

Remark 1. A more straightforward way to show the inequality in (6) is to use a specific coding scheme in which the sender first encodes the source into W = (U, V) by using an optimal point-to-point lossy compression code with distortions (D'_1, D'_2) and common rate $R_{XY}(D'_1, D'_2)$ where $D'_1 =$ $R^{-1}\left([R(D_1) - R_1]^+\right), D'_2 = R^{-1}\left([R(D_2) - R_2]^+\right)$, and then further encodes X and Y with help of U, V by using successively refinement codes with private rates $h(D'_1) - h(D_1)$ and similarly, $h(D'_1)-h(D_1) \le R_2$. This scheme is essentially same as the lossless one given below Conjecture 1.

We next derive analytical expressions for $\underline{\Upsilon}(\alpha,\beta)$ and $\overline{\Upsilon}(\alpha,\beta)$. Define

$$\mathcal{I}_0^* := \left\{ (\alpha, \beta) \in [0, 1]^2 : \beta \ge \alpha - \alpha h(p/\alpha) \right\}$$
$$\alpha \ge \beta - \beta h(p/\beta) \right\}.$$

Define

$$\begin{split} \mathcal{D}'_{3} &:= \left\{ (\alpha, \beta) \in [0, 1]^{2} : a * p < b, \ \beta \geq (1 - h(p)) \alpha \right\}, \\ \mathcal{D}'_{4} &:= \left\{ (\alpha, \beta) \in [0, 1]^{2} : b * p < a, \ \alpha \geq (1 - h(p)) \beta \right\}, \\ \mathcal{D}''_{3} &:= \left\{ (\alpha, \beta) \in [0, 1]^{2} : \alpha - \alpha h(p/\alpha) \leq \beta \\ &< (1 - h(p)) \alpha \right\}, \\ \mathcal{D}''_{4} &:= \left\{ (\alpha, \beta) \in [0, 1]^{2} : \beta - \beta h(p/\beta) \leq \alpha \\ &< (1 - h(p)) \beta \right\}. \end{split}$$

Then, $\mathcal{I}_0^* = \mathcal{D}_1 \cup \mathcal{D}_2 \cup \mathcal{D}'_3 \cup \mathcal{D}''_3 \cup \mathcal{D}'_4 \cup \mathcal{D}''_4$. For $(\alpha, \beta) \in \mathcal{I}_0^*$, define

$$\begin{split} \underline{\Upsilon}^*(\alpha,\beta) \\ &= \begin{cases} 1 - (1-p)h\left(\frac{a+b-p}{2(1-p)}\right) \\ -ph\left(\frac{a-b+p}{2p}\right), & (\alpha,\beta) \in \mathcal{D}_1 \\ 1+h(p)-h(a)-h(b), & (\alpha,\beta) \in \mathcal{D}_2 \\ \alpha, & (\alpha,\beta) \in \mathcal{D}_3' \\ h(p)+\beta & & , \\ -(1-\alpha)h\left(\frac{p-\alpha h^{-1}(1-\beta/\alpha)}{1-\alpha}\right), & (\alpha,\beta) \in \mathcal{D}_3'' \\ \beta, & (\alpha,\beta) \in \mathcal{D}_4' \\ h(p)+\alpha & & , \\ -(1-\beta)h\left(\frac{p-\beta h^{-1}(1-\alpha/\beta)}{1-\beta}\right), & (\alpha,\beta) \in \mathcal{D}_4'' \end{cases} \end{split}$$

where $a = h^{-1}(1 - \alpha), b = h^{-1}(1 - \beta)$. For $(\alpha, \beta) \in \mathcal{I}_0^*$, define

$$\Upsilon^*(\alpha,\beta) := h(p) + \alpha \wedge \beta$$

We now provide analytical expressions for $\underline{\Upsilon}(\alpha, \beta)$ and $\overline{\Upsilon}(\alpha, \beta)$ in the following theorem. Since Υ is determined by $\underline{\Upsilon}$, this theorem can be seen as an improved version of Theorem 1.

Theorem 2 (Mutual Information Region for DSBS). For the source DSBS(p) with $p \in (0, 1/2)$, the following hold.

1) The projection region satisfies

$$\mathcal{I}_0 = \mathcal{I}_0^*.$$

2) For $(\alpha, \beta) \in \mathcal{I}_0$, the lower and upper envelopes of the mutual information region satisfy

$$\underline{\Upsilon}(\alpha,\beta) = \underline{\Upsilon}^*(\alpha,\beta),\\ \overline{\Upsilon}(\alpha,\beta) = \overline{\Upsilon}^*(\alpha,\beta).$$

The proof is provided in Section V which follows steps same as those for Theorem 1. Note that Υ^* and $\underline{\Upsilon}^*$ differ on the regions \mathcal{D}''_3 and \mathcal{D}''_4 . The functions $\underline{\Upsilon}^*$ and $\overline{\Upsilon}^*$ are plotted in Fig. 2.

B. Mutual Information Region for Gaussian Source

We next consider Gaussian sources. In this subsection and in the corresponding proofs of results stated in this subsection, we always use the logarithm with base e, which is denoted by ln.

 $\stackrel{
ho}{1}$

Let
$$P_{XY} = \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma})$$
 with
 $\boldsymbol{\Sigma} = \begin{bmatrix} 1 \\ \rho \end{bmatrix}$

and $\rho \in (0, 1)$. We next give the analytical expression for the mutual information region for a Gaussian source. For $\alpha \ge 0$, denote $\theta_{\alpha} \in [0, \pi/2]$ such that

$$\sin\theta_{\alpha} = e^{-\alpha}$$

So, we also have $\sin \theta_{\beta} = e^{-\beta}$. Denote

$$\rho_{\alpha,\beta} := \frac{\rho - \sqrt{(1 - e^{-2\alpha})(1 - e^{-2\beta})}}{e^{-\alpha - \beta}}$$
$$= \frac{\rho - \cos\theta_{\alpha}\cos\theta_{\beta}}{\sin\theta_{\alpha}\sin\theta_{\beta}}.$$
(7)

Define several disjoint sets

$$\begin{split} \mathcal{D}_{\mathrm{G},1} &:= \left\{ (\alpha,\beta) \in [0,\infty)^2 : \cos \theta_\alpha \cos \theta_\beta \leq \rho \\ &\leq \min \left\{ \frac{\cos \theta_\beta}{\cos \theta_\alpha}, \frac{\cos \theta_\alpha}{\cos \theta_\beta} \right\} \right\}, \\ \mathcal{D}_{\mathrm{G},2} &:= \left\{ (\alpha,\beta) \in [0,\infty)^2 : \\ &\rho \leq \min \left\{ \cos \theta_\alpha \cos \theta_\beta, \frac{\cos \theta_\beta}{\cos \theta_\alpha}, \frac{\cos \theta_\alpha}{\cos \theta_\beta} \right\} \right\}, \\ \mathcal{D}_{\mathrm{G},3} &:= \left\{ (\alpha,\beta) \in [0,\infty)^2 : \rho > \frac{\cos \theta_\beta}{\cos \theta_\alpha} \right\}, \\ \mathcal{D}_{\mathrm{G},4} &:= \left\{ (\alpha,\beta) \in [0,\infty)^2 : \rho > \frac{\cos \theta_\alpha}{\cos \theta_\beta} \right\}. \end{split}$$

Define a function for $\alpha, \beta \ge 0$,

$$\Upsilon_{\mathrm{G}}^{*}(\alpha,\beta) := \begin{cases} \alpha + \beta - \frac{1}{2} \ln \frac{1 - \rho_{\alpha,\beta}^{2}}{1 - \rho^{2}} & (\alpha,\beta) \in \mathcal{D}_{\mathrm{G},1} \\ \alpha + \beta - \frac{1}{2} \ln \frac{1}{1 - \rho^{2}} & (\alpha,\beta) \in \mathcal{D}_{\mathrm{G},2} \\ \alpha & (\alpha,\beta) \in \mathcal{D}_{\mathrm{G},3} \\ \beta & (\alpha,\beta) \in \mathcal{D}_{\mathrm{G},4} \end{cases}$$
(8)

Theorem 3 (Mutual Information Region for Gaussian Source). For the bivariate Gaussian source $\mathcal{N}(\mathbf{0}, \Sigma)$, the following hold.

- 1) The projection region satisfies $\mathcal{I}_0 = [0, \infty)^2$.
- 2) For $(\alpha, \beta) \in \mathcal{I}_0$, the lower and upper envelopes of the mutual information region satisfy

$$\underline{\Upsilon}(\alpha,\beta) = \Upsilon^*_{\mathbf{G}}(\alpha,\beta),\tag{9}$$

$$\Upsilon(\alpha,\beta) = +\infty.$$
 (10)

Moreover, Υ_{G}^{*} is increasing in one parameter given the other one, and hence, the lower increasing envelope satisfies $\Upsilon(\alpha, \beta) = \Upsilon_{G}^{*}(\alpha, \beta)$.

The proof of Theorem 3 is provided in Section VI, which is similar to those of Theorems 1 and 2. More specifically, it is based on an auxiliary measure technique and the analytical expression of the optimal-transport divergence region for the Gaussian source. The analytical expression of the optimaltransport divergence region for the Gaussian source is given in Lemma 4 in Section III. Another possible way to prove Theorem 3 is based on the fact [11], [12] that it suffices to evaluate the mutual information region for the Gaussian source by using a random variable W which is jointly Gaussian with X, Y. By this fact, evaluating the mutual information region over arbitrary auxiliary random variable W reduces



Figure 3. Illustration of $\Upsilon_{\rm G}^*$ for $\rho = 0.9$.

to evaluating it over the covariance matrix of (W, X, Y) and the mean of W. Note that the resultant optimization is still nonconvex, and hence, solving it requires some additional techniques.

The function $\Upsilon_{\rm G}^*$ is plotted in Fig. 2. By the following lemma, it holds that $\cos(\theta_{\beta} - \theta_{\alpha}) \geq \min\left\{\frac{\cos\theta_{\beta}}{\cos\theta_{\alpha}}, \frac{\cos\theta_{\alpha}}{\cos\theta_{\beta}}\right\}$, which implies $0 \leq \rho_{\alpha,\beta} < 1$ for $(\alpha, \beta) \in \mathcal{D}_{{\rm G},1}$.

Lemma 1. For $0 \le \theta_1 \le \theta_2 < \pi/2$, it holds that $\cos \theta_2 \le \cos (\theta_2 - \theta_1) \cos \theta_1$.

Proof: This lemma is obviously since $\cos \theta_2 = \cos (\theta_2 - \theta_1) \cos \theta_1 - \sin (\theta_2 - \theta_1) \sin \theta_1 \leq \cos (\theta_2 - \theta_1) \cos \theta_1.$

Using Theorem 3, we obtain the analytical expression for the lossy Gray–Wyner rate region of a Gaussian source. The proof is similar to that of Corollary 1, and hence, omitted here.

Corollary 2 (Lossy Gray–Wyner Rate Region for Gaussian Source). For the bivariate Gaussian source $\mathcal{N}(\mathbf{0}, \Sigma)$, under the quadratic distortion measure, it holds that for $R_1, R_2, D_1, D_2 \geq 0$,

$$R_0(R_1, R_2, D_1, D_2) = \Upsilon_{\rm G}^*([R_{\rm G}(D_1) - R_1]^+, [R_{\rm G}(D_2) - R_2]^+),$$

where $\Upsilon_{\rm G}^*$ is defined in (8), $[x]^+ := \max\{x, 0\}$, and $R_{\rm G}(D) = \frac{1}{2} \ln \frac{1}{D}$ is the rate-distribution function of the standard Gaussian source $\mathcal{N}(0, 1)$.

A partial result of Corollary 2 was given in [7], where the analytical expression for the function $R_0(R_s, D_1, D_2) := \min_{R_1+R_2=R_s} R_0(R_1, R_2, D_1, D_2)$ was derived. Furthermore, Corollary 2 in a different form was presented in [22] by using a different method.

Note that $R_{\rm G}(D_1, D_2) = \Upsilon^*_{\rm G}(R_{\rm G}^{-1}(D_1), R_{\rm G}^{-1}(D_2))$ where $R_{\rm G}(\cdot, \cdot)$ is the rate-distortion function for the bivariate Gaussian source $\mathcal{N}(\mathbf{0}, \mathbf{\Sigma})$ under the quadratic distortion measure [24], [25]. Corollary 2 implicitly states that a layered coding scheme similar to the one given in Remark 1 is optimal for the lossy Gray–Wyner system for the bivariate Gaussian source.

C. Implications of Our Results

The Gray–Wyner rate region has many applications. It has not only been used to characterize the rate region of the Gray–Wyner coding system, but also used to characterize many other problems, including the measure of common information [16], the exponent of the maximal density of the type graph [26], the optimal exponent in the Brascamp– Lieb (BL) inequalities for uniform distributions over type classes [26], [27], the hypercontractivity region [28]–[30], Mrs. Gerber's lemma and information bottleneck [13]–[15], communication rate for channel synthesis [31], etc. See more details in [5]. So, our characterizations of the Gray–Wyner rate regions for the DSBS and the Gaussian source imply the corresponding characterizations of these results for the same sources, although some of them are already known.

Furthermore, in theoretical computer science, the DSBS is usually described as a coin toss model. Such a source has now attracted a lot of interest in theoretical computer science. For example, the joint probability of $A \times A$ under the DSBS corresponds to the generating function of the Fourier weights of the Boolean function $\mathbb{1}_A$, and hence, the DSBS (and also its hypercontractivity inequalities) plays a key role in analysis of Boolean functions; see, e.g., [32] for more details.

III. PRELIMINARIES ON OPTIMAL-TRANSPORT DIVERGENCES

Before proving the main results, we first introduce some preliminary lemmas that will be used in our proofs.

The set of all couplings with marginals Q_X and Q_Y is denoted as

$$\mathcal{C}(P_X, P_Y)$$

:= { $Q_{XY} \in \mathcal{P}(\mathcal{X} \times \mathcal{Y}) : Q_X = P_X, Q_Y = P_Y$ }.

Definition 1. The optimal transport divergence (or minimum relative entropy) between Q_X and Q_Y with respect to a probability measure P_{XY} is defined as

$$\mathsf{D}(Q_X, Q_Y \| P_{XY}) := \inf_{Q_{XY} \in \mathcal{C}(Q_X, Q_Y)} D(Q_{XY} \| P_{XY}).$$

Define the optimal-transport-divergence (or minimumrelative-entropy) region of P_{XY} as

$$\mathcal{D}(P_{XY}) := \bigcup_{Q_X \ll P_X, Q_Y \ll P_Y} \{ (D(Q_X \| P_X), D(Q_Y \| P_Y), D(Q_X, Q_Y \| P_Y)) \}.$$

Define the lower and upper envelopes of the optimal divergence region $\mathcal{D}(P_{XY})$ as for $\alpha, \beta \geq 0$,

$$\underline{\varphi}(\alpha,\beta) := \inf_{\substack{Q_{XY}: D(Q_X \| P_X) = \alpha, \\ D(Q_Y \| P_Y) = \beta}} D(Q_{XY} \| P_{XY})$$
(11)

$$= \inf_{\substack{Q_X, Q_Y: D(Q_X || P_X) = \alpha, \\ D(Q_Y || P_Y) = \beta}} \mathsf{D}(Q_X, Q_Y || P_{XY})$$
(12)

and

$$\overline{\varphi}(\alpha,\beta) := \sup_{\substack{Q_X, Q_Y: D(Q_X \| P_X) = \alpha, \\ D(Q_Y \| P_Y) = \beta}} \mathsf{D}(Q_X, Q_Y \| P_{XY})$$
(13)

Define the lower and upper increasing envelopes of $\mathcal{D}(P_{XY})$ the last infinization in (16) is equal to respectively as

$$\underline{\psi}(\alpha,\beta) := \inf_{s \ge \alpha, t \ge \beta} \underline{\varphi}(s,t) \tag{14}$$

$$\overline{\psi}(\alpha,\beta) := \sup_{s \le \alpha, t \le \beta} \overline{\varphi}(s,t).$$

We also define for q < 0,

$$\varphi_q(\alpha) := \sup_{\substack{Q_X: D(Q_X \parallel P_X) = \alpha}} \inf_{\substack{Q_Y}} \mathsf{D}(Q_X, Q_Y \parallel P_{XY}) \\ - \frac{D(Q_Y \parallel P_Y)}{q}.$$

For the DSBS, φ_q can be rewritten as

$$\varphi_q(\alpha) = \min_{0 \le \beta \le 1} \underline{\varphi}(\alpha, \beta) - \frac{\beta}{q}.$$
 (15)

The following lemma is obvious. Recall that, as mentioned in the notation part (at the end of the introduction section), $\operatorname{conv} f$ and $\operatorname{conc} f$ respectively denote the lower convex envelope and the upper concave envelope of f.

Lemma 2. It holds that

$$\operatorname{conv} \underline{\psi}(\alpha, \beta) = \inf_{\substack{s \ge \alpha, t \ge \beta}} \operatorname{conv} \underline{\varphi}(s, t) \\ = \inf_{\substack{Q_{UXY}: \\ D(Q_{X|U} \| P_X | Q_U) \ge \alpha, \\ D(Q_{Y|U} \| P_Y | Q_U) \ge \beta}} D(Q_{XY|U} \| P_{XY} | Q_U), \quad (16)$$

and

$$\operatorname{conc}\psi(\alpha,\beta) = \sup_{s \leq \alpha, t \leq \beta} \operatorname{conc}\overline{\psi}(s,t)$$

$$= \sup_{\substack{Q_U, Q_{X|U}, Q_{Y|U}:\\D(Q_{X|U} \| P_X | Q_U) \leq \alpha,\\D(Q_{Y|U} \| P_Y | Q_U) \leq \beta}} \mathsf{D}(Q_{X|U}, Q_{Y|U} \| P_{XY} | Q_U), \quad (17)$$

where

$$D(Q_{X|U}, Q_{Y|U} || P_{XY} | Q_U) := \inf_{\substack{Q_{XY|U} \in \mathcal{C}(Q_{X|U}, Q_{Y|U})}} D(Q_{XY|U} || P_{XY} | Q_U)$$

with $\mathcal{C}(Q_{X|U}, Q_{Y|U})$ denoting the set of conditional distributions $Q_{XY|U}$ whose marginals are $Q_{X|U}, Q_{Y|U}$. Furthermore, the alphabet sizes of U in the last infimization in (16) and the last supremization in (17) can be restricted to be no larger than 3.

Proof: The bound on the alphabet sizes of U follows by the support lemma [33]. Based on this, it is easily seen that

$$\inf_{\substack{(q_i,Q_{XY}^{(i)})_{i\in[3]:\\ \sum_{i}q_i=1, q_i\geq 0, \forall i\in[3]\\ \sum_{i}q_iD(Q_X^{(i)}\|P_X)\geq\alpha,\\ \sum_{i}q_iD(Q_Y^{(i)}\|P_Y)\geq\beta}} q_i D(Q_X^{(i)}\|P_Y)\geq\beta$$

$$= \inf_{\substack{(q_i,s_i,t_i)_{i\in[3]:\\ \sum_{i}q_i=1, q_i\geq 0, \forall i\in[3]\\ \sum_{i}q_is_i\geq\alpha,\sum_{i}q_it_i\geq\beta}} \inf_{\substack{(Q_{XY}^{(i)})_{i\in[3]:\\ D(Q_X^{(i)}\|P_X)=s_i,\\ D(Q_Y^{(i)}\|P_Y)=t_i}}} \sum_{i}q_iD(Q_{XY}^{(i)}\|P_{XY})$$

$$= \inf_{\substack{(q_i,s_i,t_i)_{i\in[3]:\\ \sum_{i}q_i=1, q_i\geq 0, \forall i\in[3]\\ \sum_{i}q_is_i\geq\alpha,\sum_{i}q_it_i\geq\beta}} \sum_{i}q_i \inf_{\substack{Q_{XY}^{(i)}:\\ D(Q_X^{(i)}\|P_X)=s_i,\\ D(Q_Y^{(i)}\|P_Y)=t_i}}} D(Q_{XY}^{(i)}\|P_Y)=t_i$$

$$= \inf_{\substack{(q_i,s_i,t_i)_{i\in[3]:\\ \sum_{i}q_i=1, q_i\geq 0, \forall i\in[3]\\ \sum_{i}q_i=1, q_i\geq 0, \forall i\in[3]}}} \sum_{i}q_i\underline{Q}_{XY}^{(i)}(s_i,t_i),$$
(19)

where $(q_i)_{i \in [3]}$ denotes the probability values of U, $Q_{XY}^{(i)}$ denotes $Q_{XY|U=i}$, and (19) follows since the inner infimization in (18) can be taken pointwise for each *i*. By definition, it is easily verified that both $\operatorname{conv}\psi(\alpha,\beta)$ and $\inf_{s \ge \alpha, t \ge \beta} \operatorname{conv} \underline{\varphi}(s, t)$ are also equal to the last formula above. So, equalities in (16) hold. Similarly, one can prove that equalities in (17) hold as well.

The analytic expressions for various envelopes of the optimal divergence region for the DSBS are given in the following lemma.

Lemma 3. [21] For the source DSBS(p) with $p \in (0, 1/2)$, the following hold.

1) It holds that for $\alpha, \beta \in [0,1]^2$, the optimal distribution Q_{XY} attaining $\varphi(\alpha,\beta)$ (in (11)) is

$$Q_{XY} = \begin{bmatrix} 1+q-a-b & b-q \\ a-q & q \end{bmatrix},$$

where $a = h^{-1}(1 - \alpha), b = h^{-1}(1 - \beta)$, and

$$q = q_{a,b}(p) := \frac{1}{2(\kappa - 1)} \times \left((\kappa - 1)(a + b) + 1 - \sqrt{((\kappa - 1)(a + b) + 1)^2 - 4\kappa(\kappa - 1)ab} \right)$$

with $\kappa = \left(\frac{1-p}{p}\right)^2$. Similarly, the optimal distribution Q_{XY} attaining $\overline{\varphi}(\alpha,\beta)$ (in (13)) is still Q_{XY} but with b replaced by $b = 1 - h^{-1}(1 - \beta)$ (or alternatively, with a replaced by $a = 1 - h^{-1}(1 - \alpha)$).

2) Given $\alpha \in [0,1]$, $\beta \mapsto \varphi(\alpha,\beta)$ is strictly decreasing for β such that $a * p \leq b$ and strictly increasing for β such that a * p > b, and moreover, its minimum is α which is attained by the β such that a * p = b. Symmetrically, given $\beta \in [0,1]$, $\alpha \mapsto \varphi(\alpha,\beta)$ is strictly decreasing for α such that $b * p \leq a$ and strictly increasing for α such that $b * p \ge a$, and moreover, its minimum is β which is attained by the α such that b * p = a.

$$\underline{\psi}(\alpha,\beta) = \begin{cases} \underline{\varphi}(\alpha,\beta) & a*p \ge b, \ b*p \ge a \\ \alpha & a*p < b \\ \beta & b*p < a \end{cases}$$

Moreover, $\underline{\psi}$ is convex on $[0,1]^2$ and strictly convex on $\{(\alpha,\beta): a * p \ge b, b * p \ge a\}$, where $a = h^{-1}(1 - \alpha), b = h^{-1}(1 - \beta)$.

4) It holds that for $\alpha, \beta \in [0, 1]^2$,

$$\operatorname{conv}\underline{\varphi}(\alpha,\beta) = \begin{cases} \underline{\varphi}(\alpha,\beta), & (\alpha,\beta) \in \hat{\mathcal{D}}_1 \\ \alpha, & (\alpha,\beta) \in \hat{\mathcal{D}}_2 \\ \alpha + \alpha D \big((1-h^{-1}(1-\beta/\alpha), \\ h^{-1}(1-\beta/\alpha)) \| (1-p,p) \big), & (\alpha,\beta) \in \hat{\mathcal{D}}_4 20 \\ \beta, & (\alpha,\beta) \in \hat{\mathcal{D}}_3 \\ \beta + \beta D \big((1-h^{-1}(1-\alpha/\beta), \\ h^{-1}(1-\alpha/\beta)) \| (1-p,p) \big), & (\alpha,\beta) \in \hat{\mathcal{D}}_5 \end{cases}$$

where

$$\begin{split} \hat{\mathcal{D}}_{1} &:= \mathcal{D}_{1} \cup \mathcal{D}_{2} = \left\{ (\alpha, \beta) \in [0, 1]^{2} : \\ a * p \geq b, \ b * p \geq a \right\}, \\ \hat{\mathcal{D}}_{2} &:= \mathcal{D}'_{3} = \left\{ (\alpha, \beta) \in [0, 1]^{2} : \\ a * p < b, \ \beta \geq (1 - h(p)) \alpha \right\}, \\ \hat{\mathcal{D}}_{3} &:= \mathcal{D}'_{4} = \left\{ (\alpha, \beta) \in [0, 1]^{2} : \\ b * p < a, \ \alpha \geq (1 - h(p)) \beta \right\}, \\ \hat{\mathcal{D}}_{4} &:= \left\{ (\alpha, \beta) \in [0, 1]^{2} : \beta < (1 - h(p)) \alpha \right\}, \\ \hat{\mathcal{D}}_{5} &:= \left\{ (\alpha, \beta) \in [0, 1]^{2} : \alpha < (1 - h(p)) \beta \right\}. \end{split}$$

Moreover, $\operatorname{conv} \varphi(\alpha, \beta)$ for the second clause above is attained by a convex combination of (0,0) (with probability $1-\theta$) and (1-h(a'), 1-h(a'*p)) (with probability θ), where $a' \in [0,1/2]$ is the unique solution to the equation $\frac{1-h(a'*p)}{1-h(a')} = \frac{\beta}{\alpha}$, and $\theta = \frac{\alpha}{1-h(a')}$. Similarly, $\operatorname{conv} \varphi(\alpha, \beta)$ for the third clause above is attained by a convex combination of (0,0) (with probability $1-\alpha$) and $(1, \beta/\alpha)$ (with probability α).

- 5) It holds that $\overline{\varphi}$ is increasing in one argument given the other one. Moreover, $\overline{\varphi}$ is strictly concave on $[0,1]^2$.
- 6) For q < 0, φ_q is increasing and strictly concave on [0, 1].

Remark 2. In other words, the optimal distribution Q_{WXY} (with W denoting the time-sharing random variable in the convex combination operation) attaining $\operatorname{conv} \varphi(\alpha, \beta)$ for the second clause in (20) is given by $Q_W = \operatorname{Bern}(\theta)$, $Q_{XY|W=0} = P_{XY}$, and $Q_{XY|W=1} = \operatorname{Bern}(a')P_{Y|X}$; the optimal distribution Q_{WXY} attaining $\operatorname{conv} \varphi(\alpha, \beta)$ for the third clause in (20) is given by $Q_W = \operatorname{Bern}(\alpha)$, $Q_{XY|W=0} = P_{XY}$, and

$$Q_{XY|W=1} = \begin{bmatrix} 1 - h^{-1}(1 - \beta/\alpha) & h^{-1}(1 - \beta/\alpha) \\ 0 & 0 \end{bmatrix}.$$

The functions appearing in Lemma 3 are plotted in Fig. 4. All statements in Lemma 3 were proven in [21] except for Statements 2 and 4. The proofs of Statements 2 and 4 are given in Appendix A.

As for the Gaussian source, the analytic expressions for envelopes are given in the following lemma, which is a consequence of classic hypercontractivity inequalities. See details in Appendix B.

Lemma 4. For the bivariate Gaussian source $\mathcal{N}(\mathbf{0}, \mathbf{\Sigma})$ with $\mathbf{\Sigma} = \begin{bmatrix} 1 & \rho \\ \rho & 1 \end{bmatrix}$ and $\rho \in (0, 1)$, the following hold. 1) It holds that for $\alpha, \beta \geq 0$,

$$\operatorname{conv}\underline{\varphi}(\alpha,\beta) = \underline{\psi}(\alpha,\beta) \\ = \begin{cases} \underline{\varphi}(\alpha,\beta) = \frac{\alpha+\beta-2\rho\sqrt{\alpha\beta}}{1-\rho^2}, & \rho^2\alpha \le \beta \le \frac{\alpha}{\rho^2} \\ \alpha, & \beta < \rho^2\alpha \\ \beta, & \alpha < \rho^2\beta \end{cases}$$

Moreover, they are convex on $[0, \infty)^2$. An optimal distribution attaining $\underline{\varphi}(\alpha, \beta)$ for the case $\rho^2 \alpha \leq \beta \leq \frac{\alpha}{\rho^2}$ is $Q_{XY} = \mathcal{N}((a, b), \Sigma)$, where $a = \sqrt{2\alpha}, b = \sqrt{2\beta}$.

2) It holds that

$$\overline{\varphi}(\alpha,\beta) = \frac{\alpha + \beta + 2\rho\sqrt{\alpha\beta}}{1 - \rho^2}$$

which is increasing in one argument given the other one. Moreover, $\overline{\varphi}$ is strictly concave on $[0, \infty)^2$.

3) It holds that for q < 0,

$$\varphi_q(\alpha) = \frac{(1-q)\alpha}{1-q-\rho^2},$$

which is increasing and linear on $[0, \infty)$.

The functions appearing in Lemma 4 are plotted in Fig. 5.

IV. PROOF OF THEOREM 1

Proof of $\Upsilon(\alpha, \beta) \leq \Upsilon^*(\alpha, \beta)$: We denote U, V both following $\operatorname{Bern}(\frac{1}{2})$ such that $X \xrightarrow{\operatorname{BSC}(a)} U \xrightarrow{\operatorname{BSC}(c)} V \xrightarrow{\operatorname{BSC}(b)} Y$, where a * b * c = p. Such (a, b, c) exists if $a * b \leq p$. If we set W = (U, V), then

$$I(X, Y; W) = 1 + h(p) - h(a) - h(b)$$

$$I(X; W) = 1 - h(a)$$

$$I(Y; W) = 1 - h(b).$$

This leads to the desired result for $(\alpha, \beta) \in \mathcal{D}_2$.

For the third clause, we set $W \sim \text{Bern}(\frac{1}{2})$ such that $W \xrightarrow{\text{BSC}(a)} X \xrightarrow{\text{BSC}(p)} Y$. For such W, we have

$$I(X, Y; W) = 1 - h(a)$$

 $I(X; W) = 1 - h(a)$
 $I(Y; W) = 1 - h(a * p)$

If $a * p \le b$, then $I(Y; W) \ge \beta$, i.e., this W is feasible. This leads to the desired result for $(\alpha, \beta) \in \mathcal{D}_3$, and by symmetry, also leads to the one for $(\alpha, \beta) \in \mathcal{D}_4$.



Figure 4. Illustration of $\underline{\varphi}, \psi, \overline{\psi} = \overline{\varphi}$, and φ_q for the DSBS(p) with p = 0.05 (equivalently, the correlation coefficient $\rho = 0.9$). Lemma 3 implies that $\underline{\psi}$ is convex, $\overline{\psi} = \overline{\varphi}$ is concave, and φ_q is convex for q < 0.

For $(\alpha, \beta) \in \mathcal{D}_1$, we set $W \sim \text{Bern}(\frac{1}{2})$ such that $W \xrightarrow{\text{BSC}(a)} X$ and $W \xrightarrow{\text{BSC}(b)} Y$, and moreover, $P_{XY|W}$ is a coupling of two channels BSC(a) and BSC(b), given by

$$P_{XY|W=0} = \begin{bmatrix} 1 - \frac{a+b+p}{2} & \frac{-a+b+p}{2} \\ \frac{a-b+p}{2} & \frac{a+b-p}{2} \end{bmatrix},$$
$$P_{XY|W=1} = \begin{bmatrix} \frac{a+b-p}{2} & \frac{a-b+p}{2} \\ \frac{-a+b+p}{2} & 1 - \frac{a+b+p}{2} \end{bmatrix}.$$

For such (W, X, Y), the marginal distribution on (X, Y) is

$$P_{XY} = \frac{1}{2} P_{XY|W=0} + \frac{1}{2} P_{XY|W=1} = \begin{bmatrix} \frac{1-p}{2} & \frac{p}{2} \\ \frac{p}{2} & \frac{1-p}{2} \end{bmatrix},$$

which coincides with the given distribution. So, such W is feasible. This leads to the desired result for $(\alpha, \beta) \in \mathcal{D}_1$.

Proof of $\Upsilon(\alpha, \beta) \geq \Upsilon^*(\alpha, \beta)$: Observe that

$$\begin{split} &\Upsilon(\alpha,\beta) - \alpha - \beta \\ &\geq \inf_{\substack{P_{W|XY}: I(X;W) \geq \alpha, I(Y;W) \geq \beta \\ - I(X;W) - I(Y;W)}} I(X,Y;W) \\ &\geq \inf_{\substack{P_{W|XY}}} I(X,Y;W) - I(X;W) - I(Y;W) \\ &= \inf_{\substack{P_{W|XY}}} -I(X;Y) + I(X;Y|W) \\ &\geq -I(X;Y). \end{split}$$

Hence,

$$\mathbf{f}(\alpha,\beta) \ge \alpha + \beta - I(X;Y) \\
= 1 + h(p) - h(a) - h(b)$$

This implies the desired result for $(\alpha, \beta) \in \mathcal{D}_2$. Furthermore,

$$\begin{split} \Upsilon(\alpha,\beta) &- \alpha \\ &\geq \inf_{\substack{P_{W|XY}: I(X;W) \geq \alpha, I(Y;W) \geq \beta}} I(X,Y;W) - I(X;W) \\ &\geq 0. \end{split}$$

Hence, $\Upsilon(\alpha, \beta) \ge \alpha = 1 - h(a)$, which implies the desired result for $(\alpha, \beta) \in \mathcal{D}_3$, and by symmetry, also implies the one for $(\alpha, \beta) \in \mathcal{D}_4$.



Figure 5. Illustration of $\underline{\psi}, \overline{\psi} = \overline{\varphi}$, and φ_q for the bivariate Gaussian source with the correlation coefficient $\rho = 0.9$. Lemma 4 implies that $\underline{\psi}$ is convex, $\overline{\psi} = \overline{\varphi}$ is concave, and $\overline{\varphi_q}$ is linear for q < 0. In fact, both the graphs of $\underline{\psi}$ and $\overline{\psi} = \overline{\varphi}$ consist of half lines emanating from the origin.

We now consider $(\alpha, \beta) \in \mathcal{D}_1$. Observe that for any R_{XY} ,

$$\begin{split} \Upsilon(\alpha,\beta) &= \inf_{\substack{Q_{WXY}: I(X;W) \geq \alpha, I(Y;W) \geq \beta}} I(X,Y;W) \\ &= \inf_{\substack{Q_{WXY}: Q_{XY} = P_{XY}, \\ D(Q_{X|W} \| R_X | Q_W) - D(P_X \| R_X) \geq \alpha, \\ D(Q_{Y|W} \| R_X | Q_W) - D(P_Y \| R_Y) \geq \beta} \\ &= D(Q_{XY|W} \| R_{XY} | Q_W) - D(P_{XY} \| R_{XY}) \\ &\geq \inf_{\substack{Q_{WXY}: \\ D(Q_{X|W} \| R_X | Q_W) - D(P_X \| R_X) \geq \alpha, \\ D(Q_{Y|W} \| R_X | Q_W) - D(P_Y \| R_Y) \geq \beta} \\ &= D(Q_{XY|W} \| R_{XY} | Q_W) - D(P_{XY} \| R_{XY}) \\ &= \operatorname{conv} \psi(\alpha + D(P_X \| R_X), \beta + D(P_Y \| R_Y)) \\ &- D(P_{XY} \| R_{XY}) \qquad (21) \\ &= \underline{\psi}(\alpha + D(P_X \| R_X), \beta + D(P_Y \| R_Y)) \\ &- D(P_{XY} \| R_{XY}), \qquad (22) \end{split}$$

where ψ is defined in (14) but for R_{XY} , (21) follows by Lemma 2 (recall that $\mathrm{conv}\psi$ denotes the lower convex envelope of ψ), and the last line follows by the convexity of ψ shown in Statement 3 of Lemma 3.

We now choose $R_{XY} = \text{DSBS}(\hat{p})$ with $\hat{p} \in (0, 1/2)$. The value of \hat{p} will be specified later. For such R_{XY} , it holds that

$$D(P_X || R_X) = D(P_Y || R_Y) = 0.$$

Moreover, by Lemma 3 again, for the case of $b \le a * \hat{p}, a \le$ $b * \hat{p}$, it holds that

$$\begin{split} \underline{\psi}(\alpha,\beta) &= \underline{\varphi}(\alpha,\beta) \\ &= D\left(\begin{bmatrix} 1+q-a-b & b-q \\ a-q & q \end{bmatrix} \| \begin{bmatrix} \frac{1-\hat{p}}{2} & \frac{\hat{p}}{2} \\ \frac{\hat{p}}{2} & \frac{1-\hat{p}}{2} \end{bmatrix} \right), \end{split}$$

where $a = h^{-1}(1 - \alpha), b = h^{-1}(1 - \beta)$, and

$$q = q_{a,b}(\hat{p}) := \frac{1}{2(\kappa - 1)} \times \left((\kappa - 1)(a + b) + 1 - \sqrt{((\kappa - 1)(a + b) + 1)^2 - 4\kappa(\kappa - 1)ab} \right)$$

with $\kappa = \left(\frac{1-\hat{p}}{\hat{p}}\right)^2$. Under the condition that $a \leq b$, the conditions that $b \leq a * \hat{p}, a \leq b * \hat{p}$ are equivalent to $\hat{p} \geq \frac{b-a}{1-2a}$. Observe that

 $q_{a,b}(\hat{p})$ is continuous in \hat{p} . Moreover, by definition, it is easily verified that

$$\lim_{\hat{p}\uparrow 1/2} q_{a,b}(\hat{p}) = ab,$$
$$\lim_{\hat{p}\downarrow \frac{b-a}{1-2a}} q_{a,b}(\hat{\rho}) = \frac{a(1-a-b)}{1-2a}$$

On the other hand, for the case of a * p > b, a * b > p, it holds that $ab < \frac{a+b-p}{2} < \frac{a(1-a-b)}{1-2a}$. So, there is a $\hat{p}^* \in (\frac{b-a}{1-2a}, 1/2)$ such that $q_{a,b}(\hat{p}^*) = \frac{a+b-p}{2}$. For such \hat{p}^* , the optimal distribution Q_{XY} attaining $\underline{\varphi}(\alpha, \beta)$ with $R_{XY} = \text{DSBS}(\hat{p}^*)$ is

$$Q_{XY} = \begin{bmatrix} 1 - \frac{a+b+p}{2} & \frac{-a+b+p}{2} \\ \frac{a-b+p}{2} & \frac{a+b-p}{2} \end{bmatrix}$$

We choose $\hat{p} = \hat{p}^*$, i.e., $R_{XY} = \text{DSBS}(\hat{p}^*)$. We then obtain that for $(\alpha, \beta) \in \mathcal{D}_1$,

$$\begin{split} \Upsilon(\alpha,\beta) &\geq \underline{\varphi}(\alpha,\beta) - D(P_{XY} \| R_{XY}) \\ &= D(Q_{XY} \| R_{XY}) - D(P_{XY} \| R_{XY}) \\ &= -H_Q(X,Y) - \mathbb{E}_Q \log R_{XY}(X,Y) \\ &+ H_P(X,Y) - \mathbb{E}_P \log R_{XY}(X,Y) \\ &= H_P(X,Y) - H_Q(X,Y) \\ &= 1 + h\left(p\right) - H\left(\begin{bmatrix} 1 - \frac{a+b+p}{2} & \frac{-a+b+p}{2} \\ \frac{a-b+p}{2} & \frac{a+b-p}{2} \end{bmatrix} \right). \end{split}$$

The last line is exactly the expression for $(\alpha, \beta) \in \mathcal{D}_1$. This proves the desired result for $(\alpha, \beta) \in \mathcal{D}_1$. We hence complete the proof.

V. PROOF OF THEOREM 2

A. Proof of Statement 2

We first prove Statement 2. That is, for $(\alpha, \beta) \in \mathcal{I}_0^*$,

$$\underline{\Upsilon}(\alpha,\beta) = \underline{\Upsilon}^*(\alpha,\beta), \tag{23}$$

$$\overline{\Upsilon}(\alpha,\beta) = \overline{\Upsilon}^*(\alpha,\beta). \tag{24}$$

Note that here $(\alpha, \beta) \in \mathcal{I}_0^*$ instead of $(\alpha, \beta) \in \mathcal{I}_0$.

Proof of (23): We first consider the equality in (23). By definition, $\underline{\Upsilon}(\alpha,\beta) \geq \Upsilon(\alpha,\beta)$. Moreover, for $(\alpha,\beta) \in$ $\mathcal{D}_1 \cup \mathcal{D}_2, \Upsilon^*(\alpha, \beta) = \Upsilon^*(\alpha, \beta).$ So, by Theorem 1, $\Upsilon(\alpha, \beta) \geq$ $\Upsilon(\alpha,\beta) = \Upsilon^*(\alpha,\beta) = \Upsilon^*(\alpha,\beta)$. On the other hand, the random variable W constructed in the proof of Theorem 1 in fact satisfies $I(X; W) = \alpha$, $I(Y; W) = \beta$, and $I(X, Y; W) = \beta$ $\Upsilon^*(\alpha,\beta) = \underline{\Upsilon}^*(\alpha,\beta)$. So, $\underline{\Upsilon}(\alpha,\beta) = \underline{\Upsilon}^*(\alpha,\beta)$ for $(\alpha,\beta) \in$ $\mathcal{D}_1 \cup \mathcal{D}_2$. We next consider $(\alpha, \beta) \in \mathcal{D}'_3 \cup \mathcal{D}''_3 \cup \mathcal{D}'_4 \cup \mathcal{D}''_4$.

By replacing the inequality constraints in the infinizations with the corresponding equality constraints in the equation chain in (22), it holds that for any R_{XY} ,

$$\underline{\Upsilon}(\alpha,\beta) \ge \operatorname{conv}\underline{\varphi}(\alpha + D(P_X \| R_X), \beta + D(P_Y \| R_Y)) - D(P_{XY} \| R_{XY}), \qquad (25)$$

where φ is defined in (12) but for R_{XY} . We now choose $R_{XY} = \text{DSBS}(\hat{p})$ with $\hat{p} > 0$. For such R_{XY} , it holds that

$$D(P_X || R_X) = D(P_Y || R_Y) = 0.$$

We now consider the case $(\alpha, \beta) \in \mathcal{D}'_3$, i.e., $h^{-1}(1-\beta/\alpha) \leq \beta$ $p < \frac{b-a}{1-2a}$. For this case, we choose \hat{p} in the same range $h^{-1}(1-\beta/\alpha) \leq \hat{p} < \frac{b-a}{1-2a}$. For this case, we choose $\hat{p} \leq h^{-1}(1-\beta/\alpha)$. By Statement 4 in Lemma 3 (more precisely, by Remark 2), the optimal distribution Q_{WXY} attaining $\operatorname{conv}\varphi(\alpha,\beta)$ is given by $Q_W = \operatorname{Bern}(\theta)$, and

$$Q_{XY|W=0} = \begin{bmatrix} \frac{1-\hat{p}}{2} & \hat{p}\\ \frac{\hat{p}}{2} & \frac{1-\hat{p}}{2} \end{bmatrix},$$
$$Q_{XY|W=1} = \begin{bmatrix} (1-a')(1-\hat{p}) & (1-a')\hat{p}\\ a'\hat{p} & a'(1-\hat{p}) \end{bmatrix}.$$

where $a' \in [0, 1/2]$ is the unique solution to the equation $\frac{1-h(a'*\hat{p})}{1-h(a')} = \frac{\beta}{\alpha}$, and $\theta = \frac{\alpha}{1-h(a')}$. This distribution satisfies

$$D(Q_{X|W} || R_X) = \alpha,$$

$$D(Q_{Y|W} || R_Y) = \beta,$$

$$D(Q_{XY|W} || R_{XY} |Q_W) = \operatorname{conv} \underline{\varphi}(\alpha, \beta).$$

For such a distribution,

$$Q_{XY}(0,1) + Q_{XY}(1,0) = (1-\theta)\hat{p} + \theta\hat{p} = \hat{p}.$$

We choose $\hat{p} = p$. Substituting such a choice of \hat{p} into the inequality in (25) yields that

$$\begin{split} \underline{\Upsilon}(\alpha,\beta) &\geq \operatorname{conv}\underline{\varphi}(\alpha,\beta) - D(P_{XY} \| R_{XY}) \\ &= D(Q_{XY|W} \| R_{XY} | Q_W) - D(P_{XY} \| R_{XY}) \\ &= -H_Q(X,Y|W) - \mathbb{E}_Q \log R_{XY}(X,Y) \\ &+ H_P(X,Y) - \mathbb{E}_P \log R_{XY}(X,Y) \\ &= H_P(X,Y) - H_Q(X,Y|W) \\ &= 1 + h(p) - (1 - \theta) (1 + h(p)) \\ &- \theta H \left(\begin{bmatrix} (1 - a') (1 - p) & (1 - a')p \\ a'p & a' (1 - p) \end{bmatrix} \right) \\ &= 1 + h(p) - (1 - \theta) (1 + h(p)) \\ &- \theta (h(a') + h(p)) \\ &= \theta (1 - h(a')) \\ &= \alpha. \end{split}$$

This completes the proof of the case $(\alpha, \beta) \in \mathcal{D}'_3$. By

symmetry, the desired result still holds for $(\alpha, \beta) \in \mathcal{D}'_4$. We next consider the case $(\alpha, \beta) \in \mathcal{D}''_3$, i.e., $\alpha h^{-1}(1 - 1)$ $\beta/\alpha) \leq p \leq h^{-1}(1-\beta/\alpha)$. For this case, we choose \hat{p} such that $\hat{p} \leq h^{-1}(1-\beta/\alpha)$. By Statement 4 in Lemma 3 (more precisely, by Remark 2), the optimal distribution Q_{WXY} attaining $\operatorname{conv}\varphi(\alpha,\beta)$ is given by $Q_W = \operatorname{Bern}(\alpha)$, and

$$Q_{XY|W=0} = \begin{bmatrix} \frac{1-\hat{p}}{2} & \frac{\hat{p}}{2} \\ \frac{\hat{p}}{2} & \frac{1-\hat{p}}{2} \end{bmatrix},$$
$$Q_{XY|W=1} = \begin{bmatrix} 1-h^{-1}(1-\beta/\alpha) & h^{-1}(1-\beta/\alpha) \\ 0 & 0 \end{bmatrix}.$$

This distribution satisfies that

$$D(Q_{X|W} || R_X) = \alpha,$$

$$D(Q_{Y|W} || R_Y) = \beta,$$

$$D(Q_{XY|W} || R_{XY} |Q_W) = \operatorname{conv} \underline{\varphi}(\alpha, \beta)$$

For such a distribution,

$$Q_{XY}(0,1) + Q_{XY}(1,0) = (1-\alpha)\hat{p} + \alpha h^{-1}(1-\beta/\alpha).$$

We choose $\hat{p} \in [0, h^{-1}(1 - \beta/\alpha)]$ such that

$$\hat{p}(1-\alpha) + \alpha h^{-1}(1-\beta/\alpha) = p.$$

Such \hat{p} always exists for the case of $(\alpha, \beta) \in \mathcal{D}_{3}^{\prime\prime}$, since for this case, $\alpha h^{-1}(1-\beta/\alpha) \le p \le h^{-1}(1-\beta/\alpha)$.

Substituting such a choice of \hat{p} into the inequality in (25) yields that

$$\begin{split} \underline{\Upsilon}(\alpha,\beta) \\ &\geq \operatorname{conv}\underline{\varphi}(\alpha,\beta) - D(P_{XY} \| R_{XY}) \\ &= D(Q_{XY|W} \| R_{XY} | Q_W) - D(P_{XY} \| R_{XY}) \\ &= -H_Q(X,Y|W) - \mathbb{E}_Q \log R_{XY}(X,Y) \\ &+ H_P(X,Y) - \mathbb{E}_P \log R_{XY}(X,Y) \\ &= H_P(X,Y) - H_Q(X,Y|W) \\ &= 1 + h(p) - (1-\alpha) \left(1 + h(\hat{p})\right) - \alpha \left(1 - \beta/\alpha\right) \\ &= h(p) + \beta - (1-\alpha)h\left(\frac{p - \alpha h^{-1}(1 - \beta/\alpha)}{1 - \alpha}\right). \end{split}$$

This completes the proof of the case $(\alpha, \beta) \in \mathcal{D}_3''$. By symmetry, the desired result still holds for $(\alpha, \beta) \in \mathcal{D}_{4}^{\prime\prime}$.

Proof of (24): We next prove the equality in (24). On one hand,

$$\begin{split} \overline{\mathbf{T}}(\alpha,\beta) &= \sup_{\substack{P_{W|XY}:I(X;W)=\alpha,\\I(Y;W)=\beta}} I(X,Y;W) \\ &= \sup_{\substack{P_{W|XY}:I(X;W)=\alpha,\\I(Y;W)=\beta}} H(X,Y) - H(X,Y|W) \\ &\leq \sup_{\substack{P_{W|XY}:I(X;W)=\alpha,\\I(Y;W)=\beta}} H(X,Y) - H(Y|W) \\ &= \sup_{\substack{P_{W|XY}:I(X;W)=\alpha,\\I(Y;W)=\beta}} H(X|Y) + I(Y;W) \\ &= h(p) + \beta. \end{split}$$

By symmetry, $\overline{\Upsilon}(\alpha, \beta) \leq h(p) + \alpha$. That is, $\overline{\Upsilon}(\alpha, \beta) \leq h(p) + \alpha$

 $\alpha \wedge \beta = \overline{\mathbf{T}}^*(\alpha, \beta).$ We set $W' \xrightarrow{\text{BSC}(a)} X \xrightarrow{\text{BSC}(p)} Y$, or equivalently, $X = W' \oplus Y$ $Z', Y = X \oplus Z$ where $W' \sim \operatorname{Bern}(\frac{1}{2}), Z' \sim \operatorname{Bern}(a)$, and $Z \sim \text{Bern}(p)$ are mutually independent. Here \oplus denotes the XOR operation (i.e., the module-2 sum). Set W = (W', Z). For such W, we have

$$\begin{split} I(X,Y;W) &= I(X;W) + I(Y;W|X) \\ &= I(X;W) + H(Y|X) \\ &= 1 - h(a) + h(p), \\ I(X;W) &= I(X;W',Z) = I(X;W') \\ &= 1 - h(a), \\ I(Y;W) &= I(Y;W',Z) = 1 - H(Y|W',Z) \\ &= 1 - H(Z'|W',Z) = 1 - H(Z') \\ &= 1 - h(a). \end{split}$$

So,

$$\overline{\Upsilon}(\alpha, \alpha) \ge h(p) + \alpha = \overline{\Upsilon}^*(\alpha, \alpha).$$
(26)

Moreover, from the expression derived for the lower envelope, we observe that for $\beta = \alpha - \alpha h(p/\alpha)$,

$$\overline{\Upsilon}(\alpha,\beta) \ge \underline{\Upsilon}(\alpha,\beta) = \underline{\Upsilon}^*(\alpha,\beta) = h(p) + \beta,$$

and for $\alpha = \beta - \beta h(p/\beta)$,

$$\overline{\Upsilon}(\alpha,\beta) \ge \underline{\Upsilon}(\alpha,\beta) = \underline{\Upsilon}^*(\alpha,\beta) = h(p) + \alpha.$$
 (27)

Combining (26)-(27) yields $\overline{\Upsilon}(\alpha,\beta) \geq h(p) + \alpha \wedge \beta =$ $\overline{\Upsilon}^*(\alpha,\beta)$. Hence, $\overline{\Upsilon}(\alpha,\beta) = \overline{\Upsilon}^*(\alpha,\beta)$ for $(\alpha,\beta) \in \mathcal{I}_0^*$.

B. Proof of Statement 1

Observe that the upper envelope $\overline{\Upsilon}$ and the lower envelope Υ coincide on the curves $\beta = \alpha - \alpha h(p/\alpha)$ and $\alpha = \beta - \beta$ $\beta h(p/\beta)$. By the monotonicity of $\overline{\Upsilon}$ and $\underline{\Upsilon}$, the projection region \mathcal{I}_0 must be exactly \mathcal{I}_0^* , since, otherwise, $\overline{\Upsilon} < \underline{\Upsilon}$ holds on the region $\mathcal{I}_0 \setminus \mathcal{I}_0^*$ which contradicts with the obvious fact that $\overline{\Upsilon} > \Upsilon$.

VI. PROOF OF THEOREM 3

We first prove Statement 2. We now consider the equality in (9). We first prove the " \leq " part. We denote $W \sim \mathcal{N}(0, 1)$ and $(\hat{X}, \hat{Y}) \sim \mathcal{N}((a, b), \hat{\Sigma})$ with

$$\hat{\boldsymbol{\Sigma}} = \begin{bmatrix} 1 & \hat{\rho} \\ \hat{\rho} & 1 \end{bmatrix}.$$

Assume W and (\hat{X}, \hat{Y}) are independent. Denote

$$\begin{split} X &= \sqrt{1 - N_1} W + \sqrt{N_1} \hat{X} \\ Y &= \sqrt{1 - N_2} W + \sqrt{N_2} \hat{Y} \end{split}$$

with $N_1, N_2 \in [0, 1]$. Then the correlation coefficient between X and Y is

$$\mathbb{E}\left[(\sqrt{1 - N_1}W + \sqrt{N_1}\hat{X})(\sqrt{1 - N_2}W + \sqrt{N_2}\hat{Y}) \right] \\ = \sqrt{(1 - N_1)(1 - N_2)} + \hat{\rho}\sqrt{N_1N_2}.$$

We choose $\hat{\rho} \in [0,1]$ such that the resultant correlation coefficient is exactly ρ , i.e.,

$$\hat{\rho} = \frac{\rho - \sqrt{(1 - N_1)(1 - N_2)}}{\sqrt{N_1 N_2}}.$$

For this case, the joint distribution of X, Y is exactly P_{XY} . The induced mutual informations are respectively

$$I(X,Y;W) = \frac{1}{2} \ln \left(\frac{1-\rho^2}{N_1 N_2 (1-\hat{\rho}^2)} \right)$$
$$I(X;W) = \frac{1}{2} \ln \frac{1}{N_1}$$
$$I(Y;W) = \frac{1}{2} \ln \frac{1}{N_2}.$$

Let $I(X;W) = \alpha$, $I(Y;W) = \beta$. Then, $N_1 = e^{-2\alpha}$, $N_2 =$ $e^{-2\beta}$, which then implies

$$\hat{\rho} = \rho_{\alpha,\beta},$$

$$I(X,Y;W) = \alpha + \beta + \frac{1}{2} \ln\left(\frac{1-\rho^2}{1-\hat{\rho}^2}\right).$$

Recall the definition of $\rho_{\alpha,\beta}$ in (7). Therefore,

$$\underline{\Upsilon}(\alpha,\beta) \le \alpha + \beta + \frac{1}{2} \ln\left(\frac{1-\rho^2}{1-\hat{\rho}_{\alpha,\beta}^2}\right)$$
(28)

as long as $0 \leq \rho_{\alpha,\beta} < 1$. Hence, this inequality holds for $(\alpha,\beta) \in \mathcal{D}_{G,1}$.

For $(\alpha, \beta) \in \mathcal{D}_{G,2}$, we choose $\hat{\rho} = 0$, which leads to $\underline{\Upsilon}(\alpha, \beta) \leq \alpha + \beta - \frac{1}{2} \ln \frac{1}{1 - \rho^2}$.

For $(\alpha, \beta) \in \mathcal{D}_{G,3}$, although the bound in (28) still holds, we can derive a better bound by choosing a better W. Note that the curve $\left\{ (\alpha, \beta) : \rho^2 = \frac{1-e^{-2\beta}}{1-e^{-2\alpha}} \right\} \subseteq \mathcal{D}_{G,1}$ since $\beta \leq \alpha$ and $\rho_{\alpha,\beta} = e^{\beta-\alpha}\rho \in (0,1)$ for (α,β) on the curve. So, as proven above, $\underline{\Upsilon}(\alpha,\beta) = \alpha$ on this curve. Rewrite the curve equation as $\beta = f(\alpha) := -\frac{1}{2} \ln \left(1 - \rho^2 + \rho^2 e^{-2\alpha}\right)$, and note that the derivative of f is

$$f'(\alpha) = -\frac{\rho^2 e^{-2\alpha}}{1 - \rho^2 + \rho^2 e^{-2\alpha}}$$

which decreases from ρ^2 to 0 as α increases from 0 to $+\infty$. Hence, the closed convex hull of the curve $\{(\alpha, f(\alpha)) : \alpha \ge 0\}$ (i.e., the graph of f) is the set $\{(\alpha, \beta) : 0 \le \beta \le f(\alpha), \alpha \ge 0\}$. By convex combination of points on the curve, we obtain that $\underline{\Upsilon}(\alpha, \beta) = \alpha$ on the set $\{(\alpha, \beta) : 0 \le \beta \le f(\alpha), \alpha \ge 0\}$, i.e., on $\mathcal{D}_{G,3}$. By symmetry, $\underline{\Upsilon}(\alpha, \beta) = \beta$ on $\mathcal{D}_{G,4}$.

We next prove the other direction, i.e., the " \geq " part. Observe that for any R_{XY} ,

$$\underline{f}(\alpha,\beta) = \inf_{\substack{P_{W|XY}:I(X;W)=\alpha,I(Y;W)=\beta}} I(X,Y;W) \\
= \inf_{\substack{Q_{WXY}:Q_{XY}=P_{XY},\\D(Q_{X|W}||R_X|Q_W)-D(P_X||R_X)=\alpha,\\D(Q_{Y|W}||R_Y|Q_W)-D(P_Y||R_Y)=\beta} \\
D(Q_{XY|W}||R_{XY}|Q_W) - D(P_{XY}||R_{XY}) \\
\geq \inf_{\substack{Q_{WXY}:\\D(Q_{X|W}||R_X|Q_W)-D(P_X||R_X)=\alpha,\\D(Q_{Y|W}||R_X|Q_W)-D(P_Y||R_Y)=\beta} \\
D(Q_{XY|W}||R_{XY}|Q_W) - D(P_{XY}||R_{XY}) \\
= \operatorname{conv}\underline{\varphi}(\alpha',\beta') - D(P_{XY}||R_{XY}), \quad (29)$$

where $\alpha' := \alpha + D(P_X || R_X), \beta' := \beta + D(P_Y || R_Y)$, and $\underline{\varphi}$ and $\underline{\psi}$ are defined in (12) and (14) but for R_{XY} . The last line above follows by Statement 1 of Lemma 4.

We now choose
$$R_{XY} = \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma}_R)$$
 with $\boldsymbol{\Sigma}_R = \begin{bmatrix} N_1 & \hat{\rho}\sqrt{N_1N_2} \\ \hat{\rho}\sqrt{N_1N_2} & N_2 \end{bmatrix}$, $N_1 = e^{-2\alpha}$, $N_2 = e^{-2\beta}$, and $\hat{\rho} \ge 0$

For such R_{XY} , it holds that

$$D(P_X || R_X) = \frac{1}{2} \left(\ln N_1 + \frac{1}{N_1} - 1 \right)$$

$$D(P_Y || R_Y) = \frac{1}{2} \left(\ln N_2 + \frac{1}{N_2} - 1 \right)$$

$$D(P_{XY} || R_{XY}) = \frac{1}{2} \left(\ln \frac{|\boldsymbol{\Sigma}_R|}{|\boldsymbol{\Sigma}|} + \operatorname{trace} \left(\boldsymbol{\Sigma}_R^{-1} \boldsymbol{\Sigma} \right) - 2 \right)$$

$$= \frac{1}{2} \left(\ln \frac{N_1 N_2 \left(1 - \hat{\rho}^2 \right)}{1 - \rho^2} + \frac{N_1 + N_2 - 2\rho \hat{\rho} \sqrt{N_1 N_2}}{N_1 N_2 \left(1 - \hat{\rho}^2 \right)} - 2 \right). \quad (30)$$

So,

$$\begin{aligned} \alpha' &= \frac{1}{2} \left(e^{2\alpha} - 1 \right) = \frac{1}{2} \left(\frac{1}{N_1} - 1 \right), \\ \beta' &= \frac{1}{2} \left(e^{2\beta} - 1 \right) = \frac{1}{2} \left(\frac{1}{N_2} - 1 \right). \end{aligned}$$

We now consider the case of $(\alpha, \beta) \in \mathcal{D}_{G,1}$. For this case, we choose $\hat{\rho} \geq 0$ such that $\hat{\rho}^2 \alpha' \leq \beta' \leq \frac{\alpha'}{\hat{\rho}^2}$ (the specific value of $\hat{\rho}$ will be given below), and by Statement 1 of Lemma 4, an optimal distribution attaining $\underline{\psi}(\alpha', \beta')$ (or $\underline{\varphi}(\alpha', \beta')$) is $Q_{XY} = \mathcal{N}((a, b), \Sigma_R)$ with $a = \sqrt{2\alpha' N_1}, b = \sqrt{2\beta' N_2}$. The value of $\psi(\alpha', \beta')$ is

$$\underline{\psi}(\alpha',\beta') = D(Q_{XY} || R_{XY})
= \frac{1}{2} \left(\frac{a^2 N_2 + b^2 N_1 - 2ab\hat{\rho}\sqrt{N_1 N_2}}{N_1 N_2 (1 - \hat{\rho}^2)} \right)
= \frac{1}{2N_1 N_2 (1 - \hat{\rho}^2)} \left((1 - N_1) N_2 + (1 - N_2) N_1 - 2\hat{\rho}\sqrt{N_1 N_2 (1 - N_1) (1 - N_2)} \right).$$
(31)

We choose

$$\hat{o} = \rho_{\alpha,\beta},\tag{32}$$

with $\rho_{\alpha,\beta}$ defined in (7), which satisfies $0 \leq \rho_{\alpha,\beta} < 1$ for $(\alpha,\beta) \in \mathcal{D}_{G,1}$; see the argument below Theorem 3. Such $\hat{\rho}$ also satisfies $\hat{\rho}^2 \alpha' \leq \beta' \leq \frac{\alpha'}{\hat{\rho}^2}$, i.e., $\hat{\rho} \leq \min\left\{\sqrt{\frac{\alpha'}{\beta'}}, \sqrt{\frac{\beta'}{\alpha'}}\right\}$, as desired, since this condition is equivalent to that

$$\rho \le \min\left\{\frac{\cos\theta_{\beta}}{\cos\theta_{\alpha}}, \frac{\cos\theta_{\alpha}}{\cos\theta_{\beta}}\right\}$$

Substituting (30), (31), and (32) into (29) yields that

$$\underline{\Upsilon}(\alpha,\beta) \ge \alpha + \beta + \frac{1}{2} \ln \left(\frac{1-\rho^2}{1-\rho_{\alpha,\beta}^2} \right).$$

We now consider the case $(\alpha, \beta) \in \mathcal{D}_{G,2}$ in which $\rho_{\alpha,\beta} \leq 0$. For this case, we choose $\hat{\rho} = 0$ which yields

$$\underline{\Upsilon}(\alpha,\beta) \ge \alpha + \beta + \frac{1}{2}\ln\left(1-\rho^2\right).$$

We now consider the case of $(\alpha, \beta) \in \mathcal{D}_{G,3}$. For this case, we choose $\hat{\rho} = \rho$, i.e., $R_{XY} = P_{XY}$. For this case, by Statement 1 of Lemma 4, it holds that $\underline{\Upsilon}(\alpha, \beta) = \underline{\psi}(\alpha, \beta) \ge \alpha$, since for this case, $\rho > \frac{\cos \theta_{\beta}}{\cos \theta_{\alpha}} = \sqrt{\frac{1-e^{-2\beta}}{1-e^{-2\alpha}}} \ge \sqrt{\frac{\beta}{\alpha}}$ by the facts that $t \mapsto \frac{1-e^{-2t}}{t}$ is decreasing and $\beta < \alpha$. By symmetry, $\underline{\Upsilon}(\alpha, \beta) \ge \beta$ for $(\alpha, \beta) \in \mathcal{D}_{G,4}$.

Combining all cases above, (9) holds.

The finiteness of $\underline{\Upsilon}(\alpha,\beta)$ on $[0,\infty)^2$ implies the projection region $\mathcal{I}_0 = [0,\infty)^2$, i.e., Statement 1.

We next prove (10). Denote

$$\begin{split} X &= \sqrt{1 - N} \hat{W} + \sqrt{N} \hat{X} \\ Y &= \rho X + \sqrt{1 - \rho^2} \hat{Y} \end{split}$$

with $N \in (0,1)$ and independent standard Gaussian random variables $\hat{W}, \hat{X}, \hat{Y}$. Denote $W = (\hat{W}, \hat{Y})$. For this case,

$$I(X; W) = I(X; \hat{W})$$

= $\frac{1}{2} \ln \frac{1}{N} < +\infty,$
 $I(Y; W) = h_d(Y) - h_d(Y|\hat{W}, \hat{Y})$
= $\frac{1}{2} \ln \frac{1}{N\rho^2} < +\infty,$
 $I(X, Y; W) = I(X; W) + I(Y; W|X)$
= $\frac{1}{2} \ln \frac{1}{N} + h_d(Y|X) - h_d(Y|X, \hat{W}, \hat{Y})$
= $+\infty.$

where $h_{\rm d}$ denotes the differential entropy. Hence, $\overline{\Upsilon}(\alpha, \beta) = +\infty$ for some finite point (α, β) . By the concavity of $\overline{\Upsilon}$, it holds that $\overline{\Upsilon}(\alpha, \beta) = +\infty$ for all $\alpha, \beta \ge 0$, i.e., (10).

APPENDIX A PROOFS OF STATEMENTS 2 AND 4 IN LEMMA 3

A. Proof of Statement 2 in Lemma 3

The monotonicity in fact follows by the convexity of the relative entropy. Specifically, by the strict convexity of the relative entropy, it holds that $(a, b) \mapsto D((1 - a, a), (1 - b, b) || P_{XY})$ is strictly convex, since for $Q_{XY}^{(i)}$ attaining $D((1 - a_i, a_i), (1 - b_i, b_i) || P_{XY})$, i = 0, 1,

$$\begin{aligned} &(1-\lambda)D(Q_{XY}^{(0)} \| P_{XY}) + \lambda D(Q_{XY}^{(1)} \| P_{XY}) \\ &> D((1-\lambda)Q_{XY}^{(0)} + \lambda Q_{XY}^{(1)} \| P_{XY}) \\ &\ge \mathsf{D}((1-a_{\lambda},a_{\lambda}), (1-b_{\lambda},b_{\lambda}) \| P_{XY}), \end{aligned}$$

where $a_{\lambda} = (1 - \lambda)a_0 + \lambda a_1$, $b_{\lambda} = (1 - \lambda)b_0 + \lambda b_1$. So, given $\alpha \in [0, 1]$ (or equivalently, given $a = h^{-1}(1 - \alpha) \in [0, 1/2]$), the function $b \mapsto D((1 - a, a), (1 - b, b) || P_{XY})$ is strictly convex, and its minimum is α which is attained at b = a * p. On the other hand, observe that

$$\inf_{\hat{\beta} \ge \beta} \underline{\varphi}(\alpha, \beta)
= \inf_{\hat{b} \in [0, 1/2]: 1-h(\hat{b}) \ge \beta} \mathsf{D}((1-a, a), (1-\hat{b}, \hat{b}) \| P_{XY})
= \inf_{\hat{b} \in [0, b]} \mathsf{D}((1-a, a), (1-\hat{b}, \hat{b}) \| P_{XY}).$$
(33)

By the strict convexity of the objective function at the last line, the minimum is uniquely attained by $\hat{b} = b$ when $b \le a * p$. Hence, $\varphi(\alpha, \hat{\beta}) > \varphi(\alpha, \beta)$ for all $\hat{\beta}, \beta$ such that $\hat{\beta} > \beta$ and $b \leq a * p$. That is, $\beta \mapsto \underline{\varphi}(\alpha, \beta)$ is strictly decreasing for β such that $a * p \leq b$.

The strict monotonicity of $\beta \mapsto \underline{\varphi}(\alpha, \beta)$ on the interval $a * p \ge b$ can be proven similarly (by replacing the constraints $\hat{\beta} \ge \beta$, $1 - h(\hat{b}) \ge \beta$, and $\hat{b} \in [0, b]$ in (33) respectively with $\hat{\beta} \le \beta$, $1 - h(\hat{b}) \le \beta$, and $\hat{b} \in [b, 1/2]$).

B. Proof of Statement 4 in Lemma 3

We first make the following claim.

Claim 1: $\operatorname{conv} \underline{\varphi}(\alpha, \beta) = \underline{\psi}(\alpha, \beta)$ for (α, β) such that $\beta \ge (1 - h(p)) \alpha$ and $\alpha \ge (1 - h(p)) \beta$. In other words, the formula in (20) holds for $(\alpha, \beta) \in \hat{\mathcal{D}}_1 \cup \hat{\mathcal{D}}_2 \cup \hat{\mathcal{D}}_3$.

We now prove this claim. On one hand, by Statement 3 and the definition of ψ ,

$$\operatorname{conv}\varphi(\alpha,\beta) \ge \operatorname{conv}\psi(\alpha,\beta) = \psi(\alpha,\beta).$$
 (34)

On the other hand, $\operatorname{conv}\underline{\varphi}(\alpha,\beta) \leq \underline{\varphi}(\alpha,\beta) = \underline{\psi}(\alpha,\beta)$ for (α,β) such that $a * p \geq b$, $b * p \geq a$ (i.e., $(\alpha,\beta) \in \hat{\mathcal{D}}_1$). So, (20) holds for $(\alpha,\beta) \in \hat{\mathcal{D}}_1$.

Denote $\beta^*(\alpha)$ as the value β such that a * p = b where $a = h^{-1}(1 - \alpha), b = h^{-1}(1 - \beta)$. By definition of $\underline{\varphi}$, it is easily verified that $\underline{\varphi}(\alpha, \beta^*(\alpha)) = \alpha$, and hence, all points $(\alpha, \beta^*(\alpha), \underline{\varphi}(\alpha, \beta^*(\alpha)))$ with $\alpha \in [0, 1]$ are coplanar. That is, they are on the plane $\{(\alpha, \beta, \alpha) : \alpha, \beta \in [0, 1]\}$. So, $\operatorname{conv}\underline{\varphi}(\alpha, \beta) \leq \alpha$ for (α, β) such that $a * p \leq b, \beta \geq (1 - h(p)) \alpha$ (i.e., $(\alpha, \beta) \in \hat{\mathcal{D}}_2$; see this region in the subfigure (a) in Fig. 4). Since (34) still holds and $\underline{\psi}(\alpha, \beta) = \alpha$ for this case (by Statement 3), it holds that $\operatorname{conv}\underline{\varphi}(\alpha, \beta) = \alpha$ for $(\alpha, \beta) \in \hat{\mathcal{D}}_2$. Similarly, $\operatorname{conv}\underline{\varphi}(\alpha, \beta) = \beta$ for $(\alpha, \beta) \in \hat{\mathcal{D}}_3$. This completes the proof of the claim above.

We next consider the case $(\alpha, \beta) \in \mathcal{D}_4$. By Statement 2, given $\alpha, \beta \mapsto \underline{\varphi}(\alpha, \beta)$ is strictly decreasing for $a * p \leq b$ (and hence also for $\beta < (1 - h(p)) \alpha$). Based on these observations, if we denote (1/u, 1/v) as a subgradient of $\operatorname{conv}\underline{\varphi}$ at (α, β) with $\beta < (1 - h(p)) \alpha$, then v < 0.

If $(\alpha_i, \beta_i, \underline{\varphi}(\alpha_i, \beta_i)), i \in [3]$ are on the supporting plane of $\operatorname{conv}\underline{\varphi}$ at $(\alpha, \overline{\beta})$, then $(\alpha_i, \beta_i), i \in [3]$ must attain the following minimum:,

$$\Gamma := \min_{s,t \ge 0} \underline{\varphi}(s,t) - \frac{s}{u} - \frac{t}{v}.$$

We now make the second claim.

Claim 2: Any optimal (s^*, t^*) attaining the minimum above must be either (0, 0) or $(1, \beta')$ for some $\beta' \in [0, 1]$.

We next prove this claim. By the definition of φ_q in (15), we can rewrite

$$\Gamma = \min_{s \ge 0} \varphi_v(s) - \frac{s}{u}.$$

By Statement 5 in Lemma 3, for v < 0, φ_v is strictly concave on [0, 1]. So, the infimum above is only attained at s = 0 or 1. Moreover, for s = 0, it holds that

$$\varphi_v(0) = \min_{0 \le t \le 1} \underline{\varphi}(0, t) - \frac{t}{v} = 0,$$

since $\underline{\varphi}(0,t) - \frac{t}{v} \ge 0$ (note v < 0) and this lower bound is and uniquely attained at t = 0. So, the unique minimizer above is t = 0. For s = 1, it holds that

$$\begin{aligned} \varphi_v(1) &= \min_{0 \le t \le 1} \underline{\varphi}(1, t) - \frac{t}{v} \\ &= \min_{0 \le b \le 1} \mathsf{D}((1, 0), (1 - b, b) \| P_{XY}) \\ &- \frac{D((1 - b, b) \| P_Y)}{v} \\ &= \min_{0 \le b \le 1} D\left(\begin{bmatrix} 1 - b & b \\ 0 & 0 \end{bmatrix} \| P_{XY} \right) \\ &- \frac{D((1 - b, b) \| P_Y)}{v} \\ &= \min_{0 \le b \le 1} \left(\frac{1}{v} - 1 \right) h(b) - (1 - b) \log \left(1 - \frac{p}{2} \right) \\ &- b \log \frac{p}{2} - \frac{1}{v}. \end{aligned}$$

Since v < 0, it holds that the objective function in the last line is strictly convex, the minimum is attained by a unique *b*. This completes the proof of Claim 2.

By Claim 2, $(\alpha, \beta, \operatorname{conv} \underline{\varphi}(\alpha, \beta))$ is the convex combination of (0, 0, 0) and $(1, \beta', \underline{\varphi}(\overline{1, \beta'}))$ for some $\beta' \in [0, 1]$ (see the subfigure (a) in Fig. 4 for better understanding this statement). That is,

$$(\alpha, \beta, \operatorname{conv}\underline{\varphi}(\alpha, \beta)) = (1 - \theta)(0, 0, 0) + \theta(1, \beta', \underline{\varphi}(1, \beta')),$$

which implies

$$\beta' = \beta/\alpha$$
$$\theta = \alpha.$$

These parameters induce the following optimal distribution Q_{WXY} which attains $\operatorname{conv}\underline{\varphi}(\alpha,\beta)$. Here W denotes the time-sharing (or convex-combination) variable. The optimal distribution Q_{WXY} is given by $Q_W = \operatorname{Bern}(\alpha)$, and

$$Q_{XY|W=0} = \begin{bmatrix} \frac{1-p}{2} & \frac{p}{2} \\ \frac{p}{2} & \frac{1-p}{2} \end{bmatrix},$$
$$Q_{XY|W=1} = \begin{bmatrix} 1-h^{-1}(1-\beta/\alpha) & h^{-1}(1-\beta/\alpha) \\ 0 & 0 \end{bmatrix}.$$

Hence, for this case,

$$\operatorname{conv}\underline{\varphi}(\alpha,\beta) = D(Q_{XY|W} || R_{XY} |Q_W)$$
$$= \alpha + \alpha D\big((1 - h^{-1}(1 - \beta/\alpha), h^{-1}(1 - \beta/\alpha)) || (1 - p, p)\big).$$

This proves (20) for $(\alpha, \beta) \in \hat{\mathcal{D}}_4$. The case $(\alpha, \beta) \in \hat{\mathcal{D}}_5$ follows by symmetry.

APPENDIX B PROOF OF LEMMA 4

The forward and reverse hypercontractivity regions for a joint distribution P_{XY} are respectively

$$\mathcal{R}_{\mathrm{FH}}(P_{XY}) := \left\{ (p,q) \in [1,\infty)^2 : \\ \langle f,g \rangle \le \|f\|_p \|g\|_q, \ \forall f,g \ge 0 \right\}$$

$$\mathcal{R}_{\mathrm{RH}}(P_{XY}) := \left\{ (p,q) \in (-\infty,1]^2 : \\ \langle f,g \rangle \ge \|f\|_p \|g\|_q, \ \forall f,g \ge 0 \right\},$$

where $f: \mathcal{X} \to [0, \infty)$ and $g: \mathcal{Y} \to [0, \infty)$ denote nonnegative measurable functions, $\langle f, g \rangle := \mathbb{E}_P [f(X)g(Y)]$ denote the inner product of f and g, and $||f||_p := \mathbb{E}_P [f^p(X)]^{1/p}$ and $||g||_q := \mathbb{E}_P [g^q(Y)]^{1/q}$ are respectively the (pseudo) pnorm of f and the (pseudo) q-norm of g. In other words, the forward and reverse hypercontractivity regions are respectively the sets of parameters (p, q) such that the forward and reverse hypercontractivity inequalities hold.

We can write $\mathcal{R}_{RH}(P_{XY})$ as the disjoint union of four sets

$$\begin{aligned} \mathcal{R}_{\mathrm{RH}}^{++}(P_{XY}) &:= (0,1]^2 \cap \mathcal{R}_{\mathrm{RH}}(\pi_{XY}), \\ \mathcal{R}_{\mathrm{RH}}^{+-}(P_{XY}) &:= \left((0,1] \times (-\infty,0) \right) \cap \mathcal{R}_{\mathrm{RH}}(\pi_{XY}), \\ \mathcal{R}_{\mathrm{RH}}^{-+}(P_{XY}) &:= \left((-\infty,0) \times (0,1] \right) \cap \mathcal{R}_{\mathrm{RH}}(\pi_{XY}), \\ \mathcal{R}_{\mathrm{RH}}^{--}(P_{XY}) &:= (-\infty,0]^2. \end{aligned}$$

The forward and reverse hypercontractivity regions admit the information-theoretic characterizations [12], [28], [30], [34]–[37]:

$$\mathcal{R}_{\rm FH}(P_{XY}) = \left\{ (p,q) \in [1,\infty)^2 : \\ \underline{\psi}(\alpha,\beta) \ge \frac{\alpha}{p} + \frac{\beta}{q}, \, \forall \, \alpha, \beta \ge 0 \right\}, \\ \mathcal{R}_{\rm RH}^{++}(P_{XY}) = \left\{ (p,q) \in (0,1]^2 : \\ \overline{\varphi}(\alpha,\beta) \le \frac{\alpha}{p} + \frac{\beta}{q}, \, \forall \, \alpha, \beta \ge 0 \right\}, \\ \mathcal{R}_{\rm RH}^{+-}(P_{XY}) = \left\{ (p,q) \in (0,1] \times (-\infty,0) : \\ \varphi_q(\alpha) \le \frac{\alpha}{p}, \, \forall \, \alpha \ge 0 \right\}.$$
(35)

By symmetry, $\mathcal{R}_{\mathrm{RH}}^{-+}(P_{XY})$ can be characterized in an analogous manner to $\mathcal{R}_{\mathrm{RH}}^{+-}(P_{XY})$ in (35).

Furthermore, for the bivariate Gaussian source P_{XY} with correlation coefficient $\rho \in (0, 1)$, it is well known (e.g., [32]) that the forward and reverse hypercontractivity regions are respectively explicitly given by

$$\mathcal{R}_{\rm FH}(P_{XY}) = \left\{ (p,q) \in [1,\infty)^2 : (p-1)(q-1) \ge \rho^2 \right\},\\ \mathcal{R}_{\rm RH}(P_{XY}) = \left\{ (p,q) \in (-\infty,1]^2 : (p-1)(q-1) \ge \rho^2 \right\}.$$

Therefore, by the information-theoretic characterizations

above, for such a source,

$$\underline{\psi}(\alpha,\beta) \geq \sup_{(p,q)\in[1,\infty)^2:(p-1)(q-1)\geq\rho^2} \frac{\alpha}{p} + \frac{\beta}{q} \qquad (36)$$
$$= \begin{cases} \frac{\alpha+\beta-2\rho\sqrt{\alpha\beta}}{1-\rho^2} & \rho^2\alpha\leq\beta\leq\frac{\alpha}{\rho^2}\\ \alpha & \beta<\rho^2\alpha\\ \beta & \beta>\frac{\alpha}{\rho^2} \end{cases}$$

$$\overline{\varphi}(\alpha,\beta) \leq \inf_{\substack{(p,q)\in(0,1]^2:(p-1)(q-1)\geq\rho^2}} \frac{\alpha}{p} + \frac{\beta}{q} \qquad (37)$$
$$= \frac{\alpha+\beta+2\rho\sqrt{\alpha\beta}}{1-\rho^2},$$

$$\varphi_q(\alpha) \le \inf_{p \in (0,1]: (p-1)(q-1) \ge \rho^2} \frac{\alpha}{p}$$
(38)

$$= \frac{(1-q)\alpha}{1-q-\rho^2} \text{ for } q < 0.$$
 (39)

The optimal choice of (p,q) attaining the supremum in (36) is $p = \frac{(1-\rho^2)\sqrt{\alpha}}{\sqrt{\alpha}-\rho\sqrt{\beta}}, q = \frac{(1-\rho^2)\sqrt{\beta}}{\sqrt{\beta}-\rho\sqrt{\alpha}}$ for the case of $\rho^2 \alpha < \beta < \frac{\alpha}{\rho^2}$. The optimal choice of (p,q) attaining the infimum in (37) is $p = \frac{(1-\rho^2)\sqrt{\alpha}}{\sqrt{\alpha}+\rho\sqrt{\beta}}, q = \frac{(1-\rho^2)\sqrt{\beta}}{\sqrt{\beta}+\rho\sqrt{\alpha}}$ for all $\alpha, \beta \ge 0$. The optimal choice of p attaining the infimum in (38) is $p = 1 + \frac{\rho^2}{1-q}$ for all $\alpha \ge 0$.

We now prove that the inequalities in (36)-(39) are in fact equalities. For the Gaussian source $P_{XY} = \mathcal{N}(\mathbf{0}, \mathbf{\Sigma})$ with $\mathbf{\Sigma} = \begin{bmatrix} 1 & \rho \\ \rho & 1 \end{bmatrix}$, if we choose $Q_X = \mathcal{N}(a, 1)$ and $Q_Y = \mathcal{N}(b, 1)$, then

$$D(Q_X || P_X) = \frac{a^2}{2}$$

$$D(Q_Y || P_Y) = \frac{b^2}{2}$$
(40)

$$\mathsf{D}(Q_X, Q_Y \| P_{XY}) = \frac{1}{2} \left(\frac{a^2 + b^2 - 2\rho ab}{1 - \rho^2} \right).$$
(41)

The last equality above follows since

$$D(Q_X, Q_Y || P_{XY})$$

$$= \inf_{Q_{XY} \in \mathcal{C}(Q_X, Q_Y)} D(Q_{XY} || P_{XY})$$

$$\geq \inf_{\rho' \in [0,1]} D(Q_{XY}^{(\Sigma')} || P_{XY})$$

$$= \inf_{\rho' \in [0,1]} D(Q_{XY}^{(\Sigma')} || \mathcal{N}((a, b), \Sigma'))$$

$$+ D(\mathcal{N}((a, b), \Sigma') || P_{XY})$$

$$\geq \inf_{\rho' \in [0,1]} D(\mathcal{N}((a, b), \Sigma') || P_{XY})$$

$$= D(\mathcal{N}((a, b), \Sigma) || P_{XY})$$

$$= \frac{1}{2} \left(\frac{a^2 + b^2 - 2\rho ab}{1 - \rho^2} \right),$$

and this lower bound is attained at $Q_{XY} = \mathcal{N}((a, b), \Sigma)$, where $\Sigma' := \begin{bmatrix} 1 & \rho' \\ \rho' & 1 \end{bmatrix}$, and $Q_{XY}^{(\Sigma')}$ denotes a joint distribution with covariance matrix Σ' . For $\rho^2 \alpha \leq \beta \leq \frac{\alpha}{\rho^2}$, we choose $a = \sqrt{2\alpha}, b = \sqrt{2\beta}$ and then obtain $\underline{\psi}(\alpha, \beta) \leq \underline{\varphi}(\alpha, \beta) \leq \frac{\alpha+\beta-2\rho\sqrt{\alpha\beta}}{1-\rho^2}$, which, combined with (36), implies the equality in (36) for the case of $\rho^2 \alpha \leq \beta \leq \frac{\alpha}{\rho^2}$ (and also $\underline{\psi}(\alpha, \beta) =$ 17

 $\underline{\varphi}(\alpha,\beta)$ for this case). By the monotonicity, the equality in $\overline{(36)}$ also holds for the case of $\beta < \rho^2 \alpha$ or $\beta > \frac{\alpha}{\rho^2}$. For the inequality in (37), we choose $a = \sqrt{2\alpha}, b = -\sqrt{2\beta}$ which verifies the inequality in (37).

Similarly, for $Q_X = \mathcal{N}(a, 1)$, it holds that for q < 0,

$$\begin{split} \inf_{Q_{Y}} \mathsf{D}(Q_{X}, Q_{Y} \| P_{XY}) &- \frac{D(Q_{Y} \| P_{Y})}{q} \\ &= \inf_{Q_{Y|X}} D(Q_{XY} \| P_{XY}) - \frac{D(Q_{Y} \| P_{Y})}{q} \\ &\geq \inf_{b \in \mathbb{R}, \rho'' \in [0,1], N_{2} \geq 0} D(Q_{XY}^{(\Sigma'')} \| P_{XY}) - \frac{D(Q_{Y}^{(\Sigma'')} \| P_{Y})}{q} \\ &= \inf_{b \in \mathbb{R}, \rho'' \in [0,1], N_{2} \geq 0} D(Q_{XY}^{(\Sigma'')} \| \mathcal{N}((a,b), \Sigma'')) \\ &+ D(\mathcal{N}((a,b), \Sigma'') \| P_{XY}) \\ &- \frac{D(Q_{Y}^{(\Sigma'')} \| \mathcal{N}(b, N_{2})) + D(\mathcal{N}(b, N_{2}) \| P_{Y})}{q} \\ &\geq \inf_{b \in \mathbb{R}, \rho'' \in [0,1], N_{2} \geq 0} D(\mathcal{N}((a,b), \Sigma'') \| P_{XY}) \\ &- \frac{D(\mathcal{N}(b, N_{2}) \| P_{Y})}{q} \\ &= \inf_{b \in \mathbb{R}} D(\mathcal{N}((a,b), \Sigma) \| P_{XY}) - \frac{D(\mathcal{N}(b,1) \| P_{Y})}{q} \\ &= \inf_{b \in \mathbb{R}} \frac{1}{2} \left(\frac{a^{2} + b^{2} - 2\rho ab}{1 - \rho^{2}} - \frac{b^{2}}{q} \right) \\ &= \inf_{b \in \mathbb{R}} \frac{1}{2} \left(\frac{a^{2} + b^{2} - 2\rho ab}{1 - \rho^{2}} \right), \\ &= \frac{(1 - q)a^{2}}{2(1 - q - \rho^{2})}, \end{split}$$

and this lower bound is attained at $Q_{XY} = \mathcal{N}((a, b), \Sigma)$ with) $b = \frac{-\rho q a}{1-q-\rho^2}$, where $\Sigma'' := \begin{bmatrix} 1 & \rho'' \sqrt{N_2} \\ \rho'' \sqrt{N_2} & N_2 \end{bmatrix}$, and $Q_{XY}^{(\Sigma'')}$ denotes a joint distribution with covariance matrix Σ'' . We choose $a = \sqrt{2\alpha}$ here, which verifies the equality in (39).

We now prove $\operatorname{conv} \varphi(\alpha, \beta) = \psi(\alpha, \beta)$. On one hand, $\operatorname{conv} \varphi(\alpha, \beta) \geq \operatorname{conv} \psi(\alpha, \beta) = \psi(\alpha, \beta)$. On the other hand, by choosing (40)-(41), $\operatorname{conv} \varphi(\alpha, \beta) \leq \varphi(\alpha, \beta) \leq \frac{\alpha+\beta-2\rho\sqrt{\alpha\beta}}{1-\rho^2}$ for $\rho^2 \alpha \leq \beta \leq \frac{\alpha}{\rho^2}$. So, $\operatorname{conv} \varphi(\alpha, \beta) = \psi(\alpha, \beta)$ for $\rho^2 \alpha \leq \beta \leq \frac{\alpha}{\rho^2}$.

For the case $\beta < \rho^2 \alpha$, we choose $Q_X = \mathcal{N}(a, N)$, and choose Q_Y as the output distribution of channel $P_{Y|X}$ when the input distribution is Q_X . So, $Q_Y = \mathcal{N}(\rho a, 1 - \rho^2 + \rho^2 N)$. For this case,

$$D(Q_X || P_X) = \frac{1}{2} \left(\ln N + \frac{1+a^2}{N} - 1 \right),$$

$$D(Q_Y || P_Y) = \frac{1}{2} \left(\ln \left(1 - \rho^2 + \rho^2 N \right) + \frac{1+\rho^2 a^2}{1-\rho^2 + \rho^2 N} - 1 \right),$$

$$D(Q_X, Q_Y || P_{XY}) = D(Q_X || P_X).$$

For $N \in (0, 1]$ and

$$\beta > g(\rho) := \frac{1}{2} \left(\frac{1}{1 - \rho^2} + \ln(1 - \rho^2) - 1 \right)$$

we choose

$$a = \frac{\sqrt{(1 - \rho^2 + \rho^2 N) (1 + 2\beta - \ln(1 - \rho^2 + \rho^2 N)) - 1}}{\rho}$$

which is positive and induces $D(Q_Y || P_Y) = \beta$. As N decreases from 1 to 0, $D(Q_X || P_X)$ increases from $\frac{\beta}{\rho^2}$ to $+\infty$. So, it holds that $\underline{\varphi}(\alpha, \beta) \leq \alpha$ for $g(\rho) < \beta < \rho^2 \alpha$. Note that $\underline{\varphi}(0,0) = 0$. By convex combination of (0,0) and points in the region $g(\rho) < \beta < \rho^2 \alpha$, we obtain that $\operatorname{conv}\underline{\varphi}(\alpha,\beta) \leq \alpha$ for $\beta < \rho^2 \alpha$. By symmetry, $\operatorname{conv}\underline{\varphi}(\alpha,\beta) \leq \beta$ for $\beta > \frac{\alpha}{\rho^2}$. So, $\operatorname{conv}\varphi(\alpha,\beta) = \psi(\alpha,\beta)$.

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