# Partial Information Decomposition via Deficiency for Multivariate Gaussians

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Abstract—Bivariate partial information decompositions (PIDs) characterize how the information in a "message" random variable is decomposed between two "constituent" random variables in terms of unique, redundant and synergistic information components. These components are a function of the joint distribution of the three variables, and are typically defined using an optimization over the space of all possible joint distributions. This makes it computationally challenging to compute PIDs in practice and restricts their use to low-dimensional random vectors. To ease this burden, we consider the case of jointly Gaussian random vectors in this paper. This case was previously examined by Barrett [1], who showed that certain operationally well-motivated PIDs reduce to a closed form expression for scalar messages. Here, we show that Barrett's result does not extend to vector messages in general, and characterize the set of multivariate Gaussian distributions that reduce to closed-form. Then, for all other multivariate Gaussian distributions, we propose a convex optimization framework for approximately computing a specific PID definition based on the statistical concept of deficiency. Using simplifying assumptions specific to the Gaussian case, we provide an efficient algorithm to approximately compute the bivariate PID for multivariate Gaussian variables with tens or even hundreds of dimensions. We also theoretically and empirically justify the goodness of this approximation.

#### I. INTRODUCTION

Partial information decompositions (PIDs) provide a framework for characterizing the joint information content of three or more random variables. The three-variable case is usually discussed in terms of how two random variables, X and Y, contribute to the information about a "message" variable, M, and is hence referred to as the *bivariate* decomposition. More precisely, a bivariate PID decomposes the mutual information I(M;(X,Y)) into four additive components: the information about M that is (i) unique to X; (ii) unique to Y; (iii) redundant in both X and Y; and (iv) synergistic, i.e., cannot be obtained from X or Y individually, but is present in their combination (X, Y). For an intuitive example, suppose  $M = [M_1, M_2, M_3], X = [M_1, M_2, M_3 \oplus Z],$  and  $Y = [M_2, Z]$ , where  $M_1, M_2, M_3, Z \sim \text{i.i.d. Ber}(1/2)$  and  $\oplus$ represents bitwise-XOR. Then, I(M; (X, Y)) is 3 bits, and can be decomposed as follows: X has 1 bit of unique information about M (i.e.,  $M_1$ ) that is not contained in Y, while Y has zero unique information. X and Y have 1 bit of redundant information, i.e.,  $M_2$ , which can be recovered from either Xor Y. Finally, X and Y have 1 bit of synergistic information, i.e.,  $M_3$ , which is *not* available in either X or Y individually, but can only be decoded when X and Y are taken together. Multiple competing definitions have been proposed for unique,

redundant and synergistic information [2–8], however their differences are only poorly understood (see [9] for a review).

With the development of these formal definitions, PIDs have begun to find uses in a wide variety of contexts. Many works, including ours, have used the PID to analyze biological and neural systems [11–19], e.g., to understand how neural activity and responses jointly encode stimuli. PID has also been used to characterize synergistic interactions in financial markets [20], and to define new measures of bias in machine learning [21]. Unfortunately, we find that only a few of these definitions have clear operational interpretations, and *these* definitions involve an optimization over the space of all joint distributions over (M, X, Y), making them hard to compute in practice. The absence of efficient methods to compute these PIDs, particularly for high dimensions, has been a bottleneck in their wider adoption.

Towards finding efficient ways of computing PIDs, this paper focuses on the bivariate PID for jointly Gaussian random vectors M, X and Y. Barrett [1] previously examined this problem for the case of *scalar messages* M, and showed that certain operationally well-motivated PID definitions can be reduced to a PID that has a *closed form* expression in the Gaussian case (Section II). This has enabled the efficient computation of these operationally sound PIDs for Gaussians with scalar M. However, the case of *vector* M has remained unresolved in the PID literature.

This paper has two main contributions concerning the bivariate PID for fully multivariate Gaussian random variables: (1) In Section III-A, we show that for *vector M*, Barrett's result (and hence the reduction to closed-form) does not apply in general. We introduce a key concept underpinning Barrett's result called *Blackwell sufficiency* [22], using which we characterize the condition under which Barrett's result extends to fully multivariate Gaussians. (2) For cases where this condition *does not* hold, we provide a convex optimization framework to efficiently approximate a PID definition that is based on the statistical concept of *deficiency* [23] (Section III-B). We also provide results showing how this approximation bounds the true Gaussian PID and specific cases when it is guaranteed

\*Equal contribution. The full version of this paper, including appendices, is available online [10]. Part of this work was done while P. Venkatesh was a Ph.D. student at Carnegie Mellon University, Pittsburgh, PA.

 $^1$ We use the term "fully *multivariate* Gaussian" here to refer to instances of a *bivariate* PID where M may also be a *vector* (in contrast to Barrett's work). This is not to be confused with *multivariate* PIDs, where information about M is decomposed among more than two variables.

to agree. In Section IV, we present numerical experiments that validate and go beyond our analytical results. Finally, we conclude with a discussion of open questions in Section V.

#### II. INTRODUCTION TO PID AND BARRETT'S RESULT

Let M, X and Y be random variables with sample spaces M, X and Y respectively, and joint density  $P_{MXY}$ . Then, a bivariate Partial Information Decomposition is loosely defined as a set of non-negative functions  $UI(M:X\setminus Y)$ ,  $UI(M:Y\setminus X)$ , RI(M:X;Y) and SI(M:X;Y) that satisfy:

$$I(M;(X,Y)) = UI(M:X\backslash Y) + UI(M:Y\backslash X)$$

$$+ RI(M:X;Y) + SI(M:X;Y),$$
(1)

$$I(M;X) = UI(M:X \backslash Y) + RI(M:X;Y), \quad (2)$$

$$I(M;Y) = UI(M:Y \setminus X) + RI(M:X;Y).$$
 (3)

Here,  $UI(M: X \setminus Y)$  represents the information about M uniquely<sup>2</sup> present in X and not in Y, while RI(M: X; Y) and SI(M: X; Y) represent the redundant and synergistic information about M contained between X and Y. Usually, we also require that RI and SI are symmetric in X and Y (e.g., see axioms in [2, 3]).

For brevity, we may also write the terms in the RHS of (1) as  $UI_X$ ,  $UI_Y$ , RI, and SI respectively. Since we have three equations and four unknowns, defining any one these four unknowns suffices to determine the other three.

We now state two PID definitions (which are non-identical, in general) in order to present the main result of Barrett [1]. Their interpretations are given later in Section III-A.

**Definition 1** (MMI-PID [1]). Let the redundant information about M present in both X and Y be the **M**inimum of their respective **M**utual **I**nformations with M (hence "MMI"):

$$RI_{\text{MMI}}(M:X;Y) \coloneqq \min\{I(M;X), I(M;Y)\}.$$
 (4)

Along with equations (1)–(3), this fully determines the MMI-PID, i.e.,  $UI_{\text{MMI}}(M:X\backslash Y)$ ,  $UI_{\text{MMI}}(M:Y\backslash X)$ , and  $SI_{\text{MMI}}(M:X;Y)$  are now well-defined.

**Remark 1.** When  $P_{MXY}$  is jointly Gaussian, the MMI-PID can be written in closed form using the following identity (derived in Appendix A in the full version [10]):

$$I(M; Z) = \frac{1}{2} \log \left( \frac{\det(\Sigma_M)}{\det(\Sigma_M - \Sigma_{MZ} \Sigma_Z^{-1} \Sigma_{MZ}^{\mathsf{T}})} \right), \quad (5)$$

where Z could be X, Y, or their concatenation  $[X^{\mathsf{T}}, Y^{\mathsf{T}}]^{\mathsf{T}}$ ,  $\Sigma_M$  and  $\Sigma_Z$  are the covariance matrices of M and Z, and  $\Sigma_{MZ}$  is their cross-covariance matrix. The closed-form expression follows by using (5) in (1)–(4).

**Definition 2** ( $\sim$ -PID<sup>3</sup> [3]). The unique information about M present in X and not in Y is given by

$$\widetilde{UI}(M:X\setminus Y) := \min_{Q\in\Delta_P} I_Q(M;X\mid Y),$$
 (6)

where  $\Delta_P := \{Q_{MXY}: Q_{MX} = P_{MX}, \ Q_{MY} = P_{MY}\}$  and  $I_Q$  is the conditional mutual information over the joint distribution  $Q_{MXY}$ .

**Theorem 1** (Barrett [1]). If M, X and Y are jointly Gaussian and M is scalar, then the  $\sim$ -PID of Definition 2 reduces to the (simpler) MMI-PID of Definition 1.<sup>4</sup>

**Remark 2.** Theorem 1 is significant because the  $\sim$ -PID is operationally well-motivated (as we will see), while the MMI-PID can be expressed in closed form for jointly Gaussian  $P_{MXY}$  as shown in Remark 1. This equivalence has therefore inspired usage of the MMI-PID in several studies that apply PIDs to real-world data [11–13, 20].

#### III. MAIN RESULTS

First we show that Barrett's result (Theorem 1) does not extend to vector M in general, so the closed-form expression from Remark 1 may not always apply.

Counterexample. Suppose  $M = [M_1, M_2]$ ,  $X = M_1 + Z_1$  and  $Y = M_2 + Z_2$ , with  $M_1$ ,  $M_2$ ,  $Z_1$ ,  $Z_2 \sim \text{i.i.d. } \mathcal{N}(0,1)$ . Based on the intuition from the introduction, X and Y have equal amounts of *unique* information about M, and one can show that this holds for the  $\sim$ -PID. However, since I(M;X) = I(M;Y), X and Y have only *redundant* information under the MMI-PID, and no unique information. Thus, the  $\sim$ -PID does not always reduce to the MMI-PID for vector M.

This counterexample is shown more formally in Appendix A.

A. When do Multivariate Gaussians have Closed-form PIDs?

To answer this question, we make some novel and important observations about Barrett's result by breaking it down into a few distinct steps:

- A) Given any PID definition that satisfies the basic equations (1)–(3), if  $P_{MXY}$  is such that either  $UI_X=0$  or  $UI_Y=0$ , then that PID reduces to the MMI-PID.
- B) Barrett considers a few specific PID definitions (including the  $\sim$ -PID mentioned above). In fact, we can consider all PIDs that satisfy the following property:  $UI_Y=0$  if and only if X is *Blackwell sufficient* for M with respect to Y (formally defined below). We call such PIDs *Blackwellian*.<sup>5</sup>
- C) When  $P_{MXY}$  is jointly Gaussian and M is scalar, we always have that either X is Blackwell sufficient for M w.r.t. Y, or Y is Blackwell sufficient w.r.t. X. However, this is not always the case when M is a vector.

Theorem 1 follows by reading these steps in reverse order. Thus, we observe that the concept of Blackwell sufficiency is the driving force in Barrett's result, although this is not explicitly recognized in his paper [1]. So we now proceed to formally define and understand Blackwell sufficiency.

Blackwell sufficiency. The idea of Blackwell sufficiency comes from the field of statistical decision theory [22, 24]. Suppose we are allowed to make inferences about M by observing either X or Y, but not both. Then, informally speaking, X is said to be Blackwell sufficient for M with

 $<sup>^2\</sup>mathrm{Note}$  that the  $X\setminus Y$  in the argument of UI is purely notational, and does not represent a set difference. All quantities in (1) are functions of  $P_{MXY}.$ 

<sup>&</sup>lt;sup>3</sup>This PID is also sometimes referred to as the BROJA PID in the literature.

 $<sup>^4</sup>$ Barrett's original theorem statement is actually slightly more general: all PIDs satisfying assumption (\*) of Bertschinger et al. [3] reduce to the MMI-PID for jointly Gaussian  $P_{MXY}$  and scalar M. This includes a few other well-known definitions such as [2] and [4].

<sup>&</sup>lt;sup>5</sup>Barrett actually considers all PIDs that satisfy Assumption (\*) of [3]. While this is not incorrect, it is *incidental*, and considering Blackwellian PIDs is more precise. This difference is explained in Appendix B.

respect to Y if, on average, we can make equal or better inferences about M (w.r.t. any loss function) by observing X rather than Y. This forms a useful operational interpretation for Blackwellian PIDs, which satisfy  $UI_Y=0$  if and only if X is Blackwell sufficient for M with respect to Y. Thus,  $UI_Y=0$  if and only if Y can provide no better information than X for making inferences about M, which provides a concrete intuition for the meaning of unique information [3].

For simplicity, we define an equivalent [22] notion of Blackwell sufficiency, which is more amenable to our setup here. Given random variables M, X and Y with joint density  $P_{MXY}$ , Blackwell sufficiency is formally defined for the stochastic transformations  $P_{X|M}$  and  $P_{Y|M}$  (also called "channels" from M to X and from M to Y respectively):

**Definition 3** (Blackwell sufficiency:  $\succcurlyeq_M$ ). We say that a channel  $P_{X|M}$  is Blackwell sufficient for another channel  $P_{Y|M}$  (denoted  $X \succcurlyeq_M Y$ ) if  $\exists P_{Y'|X} \in \mathcal{C}(Y \mid X)$  such that

$$P_{Y'|X} \circ P_{X|M} = P_{Y|M}, \tag{7}$$

where C(Y|X) is the set of all channels from X to Y, and  $\circ$  represents channel composition, i.e.  $\forall m \in M, y \in Y$ ,

$$(P_{Y'|X} \circ P_{X|M})(y|m) := \int P_{Y'|X}(y|x)P_{X|M}(x|m) dx.$$
 (8)

Intuitively,  $X \succcurlyeq_M Y$  means that we can generate a new random variable Y' from X (using the stochastic transformation  $P_{Y'|X}$ ), so that the effective channel from M to Y' is equivalent to the original channel from M to Y (i.e., for any M=m, samples of Y' are statistically identical to samples of Y).

**Definition 4** (Blackwellian PID). We say that a bivariate PID of I(M;(X,Y)) is Blackwellian if Y has zero unique information about M with respect to X if and only if  $X \succeq_M Y$ .

Recalling our main objective: we wish to find efficient ways of computing the fully multivariate Gaussian PID. Based on step (C) in the list above, our first goal is to characterize the conditions under which  $X \succcurlyeq_M Y$  for fully multivariate Gaussian  $P_{MXY}$ . Then, steps (B) and (A) would follow, ending with the closed form expression of the MMI-PID.

Characterizing Blackwell sufficiency for Gaussians. First, we parameterize the multivariate Gaussian distribution  $P_{MXY}$ . Let the sample spaces of M, X and Y respectively be  $\mathsf{M} = \mathbb{R}^{d_M}$ ,  $\mathsf{X} = \mathbb{R}^{d_X}$  and  $\mathsf{Y} = \mathbb{R}^{d_Y}$ . Let the joint distribution be given by  $P_{MXY} = \mathcal{N}(0,\Sigma)$ . Since Blackwell sufficiency ignores the dependence between X and Y conditional on M, we define:

$$M \sim P_M = \mathcal{N}(0, \Sigma_M) \tag{9}$$

$$X \mid M \sim P_{X \mid M} = \mathcal{N}(H_X M, \, \Sigma_{X \mid M}) \tag{10}$$

$$Y \mid M \sim P_{Y \mid M} = \mathcal{N}(H_Y M, \Sigma_{Y \mid M}) \tag{11}$$

Here,  $H_X$ ,  $H_Y$ ,  $\Sigma_{X|M}$  and  $\Sigma_{Y|M}$  can all be extracted from the full covariance matrix,  $\Sigma$ . Also, note that we *do not* assume that  $X \perp \!\!\! \perp \!\!\! \perp \!\!\! \perp \!\!\! \perp \!\!\! \perp \!\!\! \mid M$ ; this dependence is captured in  $\Sigma$ .

**Remark 3.** Without loss of generality, we assume that  $\mathbb{E}[M] = 0$  and that the noise covariance matrices  $\Sigma_{X|M}$  and  $\Sigma_{Y|M}$  are full rank. This is always valid, since removing

<sup>6</sup>Note that Blackwell sufficiency ignores potential dependencies between X and Y given M, i.e., it does not depend upon  $P_{XY|M}$  in its entirety; it only depends on the X- and Y-marginals of  $P_{XY|M}$ .

the mean of M, as well as removing linearly dependent elements within X and Y, has no effect on information-theoretic relationships (explained further in Appendix A).

We can now characterize the conditions for Blackwell sufficiency in fully multivariate Gaussian distributions.

**Theorem 2.** For jointly Gaussian random vectors M, X and Y,  $X \succcurlyeq_M Y$  if and only if

$$H_X^{\mathsf{T}} \Sigma_{X|M}^{-1} H_X \succcurlyeq H_Y^{\mathsf{T}} \Sigma_{Y|M}^{-1} H_Y, \tag{12}$$

where  $A \succcurlyeq B$  means that A - B is positive semidefinite (for positive semidefinite matrices A and B).

A proof of this theorem is provided in Appendix B in the full version of this paper [10]. The result relies on a connection between concepts from two disparate fields: Blackwell sufficiency and the *stochastic degradedness* of broadcast channels. We then leverage prior work from the literature analyzing the stochastic degradedness of MIMO Gaussian broadcast channels [26, 27] to prove our result. With this, we can formally state our extension of Barrett's result to fully multivariate Gaussians:

**Corollary 3.** Given any Blackwellian PID (e.g., the  $\sim$ -PID), if  $P_{MXY}$  is jointly Gaussian and satisfies (12), then that PID reduces to the MMI-PID and can be written in closed form as shown in Remark 1.

**Remark 4.** Since  $\Sigma_{X|M}$  and  $\Sigma_{Y|M}$  are full rank (see Remark 3), we can apply a whitening transform:

$$\widetilde{H}_X := \Sigma_{X|M}^{-\frac{1}{2}} H_X, \quad \widetilde{H}_Y := \Sigma_{Y|M}^{-\frac{1}{2}} H_Y.$$
 (13)

This simplifies (12) to  $\widetilde{H}_X^{\mathsf{T}}\widetilde{H}_X \succcurlyeq \widetilde{H}_Y^{\mathsf{T}}\widetilde{H}_Y$ . Without loss of generality, we assume henceforth that  $H_X$  and  $H_Y$  have already been whitened, and hence  $\Sigma_{X|M} = \Sigma_{Y|M} = I$ .

#### B. Efficiently Computing the Gaussian PID in General

Next, we explore how the Gaussian PID can be computed (approximately) when  $P_{MXY}$  does *not* satisfy (12). For this, we consider another PID definition based on the statistical concept of *deficiency* [5], which we call the  $\delta$ -PID.

**Definition 5** ( $\delta$ -PID [5]). Let the (weighted output) deficiency<sup>8</sup> of X with respect to Y about M be defined as<sup>9</sup>

$$\delta(M:Y\backslash X) := \inf_{P_{Y'\mid X} \in \mathcal{C}(Y\mid X)} \mathbb{E}_{P_M} \left[ D(P_{Y\mid M} \parallel P_{Y'\mid X} \circ P_{X\mid M}) \right], \tag{14}$$

where  $D(\cdot \| \cdot)$  is the KL-divergence. Then, define the deficiency-based redundant information about M in X and Y as:

$$RI_{\delta}(M:X;Y) := \min\{I(M;X) - \delta(M:X\backslash Y), I(M;Y) - \delta(M:Y\backslash X)\}.$$
 (15)

As with the MMI-PID, equations (1)–(3) fully determine the remaining components of the  $\delta$ -PID— $UI_{\delta X}$ ,  $UI_{\delta Y}$  and  $SI_{\delta}$ .

<sup>&</sup>lt;sup>7</sup>This connection was mentioned in passing by Raginsky [25], but we prove the equivalence formally in Lemma 6 (see Appendix B in the full version [10]). This connection has also never before been recognized in the context of PID.

 $<sup>^8</sup>$ There are many ways to define deficiency; Raginsky [25] provides a number of these that consider the worst-case over M. We prefer an expectation over M, since M is a random variable in our setup.

 $<sup>^9\</sup>mathrm{The}$  reason for this notation is that the deficiency of X w.r.t. Y translates to the unique information present in Y and not in X.

Deficiency finds the channel  $P_{Y'|X}$  that minimizes the expected divergence between  $P_{Y|M}$  and  $P_{Y'|X} \circ P_{X|M}$ , where the expectation is over M. The divergence goes to zero if and only if  $P_{Y|M} = P_{Y'|X} \circ P_{X|M}$ , i.e. if  $X \succcurlyeq_M Y$ , thus the  $\delta$ -PID is also Blackwellian [24]. Thus, deficiency directly measures how far  $P_{MXY}$  is from being Blackwell *sufficient* (as stated in (7)), and therefore forms a natural measure of unique information. Equation (15) plays the role of symmetrizing the redundant information, since  $I(M;X) - \delta(M:X \setminus Y)$  and  $I(M;Y) - \delta(M:Y \setminus X)$  are not necessarily equal.

Computing the deficiency as given by (14) is challenging because it requires an optimization over all continuous conditional distributions  $P_{Y'|X}$ . So, we consider the restricted problem where  $P_{Y'|X}$  lies in the set of linear additive Gaussian noise channels  $\mathcal{C}_G(Y|X) \subset \mathcal{C}(Y|X)$ . Then,  $P_{Y'|X}$  can be parameterized in terms of its channel gain and noise covariance matrices,  $T \in \mathbb{R}^{d_Y \times d_X}$  and  $\Sigma_T \in \mathbb{R}^{d_Y \times d_Y}$ ,  $\Sigma_T \succcurlyeq 0$ , as  $P_{Y'|X} \sim \mathcal{N}(TX, \Sigma_T)$ . Thus, the Gaussian deficiency can be defined as follows:

$$\delta_{G}(M:Y\setminus X) \approx \inf_{P_{Y'\mid X}\in\mathcal{C}_{G}(Y\mid X)} \mathbb{E}_{P_{M}} \left[ D(P_{Y\mid M} \parallel P_{Y'\mid X} \circ P_{X\mid M}) \right]$$
(16)
$$= \inf_{T,\Sigma_{T}\geq 0} \frac{1}{2} \left[ \mathbb{E}_{P_{M}} \left[ \left\| (TH_{X} - H_{Y})M \right\|_{\Sigma_{T} + TT^{\mathsf{T}}}^{2} \right] + \operatorname{Tr} \left\{ (\Sigma_{T} + TT^{\mathsf{T}})^{-1} \right\} + \log \det(\Sigma_{T} + TT^{\mathsf{T}}) - d_{Y} \right],$$

where  $\|a\|_B^2 \coloneqq aB^{-1}a^{\mathsf{T}}$  is the squared Mahalanobis distance, and (17) follows from the expression for the KL-divergence of normal distributions (derived in Appendix A) and using Remark 4. Unfortunately, we cannot prove that this problem is convex, since  $\mathrm{Tr}\left((\Sigma_T + TT^{\mathsf{T}})^{-1}\right)$  is the composition of a convex function  $(\mathrm{Tr}\left((\cdot)^{-1}\right))$  with a non-monotonic function of T. Therefore, we propose a convex approximation of (17) to find an approximate minimizer  $\widehat{P}_{Y'|X} = \mathcal{N}(\widehat{T}X, \widehat{\Sigma}_T)$ :

**Definition 6** (
$$\hat{\delta}_{G}$$
 and the  $\hat{\delta}_{G}$ -PID). Let
$$\hat{T} := \underset{T}{\operatorname{argmin}} \ \mathbb{E}_{P_{M}} \left[ \left\| (TH_{X} - H_{Y})M \right\|_{I + H_{Y}\Sigma_{M}H_{Y}^{\mathsf{T}}}^{2} \right]$$
(18)
s.t.  $I + H_{Y}\Sigma_{M}H_{Y}^{\mathsf{T}} - T(I + H_{X}\Sigma_{M}H_{X}^{\mathsf{T}})T^{\mathsf{T}} \succcurlyeq 0$ 

$$\widehat{\Sigma}_T := I + H_Y \Sigma_M H_Y^\mathsf{T} - \widehat{T} (I + H_X \Sigma_M H_X^\mathsf{T}) \widehat{T}^\mathsf{T}$$
 (19)

Then, we define the approximate deficiency to be:

$$\widehat{\delta}_{G}(M:Y\backslash X) := \frac{1}{2} \left[ \mathbb{E}_{P_{M}} \left[ \left\| (\widehat{T}H_{X} - H_{Y})M \right\|_{\widehat{\Sigma}_{T} + \widehat{T}\widehat{T}^{\mathsf{T}}}^{2} \right] + \operatorname{Tr}((\widehat{\Sigma}_{T} + \widehat{T}\widehat{T}^{\mathsf{T}})^{-1}) + \log |\widehat{\Sigma}_{T} + \widehat{T}\widehat{T}^{\mathsf{T}}| - d_{Y} \right]$$

$$(20)$$

Substituting  $\hat{\delta}_G$  into (15), we obtain an approximation of  $RI_{\delta}$ , and hence of the  $\delta$ -PID, which we call the  $\hat{\delta}_G$ -PID.

For brevity, we use  $\widehat{UI}_X$ ,  $\widehat{UI}_Y$ ,  $\widehat{RI}$  and  $\widehat{SI}$  to refer to the constituent atoms of the  $\widehat{\delta}_G$ -PID.

The derivation of the convex formulation in (18) has three main steps, which we summarize here and describe in detail in Appendix C in the full version [10].

- 1) First, we obtain a condition on  $\Sigma_T$  (in terms of T), which is locally optimal. This condition allows us to reduce the optimization problem from two variables ( $\Sigma_T$  and T) to just one (T alone). This step is *exact*, and is shown in Proposition 8 in Appendix C.
- Next, we reinterpret and approximate the objective to significantly simplify its functional form, while attempting to minimize the same entities.
- 3) Lastly, as part of reducing the optimization problem to a single variable, the constraint  $\Sigma_T \succcurlyeq 0$  is now replaced by a positive semidefiniteness constraint in terms of T. We approximate and simplify this constraint to make it more amenable for a convex program to handle, which yields the condition shown in (19).

This approximation can be shown to satisfy certain desirable properties. Firstly,  $\hat{\delta}_G$  is well defined, i.e.,  $\hat{\Sigma}_T + \hat{T}\hat{T}^\mathsf{T}$  is guaranteed to be invertible when using the approximation of Definition 6. This is formally stated and proved in Lemma 9, which can be found in Appendix D in the full version [10].

Secondly, the estimate in (20) provably coincides with the true deficiency in the following circumstances:

**Proposition 4.** For jointly Gaussian  $P_{MXY}$ ,

$$\widehat{\delta}_G(M:Y\setminus X) = 0 \Leftrightarrow \delta(M:Y\setminus X) = 0 \tag{21}$$

$$\delta(M:Y\backslash X) = I(M;Y) \Rightarrow \widehat{\delta}_G(M:Y\backslash X) = I(M;Y) \tag{22}$$

A proof is given in Appendix E in the full version [10].

Thirdly, since  $\widehat{P}_{Y'|X} \in \mathcal{C}_G(Y \mid X) \subset \mathcal{C}(Y \mid X)$ , we have:

$$\widehat{\delta}_G(M:Y\backslash X) \ge \delta_G(M:Y\backslash X) \ge \delta(M:Y\backslash X) \tag{23}$$

These inequalities show that the  $\hat{\delta}_G$ -PID bounds the true  $\delta$ -PID: **Proposition 5.** For jointly Gaussian random vectors M, X and Y, the  $\hat{\delta}_G$ -PID bounds the  $\delta$ -PID:

$$\widehat{UI}_X \ge UI_{\delta X} \quad \widehat{RI} \le RI_{\delta}$$

$$\widehat{UI}_Y \ge UI_{\delta Y} \quad \widehat{SI} \le SI_{\delta}$$
(24)

#### IV. EMPIRICAL RESULTS

Having established and theoretically justified a framework for approximating the  $\delta$ -PID, we address three questions using simulations: (Q1) Does  $\widehat{\delta}_G$  yield a *non-negative* PID for jointly Gaussian distributions? (Q2) Is the  $\widehat{\delta}_G$ -PID consistent with the results of Barrett [1] for the case of univariate M? (Q3) Does the  $\widehat{\delta}_G$ -PID meet our intuition for different  $d_M$ ,  $d_X$  and  $d_Y$ ? (Q4) How good is the approximation provided by the  $\widehat{\delta}_G$ -PID?

To address these questions, we sampled 80,000 joint covariance matrices  $\Sigma \in \mathbb{R}^{d \times d}$   $(d = d_M + d_X + d_Y)$  from a standard Wishart distribution, which fully characterized  $P_{MXY}$ . We sampled 20,000 matrices each from four sampling schemes:

- (S1)  $d_M \sim \text{Unif}\{1...10\}$  and  $d_X = d_Y = d_M$
- (S2)  $d_M \sim \text{Unif}\{1...9\}$  and  $d_X, d_Y \stackrel{\text{iid}}{\sim} \text{Unif}\{d_M + 1...10\}$
- (S3)  $d_M \sim \text{Unif}\{2\dots 10\}$  and  $d_X, d_Y \stackrel{\text{iid}}{\sim} \text{Unif}\{1\dots d_M 1\}$
- (S4)  $d_M \sim \text{Unif}\{2\dots 9\}, d_X \sim \text{Unif}\{1\dots d_M-1\}, \text{ and } d_Y \sim \text{Unif}\{d_M+1\dots 10\}$

Without loss of generality, we took  $d_X \leq d_Y$  (i.e., we switched their values if  $d_Y < d_X$ ). Simulations were performed on a 2.4 GHz 8-Core Intel Core i9 processor and took 188.8

minutes to complete. Details of the experimental setup and implementation are provided in Appendices F and G [10] and the code is available on Github [28].

First, we found that all estimated PID components were non-negative for *every one* of the 80,000 sampled distributions. This suggests an affirmative answer to (Q1), possibly excluding a set of distributions of measure zero. Secondly, we found that in every distribution with  $d_M=1$  (N=4277), only one of X or Y had unique information. Therefore, the  $\hat{\delta}_G$ -PID is consistent with Barrett's result in our experiments, answering (Q2) in the affirmative. Of the remaining 75,723 distributions for which  $d_M>1$ , X and Y both had unique information in 93.6% of cases (70,876 distributions). Thus, the overwhelming majority of Gaussian distributions with vector M do not satisfy Blackwell sufficiency and do not reduce to the MMI-PID, justifying the need for our approximation-based approach.

To address (Q3), we visualize the distribution of unique, redundant, and synergistic information across all four sampling schemes in Figure 1. Since the scale of the PID components varies with I(M;(X,Y)), we consider the normalized PID quantities  $\overline{UI}_X$ ,  $\overline{UI}_Y$ ,  $\overline{RI}$ , and  $\overline{SI}$  obtained by dividing each PID component by I(M;(X,Y)). These normalized values are all non-negative and satisfy  $\overline{UI}_X + \overline{UI}_Y + \overline{RI} + \overline{SI} = 1$ . In Figure 1 we represent each distribution by its location on a 3-simplex that characterizes the proportion of I(M;(X,Y)) that is accounted for by each PID component. Below the 3-simplices for each sampling scheme, we also show the distribution of  $\overline{UI}_X$ ,  $\overline{UI}_Y$ ,  $\overline{RI}$ , and  $\overline{SI}$  in the form of box plots.

Figure 1 shows how our approximate PID for multivariate Gaussians meets our intuitive expectations. Firstly, since  $d_Y \geq d_X$ , Y tends to have more unique information than X (see box plots), excepting (S1) where  $d_X = d_Y$ . Secondly, (S2) with  $d_M < d_X, d_Y$  closely mimics the scalar-M case, rarely exhibiting unique information in both X and Y simultaneously. This is seen in the simplex plot, wherein the isosceles triangle forming the lower third of the simplex (with vertices at  $\overline{UI}_X$ ,  $\overline{UI}_Y$  and the centroid of the simplex) is almost completely devoid of points. Thirdly, (S3) and (S4) have large amounts of unique information in Y (as seen in the box plots), since  $d_M$  is large and provides more dimensions of M that Y can uniquely capture.

Synergy has a strong prevalence under all four sampling schemes (see box plots), with the greatest prevalence in (S2), when  $d_M < d_X, d_Y$ . This agrees with the intuition provided by Barrett [1], who mentions the prevalence of synergy for Gaussians with  $d_M=1$ . Redundancy is never particularly prevalent—this may be due to how we sample random covariance matrices, which reduces the likelihood that X and Y capture the same dimensions of M. (S3) and (S4) have the least redundancy (as observed in the box plots), since X has fewer dimensions than M in both these cases.

To address (Q4), unfortunately, there are no alternative estimators of the  $\delta$ -PID that can serve as potential baselines. Nor are there alternative estimators of Blackwellian PIDs for Gaussian variables (excepting the scalar-M case, for which Proposition 4 already provides guarantees). Therefore, we

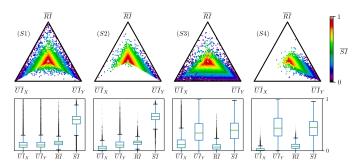


Fig. 1: Distribution of normalized unique, redundant, and synergistic information for Gaussian systems sampled from a standard Wishart distribution: (S1)  $d_M = d_X = d_Y$ ; (S2)  $d_M < d_X \leq d_Y$ ; (S3)  $d_X \leq d_Y < d_M$ ; and (S4)  $d_X < d_M < d_Y$ . Top row: scatter plots of the computed  $\overline{UI}_X$ ,  $\overline{UI}_Y$ ,  $\overline{RI}$  and  $\overline{SI}$  on the 3-simplex (3D views in Appendix I in the full version [10]). Each point is a single sampled Gaussian system. Bottom row: box plots showing the relative prevalence of each PID atom. The box shows the median and the first and third quartiles, while the whiskers extend to 1.5 times the interquartile range (difference of third and first quartiles).

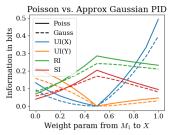


Fig. 2: A comparison of an estimate [23] of the  $\sim$ -PID evaluated on a Poisson distribution against the  $\widehat{\delta}_G$ -PID evaluated on the covariance matrix of the same distribution. We take  $M=[M_1,M_2]$ , with  $M_1,M_2\sim$  iid. Poiss(2) and  $X\sim \operatorname{Binom}(M_1,p_{X\,1})+\operatorname{Binom}(M_2,p_{X\,2})+\operatorname{Poiss}(1)$ . Y is defined similar to X.  $p_{X\,1}$  is varied between 0.0 and 1.0 in increments of 0.1, while  $p_{X\,2}$ ,  $p_{Y\,1}$  and  $p_{Y\,2}$  are kept fixed at 0.5. Despite differences in the PID definitions errors in approximating the Poisson distribution as a Gaussian, and errors in the two estimates, there is a reasonable agreement between the two PIDs.

compare the  $\hat{\delta}_G$ -PID with the best available estimator [23] for the  $\sim$ -PID. These results are explained in Figure 2, with further details in Appendix H in the full version of this paper [10].

#### V. SUMMARY AND OPEN QUESTIONS

Barrett [1] showed that a Blackwellian PID (the  $\sim$ -PID) can be easily computed for Gaussian  $P_{MXY}$  with scalar M. Theorem 2 shows that this extends to vector M only under a specific condition, which likely holds only for a small minority of Gaussian distributions. Therefore, we provided a convex optimization framework to approximate the  $\delta$ -PID, to enable applications of the PID on multivariate Gaussian data.

Our framework forms the first efficient method for computing Blackwellian PIDs (even approximately) for high-dimensional distributions. Although we have not theoretically proved that the  $\hat{\delta}_G$ -PID is non-negative, we found no negative instances empirically. Several open questions remain: Can deficiency be computed exactly? When does our approximation agree with the true deficiency (beyond Proposition 4)? Can we characterize Blackwell sufficiency for general probability distributions (e.g., see [29])? Finally, applying the  $\hat{\delta}_G$ -PID in practice also requires studying its statistical properties when estimating covariance matrices from data and providing statements of confidence.

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#### Partial Information Decomposition via Deficiency for Multivariate Gaussians

Praveen Venkatesh and Gabriel Schamberg

#### APPENDIX A

#### MISCELLANEOUS DERIVATIONS

#### A. Derivation of the Closed-form Expression for the Gaussian MMI-PID from Remark 1

Remark 1 establishes a closed-form expression for the MMI-PID of Gaussian random variables. First, we derive the expression for mutual information between two jointly Gaussian random vectors, as shown in equation (5).

$$I(M;Z) \stackrel{(a)}{=} h(M) - h(M|Z) \tag{25}$$

$$H(M) \stackrel{(b)}{=} \frac{1}{2} \log \left( (2\pi e)^{d_M} \det(\Sigma_M) \right)$$
 (26)

$$H(M \mid Z) \stackrel{(c)}{=} \frac{1}{2} \log \left( (2\pi e)^{d_M} \det(\Sigma_{M \mid Z}) \right)$$
 (27)

where (a) is the basic formula for mutual information [30, Ch. 2] and (b) is the formula for the differential entropy of a Gaussian random vector [30, Thm. 8.4.1]. Here,  $h(\cdot)$  represents differential entropy, while  $\Sigma_M$  is the covariance matrix of M. In (c), we have used the fact that  $P_{M|Z}$  is also a Gaussian distribution for jointly Gaussian  $P_{MZ}$ , so the differential entropy follows the same formula as in (b), with the difference that we use the *conditional* covariance matrix  $\Sigma_{M|Z}$  corresponding to the conditional distribution  $P_{M|Z}$ .

Next, we observe that  $\Sigma_{M|Z}$  can be written as:

$$\Sigma_{M|Z} = \Sigma_M - \Sigma_{MZ} \Sigma_Z^{-1} \Sigma_{MZ}^{\mathsf{T}} \tag{28}$$

where  $\Sigma_{MZ}$  is the cross-covariance matrix between M and Z (e.g., see [31, Sec. 8.1.3]).

Thus, the expression for mutual information reduces to

$$I(M;Z) = \frac{1}{2}\log((2\pi e)^{d_M}\det(\Sigma_M)) - \frac{1}{2}\log((2\pi e)^{d_M}\det(\Sigma_{M|Z}))$$
(29)

$$= \frac{1}{2} \log \left( \frac{\det(\Sigma_M)}{\det(\Sigma_{M|Z})} \right) \tag{30}$$

$$= \frac{1}{2} \log \left( \frac{\det(\Sigma_M)}{\det(\Sigma_M - \Sigma_{MZ} \Sigma_Z^{-1} \Sigma_{MZ}^{\mathsf{T}})} \right). \tag{31}$$

We can now write out the MMI-PID for jointly Gaussian  $P_{MXY}$  using the above expression. First, we individually substitute X and Y for Z in the RHS below, to evaluate the MMI-redundancy:

$$RI_{\text{MMI}}(M:X;Y) = \min\{I(M;X), I(M;Y)\}.$$
 (32)

Then, we can compute the MMI-unique informations by subtracting out the redundancy from the respective mutual information:

$$UI_{\text{MMI}}(M:X\setminus Y) = I(M;X) - RI_{\text{MMI}}(M:X;Y), \tag{33}$$

$$UI_{\text{MMI}}(M:Y\setminus X) = I(M;Y) - RI_{\text{MMI}}(M:X;Y). \tag{34}$$

And finally, the synergy can be computed by subtracting each of the aforementioned terms from the total mutual information:

$$SI_{\text{MMI}}(M:X;Y) = I(M;X,Y) - UI_{\text{MMI}}(M:X\setminus Y) - UI_{\text{MMI}}(M:Y\setminus X) - RI_{\text{MMI}}(M:X;Y). \tag{35}$$

Here, the total mutual information I(M; X, Y) is computed by substituting the concatenated vector,  $[X^T, Y^T]^T$ , in place of Z in (31).

#### B. Details of the Counterexample to Barrett's Result for Vector M

Recall the objective of the counterexample: we wish to show that when M is a vector, the  $\sim$ -PID of Definition 2 does not always reduce to the MMI-PID of Definition 1. Consider again the setup of the counterexample:  $M = [M_1, M_2]$ ,  $X = M_1 + Z_1$  and  $Y = M_2 + Z_2$ , with  $M_1$ ,  $M_2$ ,  $M_2$ ,  $M_3$ ,  $M_4$ ,  $M_4$ ,  $M_5$ ,  $M_4$ ,  $M_5$ ,  $M_6$ ,  $M_7$ ,  $M_8$ ,  $M_$ 

First, we show what the MMI-PID looks like in this case:

$$I(M;X) = I(M_1, M_2; X) = I(M_1; X) + I(M_2; X \mid M_1)$$
(36)

$$=I(M_1;X)+0,$$
 (37)

since  $(X, M_1) \perp M_2$ . Similarly,  $I(M; Y) = I(M_2; Y)$ . Now, by symmetry, we have that

$$I(M_1; X) = I(M_1; M_1 + Z_1) \stackrel{(a)}{=} I(M_2; M_2 + Z_2) = I(M_2; Y), \tag{38}$$

where (a) follows from the fact that  $M_1$ ,  $M_2$ ,  $Z_1$  and  $Z_2$  are all independent and identically distributed. Thus,

$$RI_{\text{MMI}}(M:X;Y) = \min\{I(M;X), I(M;Y)\} = I(M_1;X) = I(M_2;Y). \tag{39}$$

Consequently, (2) and (3) imply that  $UI_{MMI}(M:X\setminus Y)=0$  and  $UI_{MMI}(M:Y\setminus X)=0$ .

On the other hand, the  $\sim$ -PID satisfies:

$$X \perp \!\!\!\perp Y$$
 and  $X \perp \!\!\!\perp Y \mid M$ . (40)

The latter follows because

$$I(X;Y|M) = I(M_1 + Z_1; M_2 + Z_2 | M_1, M_2)$$

$$\tag{41}$$

$$= h(M_1 + Z_1 \mid M_1, M_2) - h(M_1 + Z_1 \mid M_1, M_2, M_2 + Z_2)$$

$$\tag{42}$$

$$= h(Z_1) - h(Z_1) = 0 (43)$$

Now, [3, Thm. 20] and [3, Lem. 21] state that when the two conditions in (40) hold, then  $\widetilde{RI}(M:X;Y)=0$ . Therefore, it follows that  $\widetilde{UI}_X$  and  $\widetilde{UI}_Y$  are equal to I(M;X) and I(M;Y) respectively.

Thus, we see that the  $\sim$ -PID does not always reduce to the MMI-PID for vector M.

#### C. Explanation of Remark 3

The mutual information between two random variables is invariant under invertible (and measurable) transforms applied to each of the individual variables (see, e.g., [32, Appendix]). Changing the means of M, X and Y constitutes an invertible transformation and would not affect their mutual information.

If  $\Sigma_{X|M}$  (or  $\Sigma_{Y|M}$ ) is not full-rank, that means that its rows are linearly dependent. Since  $\Sigma_{X|M} = \mathbb{E}[XX^{\mathsf{T}}|M]$  where  $\mathbb{E}[X|M] = 0$ , we can conclude that there must be linear dependencies between different elements of X (conditional on M). These can be removed by using an eigenvalue decomposition of  $\Sigma_{X|M}$  (for example), and considering only those eigenvectors corresponding to non-zero eigenvalues. That is, if  $\Sigma_{X|M} = VDV^{\mathsf{T}}$  (with eigenvalues sorted in descending order) and has rank  $k < d_X$ , then consider the transformed vector  $X' \in \mathbb{R}^k$  with elements  $X_i' = v_i^{\mathsf{T}}X$ ,  $i \in \{1...k\}$ , where  $v_i$  is the i-th column of V. Again, this constitutes an invertible transformation, since the remaining dimensions of X can be reconstructed using the linear dependencies implicit in  $\Sigma_{X|M}$ . Thus, information quantities remain unchanged under this transformation.

#### D. Derivation of the Expression for Gaussian Deficiency in Equation (17)

First, we derive the expression for the KL-divergence between two n-dimensional multivariate normal distributions. For simplicitly, suppose the distributions are given by  $p \sim \mathcal{N}(\mu_1, \Sigma_1)$  and  $q \sim \mathcal{N}(\mu_2, \Sigma_2)$ . Then,

$$D(p(x)||q(x)) = \int p(x) \log \frac{p(x)}{q(x)} dx = \mathbb{E}_p \left[ \log \frac{p(X)}{q(X)} \right]$$
(44)

$$\stackrel{(a)}{=} \mathbb{E}_p \left[ \log \left( \frac{1}{(2\pi)^{n/2} \det(\Sigma_1)^{1/2}} \exp\left( -\frac{1}{2} \|X - \mu_1\|_{\Sigma_1}^2 \right) \right) - \log \left( \frac{1}{(2\pi)^{n/2} \det(\Sigma_2)^{1/2}} \exp\left( -\frac{1}{2} \|X - \mu_2\|_{\Sigma_2}^2 \right) \right) \right]$$
(45)

$$\stackrel{(b)}{=} \mathbb{E}_p \left[ \log \frac{\det(\Sigma_2)^{1/2}}{\det(\Sigma_1)^{1/2}} - \frac{1}{2} \|X - \mu_1\|_{\Sigma_1}^2 + \frac{1}{2} \|X - \mu_2\|_{\Sigma_2}^2 \right]$$
(46)

$$\stackrel{(c)}{=} \frac{1}{2} \mathbb{E}_p \left[ \log \frac{\det(\Sigma_2)}{\det(\Sigma_1)} - (X - \mu_1)^\mathsf{T} \Sigma_1^{-1} (X - \mu_1) + (X - \mu_2)^\mathsf{T} \Sigma_2^{-1} (X - \mu_2) \right]$$
(47)

$$\stackrel{(d)}{=} \frac{1}{2} \mathbb{E}_p \left[ \log \frac{\det(\Sigma_2)}{\det(\Sigma_1)} - \text{Tr}\{(X - \mu_1)^\mathsf{T} \Sigma_1^{-1} (X - \mu_1)\} + \text{Tr}\{(X - \mu_2)^\mathsf{T} \Sigma_2^{-1} (X - \mu_2)\} \right]$$
(48)

$$\stackrel{(e)}{=} \frac{1}{2} \mathbb{E}_p \left[ \log \frac{\det(\Sigma_2)}{\det(\Sigma_1)} - \text{Tr}\{\Sigma_1^{-1}(X - \mu_1)(X - \mu_1)^\mathsf{T}\} + \text{Tr}\{\Sigma_2^{-1}(X - \mu_2)(X - \mu_2)^\mathsf{T}\} \right]$$
(49)

$$\stackrel{(f)}{=} \frac{1}{2} \left[ \log \frac{\det(\Sigma_2)}{\det(\Sigma_1)} - \text{Tr} \left\{ \Sigma_1^{-1} \mathbb{E}_p[(X - \mu_1)(X - \mu_1)^\mathsf{T}] \right\} + \text{Tr} \left\{ \Sigma_2^{-1} \mathbb{E}_p[(X - \mu_2)(X - \mu_2)^\mathsf{T}] \right\} \right]$$
(50)

$$\stackrel{(g)}{=} \frac{1}{2} \left[ \log \frac{\det(\Sigma_2)}{\det(\Sigma_1)} - \operatorname{Tr} \left\{ \Sigma_1^{-1} \Sigma_1 \right\} + \operatorname{Tr} \left\{ \Sigma_2^{-1} \left( \operatorname{Var}_p [X - \mu_2] + \mathbb{E}_p [X - \mu_2] \mathbb{E}_p [X - \mu_2]^\mathsf{T} \right) \right\} \right]$$

$$(51)$$

$$\stackrel{(h)}{=} \frac{1}{2} \left[ \log \frac{\det(\Sigma_2)}{\det(\Sigma_1)} - \text{Tr}\{I\} + \text{Tr}\left\{\Sigma_2^{-1} \left(\Sigma_1 + [\mu_1 - \mu_2][\mu_1 - \mu_2]^{\mathsf{T}}\right)\right\} \right]$$
 (52)

$$\stackrel{(i)}{=} \frac{1}{2} \left[ \log \frac{\det(\Sigma_2)}{\det(\Sigma_1)} - n + \text{Tr} \left\{ \Sigma_2^{-1} \Sigma_1 + \Sigma_2^{-1} [\mu_1 - \mu_2] [\mu_1 - \mu_2]^\mathsf{T} \right\} \right]$$
 (53)

$$\stackrel{(j)}{=} \frac{1}{2} \left[ \log \frac{\det(\Sigma_2)}{\det(\Sigma_1)} - n + \text{Tr} \left\{ \Sigma_2^{-1} \Sigma_1 \right\} + (\mu_1 - \mu_2)^{\mathsf{T}} \Sigma_2^{-1} (\mu_1 - \mu_2) \right\}$$
 (54)

$$\stackrel{(k)}{=} \frac{1}{2} \left[ \log \frac{\det(\Sigma_2)}{\det(\Sigma_1)} - n + \text{Tr}\{\Sigma_2^{-1}\Sigma_1\} + \|\mu_1 - \mu_2\|_{\Sigma_2} \} \right]$$
 (55)

where in the above steps, we have:

- (a) Expanded out the Gaussian distribution
- (b) Expanded out the logs and canceled terms
- (c) Expanded the Mahalanobis distance,  $||a||_B^2 := aB^{-1}a^T$
- (d) Used the fact that a scalar is equal to the trace of itself
- (e) Used the fact that the trace is invariant under cyclic permutations
- (f) Used linearity of trace to take the expectation inside the operator
- (g) Noted that  $\mathbb{E}_p[(X-\mu_1)(X-\mu_1)^\mathsf{T}]$  is simply  $\Sigma_1$ , and used the formula for variance in the last term.
- (h) Resolved the variance and expectation, taken with respect to p
- (i) Used the fact that the trace of the identity matrix is equal to the dimension of the matrix, n
- (j) Used the cyclic-permutation invariance of trace again
- (k) Used the formula for Mahalanobis distance again

The expression for Gaussian deficiency follows by observing that  $p = \mathcal{N}(H_Y M, \Sigma_{Y|M})$  and  $q = \mathcal{N}(TH_X M, T\Sigma_{X|M}T^\mathsf{T} + \Sigma_T)$ . Further, we make use of Remark 4 to set  $\Sigma_{X|M} = I$  and  $\Sigma_{Y|M} = I$ , so that

$$\mu_1 = H_Y M \qquad \qquad \Sigma_1 = I \tag{56}$$

$$\mu_2 = TH_X M \qquad \qquad \Sigma_2 = \Sigma_T + TT^\mathsf{T} \tag{57}$$

Finally, substituting into (55), we get

$$\mathbb{E}_{P_{M}} \left[ D(P_{Y|M} \| P_{Y'|X} \circ P_{X|M}) \right]$$

$$= \frac{1}{2} \left[ \mathbb{E}_{P_{M}} \left[ \left\| (TH_{X} - H_{Y})M \right\|_{\Sigma_{T} + TT^{\mathsf{T}}}^{2} \right] + \operatorname{Tr} \left\{ (\Sigma_{T} + TT^{\mathsf{T}})^{-1} \right\} + \log \det(\Sigma_{T} + TT^{\mathsf{T}}) - d_{Y} \right],$$
(58)

where we have used the fact that det(I) = 1 and n here is  $d_Y$ .

### APPENDIX B PROOF OF THEOREM 2

The proof of Theorem 2 consists of two steps:

- 1) First, we show that the concept of Blackwell sufficiency (Definition 3) is identical to another concept known as stochastic degradedness (defined formally below) in the literature on broadcast channels. We show this in Lemma 6.
- 2) Then, we leverage previous work from the literature characterizing the stochastic degradedness of Gaussian MIMO broadcast channels. In the process, we show how the Gaussian MIMO broadcast channel setup is precisely the same as the setup used for examining the PID of jointly Gaussian random vectors.

Finally, we provide an explanation of what is expressed in footnote 5 in a subsection at the end of this section of the Appendix.

#### A. The Equivalence of Blackwell Sufficiency and Stochastic Degradedness

**Lemma 6** (Equivalence of Blackwell sufficiency and stochastic degradedness).  $P_{X|M}$  is Blackwell sufficient for  $P_{Y|M}$  if and only if  $P_{Y|M}$  is stochastically degraded with respect to  $P_{X|M}$ .

*Proof.* Throughout this proof, we drop the arguments of probability distributions. When we equate two distributions, we mean that they are identical at all points in their shared domain. <sup>10</sup>

 $(\Leftarrow)$  Suppose  $P_{Y|M}$  is stochastically degraded w.r.t.  $P_{X|M}$ . Then,  $\exists X'$  such that

$$P_{X'|M} = P_{X|M} \text{ and } P_{YX'|M} = P_{Y|X'}P_{X'|M}.$$
 (59)

Let  $P_{Y'|X} := P_{Y|X}$ . Then, (59) implies that

$$P_{Y'|X}P_{X|M} = P_{Y|X'}P_{X'|M}. (60)$$

Therefore,

$$\int P_{Y'|X} P_{X|M} \, dx = \int P_{Y|X'} P_{X'|M} \, dx \tag{61}$$

$$= \int P_{YX'|M} dx = P_{Y|M}, \tag{62}$$

which proves that  $P_{X|M}$  is Blackwell sufficient for  $P_{Y|M}$ .

 $<sup>^{10}</sup>$ This can be extended to be more measure-theoretically accurate, to mean that they are equal  $\mu$ -almost everywhere under some measure  $\mu$  that is absolutely continuous with respect to the two distributions being equated.

 $(\Rightarrow)$  Suppose  $P_{X|M}$  is Blackwell sufficient for  $P_{Y|M}$ . Then,  $\exists P_{Y'|X}$  such that

$$\int P_{Y'|X} P_{X|M} dx = P_{Y|M}. \tag{63}$$

In other words,

$$P_{Y'|M} = P_{Y|M} \quad \text{and hence} \quad P_{Y'M} = P_{YM}. \tag{64}$$

Let X' be defined through a stochastic transformation of Y and M:  $P_{X'|YM}(x|y,m) := P_{X|Y'M}(x|y,m) \ \forall \ x \in X, \ y \in Y$ ,  $m \in M$ . Then, using (64), we find

$$P_{X'YM} = P_{X'|YM}P_{YM} \tag{65}$$

$$= P_{X|Y'M} P_{Y'M} = P_{XY'M}. (66)$$

This in turn implies

$$P_{X'Y|M} = P_{XY'|M} \stackrel{(a)}{=} P_{Y'|X} P_{X|M} \tag{67}$$

$$\stackrel{(b)}{=} P_{Y|X'} P_{X'|M}, \tag{68}$$

which proves that M - X' - Y is a Markov chain. In the above equation, (a) follows from how  $P_{Y'|X}$  is defined, while (b) follows from (66).

**Remark 5.** The equivalence stated in Lemma 6 was also mentioned in passing by Raginsky [25], though without proof. On the other hand, Cover and Thomas [30, Sec. 15.6.2] define stochastic degradedness similar to how we have defined Blackwell sufficiency. However, since we refer to the work of Gerdes et al. [26] in what follows, we have used their definition of stochastic degradedness, and proved the equivalence formally for the sake of completeness.

#### B. Characterizing the Stochastic Degradedness of Broadcast Channels

Before proceeding to the proof of Theorem 2, we introduce a lemma borrowed from Shang and Poor [27, Lemma 5] that provides an equivalent characterization of the condition in Theorem 2.

**Lemma 7.** The condition  $H_X^\mathsf{T} \Sigma_{X|M}^{-1} H_X \succcurlyeq H_Y^\mathsf{T} \Sigma_{Y|M}^{-1} H_Y$  holds if and only if

$$\exists T \quad s.t. \quad H_Y = TH_X \quad and \quad T\Sigma_{X|M}T^{\mathsf{T}} \preccurlyeq \Sigma_{Y|M}.$$
 (69)

*Proof.* Consider the whitened form of the channels:

$$\widetilde{H}_X := \Sigma_{X|M}^{-\frac{1}{2}} H_X, \ \widetilde{H}_Y := \Sigma_{Y|M}^{-\frac{1}{2}} H_Y, \tag{70}$$

as mentioned in Remark 4. Then, we need to show  $\widetilde{H}_X^{\mathsf{T}}\widetilde{H}_X\succcurlyeq \widetilde{H}_Y^{\mathsf{T}}\widetilde{H}_Y$  if and only if

$$\exists T \text{ s.t. } \widetilde{H}_Y = T\widetilde{H}_X \text{ and } TT^{\mathsf{T}} \preccurlyeq I.$$
 (71)

The remainder of the proof follows from [27, Lemma 5].

Proof of Theorem 2. This proof is derived in large part from the work of Gerdes et al. [26]. ( $\Leftarrow$ ) Suppose that  $H_X^\mathsf{T} \Sigma_{X|M}^{-1} H_X \succcurlyeq H_Y^\mathsf{T} \Sigma_{Y|M}^{-1} H_Y$ . Then, by Lemma 7,  $\exists T$  such that  $H_Y = TH_X$  and  $T \Sigma_{X|M} T^\mathsf{T} \preccurlyeq \Sigma_{Y|M}$ . In other words, we may write

$$Y' = TX + N, (72)$$

where  $N \sim \mathcal{N}(0, \Sigma_T)$ , with  $\Sigma_T \coloneqq \Sigma_{Y|M} - T\Sigma_{X|M} T^\mathsf{T}$  (the fact that  $T\Sigma_{X|M} T^\mathsf{T} \preccurlyeq \Sigma_{Y|M}$  ensures that  $\Sigma_T$  is positive semidefinite, and hence a valid covariance matrix). Therefore,  $\exists Y'$  generated by a stochastic transformation  $P_{Y'|X} = \mathcal{N}(TX, \Sigma_T)$ , such that

$$P_{Y'|M} = \mathcal{N}(TH_XM, T\Sigma_{X|M}T^\mathsf{T} + \Sigma_T) = \mathcal{N}(H_YM, \Sigma_{Y|M}) = P_{Y|M}. \tag{73}$$

Hence, by Definition 3,  $X \succcurlyeq_M Y$ .

(⇒) Next, suppose that  $X \succcurlyeq_M Y$ . Then,  $\exists Y'$  generated by  $P_{Y'|X}$ , such that  $P_{Y'|M} = P_{Y|M}$ . Since M - X - Y' is a Markov chain,

$$I(M;X) \stackrel{(a)}{\geq} I(M;Y') \stackrel{(b)}{=} I(M;Y), \tag{74}$$

where (a) follows from the Data Processing Inequality [30, Ch. 2], and (b) follows because  $P_{Y'M} = P_{YM}$ . For a Gaussian channel  $P_{X|M}$ , the mutual information is given by [30, Thm. 8.4.1]

$$I(M; X) = h(X) - h(X \mid M)$$
 (75)

$$= \frac{1}{2} \log|(2\pi e)(\Sigma_{X|M} + H_X \Sigma_M H_X^{\mathsf{T}})| - \frac{1}{2} \log|2\pi e \Sigma_{X|M}|$$
 (76)

$$= \frac{1}{2} \log \left( \frac{|\Sigma_{X|M} + H_X \Sigma_M H_X^{\mathsf{T}}|}{|\Sigma_{X|M}|} \right) \tag{77}$$

$$= \frac{1}{2} \log \left( \frac{|\Sigma_{X|M}||I + \Sigma_{X|M}^{-1} H_X \Sigma_M H_X^{\mathsf{T}}|}{|\Sigma_{X|M}|} \right)$$
 (78)

$$= \frac{1}{2} \log |I + \Sigma_{X|M}^{-1} H_X \Sigma_M H_X^{\mathsf{T}}|. \tag{79}$$

Now, suppose for the sake of contradiction that  $H_X^\mathsf{T} \Sigma_{X|M}^{-1} H_X \not\models H_Y^\mathsf{T} \Sigma_{Y|M}^{-1} H_Y$ . Then, by the definition of positive semidefiniteness,  $\exists \ c \in \mathbb{R}^{d_M}$  such that

$$c^{\mathsf{T}} H_X^{\mathsf{T}} \Sigma_{X|M}^{-1} H_X c < c^{\mathsf{T}} H_Y^{\mathsf{T}} \Sigma_{Y|M}^{-1} H_Y c. \tag{80}$$

Since  $\log |I + AB| = \log |I + BA|$ ,  $\log(\cdot)$  is an increasing function, and the determinant of a scalar is equal to itself, we have that

$$\log|1 + c^{\mathsf{T}} H_X^{\mathsf{T}} \Sigma_{X|M}^{-1} H_X c| < \log|1 + c^{\mathsf{T}} H_Y^{\mathsf{T}} \Sigma_{Y|M}^{-1} H_Y c| \tag{81}$$

$$\Rightarrow \log|I + \Sigma_{X|M}^{-1} H_X cc^{\mathsf{T}} H_X^{\mathsf{T}}| < \log|I + \Sigma_{Y|M}^{-1} H_Y cc^{\mathsf{T}} H_Y^{\mathsf{T}}|$$

$$\tag{82}$$

Now, since  $cc^{\mathsf{T}} \succcurlyeq 0$ , it is a valid covariance matrix. So if we set  $\Sigma_M := cc^{\mathsf{T}}$ , we get

$$I(M;X) = \log|I + \Sigma_{X|M}^{-1} H_X \Sigma_M H_X^{\mathsf{T}}|$$
(83)

$$<\log|I + \Sigma_{Y|M}^{-1} H_Y \Sigma_M H_Y^{\mathsf{T}}| \tag{84}$$

$$=I(M;Y). (85)$$

However, this contradicts (74), which holds no matter what  $\Sigma_M$  is. Therefore, we must have  $H_X^\mathsf{T} \Sigma_{X|M}^{-1} H_X \succcurlyeq H_Y^\mathsf{T} \Sigma_{Y|M}^{-1} H_Y$ .  $\square$ 

#### C. Explanation of Footnote 5

In footnote 5, we noted that Barrett's result applied to all PIDs satisfying Assumption (\*) from Bertschinger et al. [3], which states:

$$UI(M: X \setminus Y)$$
 is a function of only  $P_M, P_{X|M}$  and  $P_{Y|M}$  (\*)

In other words, Barrett's main result showed that for jointly Gaussian  $P_{MXY}$  with scalar M, all PIDs that satisfied the above Assumption (\*) reduced to the MMI-PID. However, we show a seemingly different result: Theorem 2 states that for fully multivariate Gaussian  $P_{MXY}$  satisfying equation (12), all *Blackwellian* PIDs reduce to the MMI-PID.

In fact, PIDs that satisfy Assumption (\*) and PIDs that are Blackwellian form two distinct and unrelated sets. All Blackwellian PIDs need not satisfy Assumption (\*), and all PIDs that satisfy Assumption (\*) need not be Blackwellian.

However, by virtue of how it is defined, UI upper bounds all PIDs that satisfy Assumption (\*) (see [3, Lem. 3]). Thus, if  $UI^{(*)}$  is an arbitrary PID that satisfies Assumption (\*), then whenever  $\widetilde{UI}_X$  goes to zero,  $UI_X^{(*)}$  must also go to zero. But, by definition, all Blackwellian PIDs have  $UI_X$  going to zero if and only if  $Y \succcurlyeq_M X$ , and thus they all have  $UI_X$  going to zero together. Since  $\widetilde{UI}$  is Blackwellian,  $\widetilde{UI}$  goes to zero if and only if all other Blackwellian PIDs go to zero too. If  $UI^{\mathrm{Bw}}$  is an arbitrary Blackwellian PID, then we can summarize these relationships as:

$$UI_X^{\text{Bw}} = 0 \quad \Leftrightarrow \quad \widetilde{U}I_X = 0 \quad \Rightarrow \quad UI_X^{(*)} = 0$$
 (86)

Therefore, our extension of Barrett's result (Corollary 3) can also be stated for PIDs satisfying Assumption (\*) rather than Blackwellian PIDs. However, while Theorem 2 can also be written (for jointly Gaussian  $P_{MXY}$ ) as

$$UI_Y^{\text{Bw}} = 0 \quad \Leftrightarrow \quad H_X^{\mathsf{T}} \Sigma_{X|M}^{-1} H_X \succcurlyeq H_Y^{\mathsf{T}} \Sigma_{Y|M}^{-1} H_Y, \tag{87}$$

we cannot write the same with  $UI_Y^{(*)}=0$ , since the backward implication ( $\Leftarrow$ ) would not always hold.

#### APPENDIX C

#### JUSTIFICATION FOR OUR CONVEX APPROXIMATION FORMULATION

First, recall the expression for Gaussian deficiency from equation (17), which we are trying to approximate through a convex objective:

$$\delta_G(M:Y\backslash X) = \inf_{T,\Sigma_T \succeq 0} \frac{1}{2} \left[ \mathbb{E}_{P_M} \left[ \left\| (TH_X - H_Y)M \right\|_{\Sigma_T + TT^{\mathsf{T}}}^2 \right] + \operatorname{Tr} \left\{ (\Sigma_T + TT^{\mathsf{T}})^{-1} \right\} + \log |\Sigma_T + TT^{\mathsf{T}}| - d_Y \right]$$

$$(88)$$

As stated in the main text, the derivation of our proposed convex approximation has three main steps:

- 1) First, we obtain a condition on  $\Sigma_T$  (in terms of T), which is locally optimal. This condition allows us to reduce the optimization problem from two variables ( $\Sigma_T$  and T) to just one (T alone). This step is *exact*, and is shown in Proposition 8.
- 2) Next, we reinterpret and approximate the objective to significantly simplify its functional form, while attempting to minimize the same entities. This objective is designed to specifically to ensure that the approximate deficiency recovers the true Gaussian deficiency at its extremal values (i.e. when  $\delta_G$  is equal to zero, or equal to the mutual information).

3) Lastly, as part of reducing the optimization problem to a single variable, the constraint  $\Sigma_T \succcurlyeq 0$  is now replaced by a positive semidefiniteness constraint in terms of T. We approximate and simplify this constraint to make it more amenable for a convex program to handle.

We first state Proposition 8, which encapsulates segments of the simplification process that are *exact*. The parts of the simplification that actually constitute approximations are described immediately afterward.

**Proposition 8.** The Gaussian deficiency, as given by equation (88), finds a local minimum at

$$\Sigma_T = I - TT^\mathsf{T} + (H_Y - TH_X)\Sigma_M (H_Y - TH_X)^\mathsf{T}. \tag{89}$$

Substituting this expression back into the optimization problem significantly simplifies the expression for the Gaussian deficiency:

$$\delta_G(M:Y\backslash X) = \inf_T \log |I + (H_Y - TH_X)\Sigma_M (H_Y - TH_X)^\mathsf{T}|$$
s.t.  $I - TT^\mathsf{T} + (H_Y - TH_X)\Sigma_M (H_Y - TH_X)^\mathsf{T} \succcurlyeq 0$ 

$$(90)$$

*Proof.* The expression in equation (88) can be simplified into a more manageable form, starting with the expectation:

$$\mathbb{E}_{P_M} \left[ \left\| (H_Y - TH_X) M \right\|_{\Sigma_T + TT^{\mathsf{T}}}^2 \right]$$

$$\stackrel{(a)}{=} \mathbb{E}_{P_M} \left[ M^{\mathsf{T}} (H_Y - TH_X)^{\mathsf{T}} (\Sigma_T + TT^{\mathsf{T}})^{-1} (H_Y - TH_X) M \right]$$
(91)

$$\stackrel{(b)}{=} \mathbb{E}_{P_M} \left[ \text{Tr} \left\{ M^\mathsf{T} (H_Y - TH_X)^\mathsf{T} (\Sigma_T + TT^\mathsf{T})^{-1} (H_Y - TH_X) M \right\} \right]$$
(92)

$$\stackrel{(c)}{=} \mathbb{E}_{P_M} \left[ \text{Tr} \left\{ (\Sigma_T + TT^\mathsf{T})^{-1} (H_Y - TH_X) M M^\mathsf{T} (H_Y - TH_X)^\mathsf{T} \right\} \right]$$
(93)

$$\stackrel{(d)}{=} \operatorname{Tr} \left\{ (\Sigma_T + TT^{\mathsf{T}})^{-1} (H_Y - TH_X) \mathbb{E}_{P_M} [MM^{\mathsf{T}}] (H_Y - TH_X)^{\mathsf{T}} \right\}$$
(94)

$$\stackrel{(e)}{=} \operatorname{Tr} \left\{ (\Sigma_T + TT^{\mathsf{T}})^{-1} (H_Y - TH_X) \Sigma_M (H_Y - TH_X)^{\mathsf{T}} \right\}, \tag{95}$$

where in (a), we have simply expanded the Mahalanobis norm; in (b), we have used the fact that a scalar is equal to the trace of itself; in (c), we have relied on the property that the trace is invariant under cyclic permutations; in (d), we have moved the expectation inside, which is possible since all these operations are linear; and finally in (e), we have equated  $\mathbb{E}[MM^T]$  to  $\Sigma_M$ .

Now that we have resolved the expectation, we can substitute this expression back into (88), and simplify the expression further:

$$\delta_G(M:Y\backslash X) = \inf_{T,\Sigma_T \geq 0} \frac{1}{2} \left[ \operatorname{Tr} \left\{ (\Sigma_T + TT^\mathsf{T})^{-1} (H_Y - TH_X) \Sigma_M (H_Y - TH_X)^\mathsf{T} \right\} + \operatorname{Tr} \left\{ (\Sigma_T + TT^\mathsf{T})^{-1} \right\} + \log |\Sigma_T + TT^\mathsf{T}| - d_Y \right]$$

$$(96)$$

$$= \inf_{T, \Sigma_T \succeq 0} \frac{1}{2} \left[ \operatorname{Tr} \left\{ (\Sigma_T + TT^{\mathsf{T}})^{-1} \left( I + (H_Y - TH_X) \Sigma_M (H_Y - TH_X)^{\mathsf{T}} \right) \right\} - d_Y + \log |\Sigma_T + TT^{\mathsf{T}}| \right]$$

$$(97)$$

From this, it might already be intuitively apparent that we would like

$$(\Sigma_T + TT^{\mathsf{T}})^{-1} (I + (H_Y - TH_X)\Sigma_M (H_Y - TH_X)^{\mathsf{T}}) = I$$
(98)

$$\Rightarrow \quad \Sigma_T = I - TT^{\mathsf{T}} + (H_Y - TH_X)\Sigma_M (H_Y - TH_X)^{\mathsf{T}},\tag{99}$$

since this would allow the trace term to perfectly cancel  $d_Y$  in (97) (as the matrix within the trace has dimension  $d_Y \times d_Y$ ). However, it is possible to show that (99) in fact gives a local optimum for  $\Sigma_T$ . This can be done by examining the partial derivative of the objective in (97) with respect to  $\Sigma_T$ , which is what we proceed to do next.

First, we lay out the following identities for matrices A and B (refer, for instance, Petersen and Pedersen [31, Sec. 2]):

$$\partial(AB) = (\partial A)B + A(\partial B) \qquad \partial \operatorname{Tr}\{A\} = \operatorname{Tr}\{\partial A\} 
\partial(A^{-1}) = -A^{-1}(\partial A)A^{-1} \qquad \partial(\log \det A) = \operatorname{Tr}\{A^{-1}\partial A\}$$
(100)

Using these identities, we can write out the partial derivative of the objective in (97) with respect to  $\Sigma_T$ , and equate it to zero:

$$0 = \frac{1}{2} \operatorname{Tr} \left\{ \frac{\partial}{\partial \Sigma_T} (\Sigma_T + TT^\mathsf{T})^{-1} \cdot \left( I + (H_Y - TH_X) \Sigma_M (H_Y - TH_X)^\mathsf{T} \right) \right\}$$

$$+ \frac{1}{2} \frac{\partial}{\partial \Sigma_T} \log \det(\Sigma_T + TT^\mathsf{T})$$
(101)

$$\Rightarrow 0 = \operatorname{Tr}\left\{-(\Sigma_T + TT^{\mathsf{T}})^{-2} \cdot \left(I + (H_Y - TH_X)\Sigma_M (H_Y - TH_X)^{\mathsf{T}}\right)\right\} + \operatorname{Tr}\left\{(\Sigma_T + TT^{\mathsf{T}})^{-1}\right\}$$

$$(102)$$

$$\Rightarrow 0 = \text{Tr}\Big\{ (\Sigma_T + TT^{\mathsf{T}})^{-1} \Big[ I - (\Sigma_T + TT^{\mathsf{T}})^{-1} \big( I + (H_Y - TH_X) \Sigma_M (H_Y - TH_X)^{\mathsf{T}} \big) \Big] \Big\}$$
 (103)

A sufficient condition for the above equation to hold is that the matrix within the trace itself goes to zero. Therefore, (103) is satisfied when

$$(\Sigma_T + TT^{\mathsf{T}})^{-1} \Big[ I - (\Sigma_T + TT^{\mathsf{T}})^{-1} \Big( I + (H_Y - TH_X) \Sigma_M (H_Y - TH_X)^{\mathsf{T}} \Big) \Big] = 0$$
 (104)

$$\Rightarrow I - (\Sigma_T + TT^{\mathsf{T}})^{-1} (I + (H_Y - TH_X)\Sigma_M (H_Y - TH_X)^{\mathsf{T}}) = 0$$
 (105)

$$\Rightarrow \qquad (\Sigma_T + TT^{\mathsf{T}})^{-1} \left( I + (H_Y - TH_X) \Sigma_M (H_Y - TH_X)^{\mathsf{T}} \right) = I \tag{106}$$

In other words, we have that

$$\Sigma_T + TT^{\mathsf{T}} = I + (H_Y - TH_X)\Sigma_M (H_Y - TH_X)^{\mathsf{T}}$$
(107)

$$\Rightarrow \qquad \Sigma_T = I - TT^\mathsf{T} + (H_Y - TH_X)\Sigma_M (H_Y - TH_X)^\mathsf{T} \tag{108}$$

Finally, we can substitute this expression back into the objective in (97) to cancel the  $Tr\{\cdot\}$  and  $d_Y$  terms, leaving only the  $\log|\cdot|$  term:

$$\delta_G(M:Y\backslash X) = \inf_T \log |\Sigma_T + TT^\mathsf{T}|$$
s.t.  $I - TT^\mathsf{T} + (H_Y - TH_X)\Sigma_M (H_Y - TH_X)^\mathsf{T} \succcurlyeq 0$  (109)

Substituting for the  $\Sigma_T$  within the  $\log |\cdot|$  yields the desired expression from the statement of the proposition.

This concludes the first step of simplifying our optimization problem, which reduces the problem to an optimization over a single variable, and which is exact. Next, we proceed to approximate the terms in this simplified formulation.

First, note that the objective seeks to minimize the log-determinant of  $I + (H_Y - TH_X)\Sigma_M(H_Y - TH_X)^T$ . This term would naturally become smaller if  $H_Y$  is made closer to  $TH_X$ . To simplify this objective, we instead look at minimizing

$$\mathbb{E}_{P_M} \left[ \left\| (H_Y - TH_X) M \right\|_{\Sigma_T + TT^{\mathsf{T}}}^2 \right], \tag{110}$$

which appears in the original optimization problem. However, to avoid having the Mahalanobis norm being taken against  $\Sigma_T + TT^\mathsf{T}$ , which depends on T and yields a non-trivial objective function, we instead minimize:

$$\mathbb{E}_{P_M} \left[ \left\| (H_Y - TH_X) M \right\|_{I + H_Y \Sigma_M H_Y^{\mathsf{T}}}^2 \right]. \tag{111}$$

This objective function is chosen such that (110) and (111) will be equivalent "at the extremes," i.e. when the deficiency is zero  $(H_Y - TH_X = 0)$  and when then deficiency is the mutual information (T = 0). This choice also enables the proof of Proposition 4 (see Appendix E), which guarantees that when the true deficiency equals zero or the mutual information, the approximation yields the true deficiency. We use this revised objective to estimate the optimal argument  $\hat{T}$ . To compute the approximate Gaussian deficiency, we substitute this value of  $\hat{T}$  back into the formula for the Gaussian deficiency, given by (17).

Finally, to arrive at the estimate of  $\widehat{\Sigma}_T$  we employ in our approximation, given in equation (19), we assume that  $H_Y - TH_X$  is small in one part of the equation:

$$\Sigma_T = I - TT^\mathsf{T} + (H_Y - TH_X)\Sigma_M(H_Y - TH_X)^\mathsf{T}$$
(112)

$$= I - TT^{\mathsf{T}} + H_Y \Sigma_M H_Y^{\mathsf{T}} - H_Y \Sigma_M H_X^{\mathsf{T}} T^{\mathsf{T}} - TH_X \Sigma_M H_Y^{\mathsf{T}} + TH_X \Sigma_M H_X^{\mathsf{T}} T^{\mathsf{T}}$$
(113)

$$\approx I - TT^{\mathsf{T}} + H_Y \Sigma_M H_Y^{\mathsf{T}} - TH_X \Sigma_M H_X^{\mathsf{T}} T^{\mathsf{T}} - TH_X \Sigma_M H_X^{\mathsf{T}} T^{\mathsf{T}} + TH_X \Sigma_M H_X^{\mathsf{T}} T^{\mathsf{T}}$$
(114)

$$= I - TT^{\mathsf{T}} + H_Y \Sigma_M H_Y^{\mathsf{T}} - TH_X \Sigma_M H_X^{\mathsf{T}} T^{\mathsf{T}}$$
(115)

$$= I + H_Y \Sigma_M H_Y^\mathsf{T} - T (I + H_X \Sigma_M H_X^\mathsf{T}) T^\mathsf{T}$$
(116)

where the approximation occurs in (114) for the two terms that are linear in T. Since  $\Sigma_T \succcurlyeq 0$  becomes a constraint in our eventual optimization problem, this approximation significantly simplifies the constraint: firstly, it removes the linear terms making this a pure quadratic form; secondly, the matrix appearing in the quadratic atom,  $I + H_X \Sigma_M H_X^\mathsf{T}$ , is now guaranteed to be invertible. Prior to the approximation, the same matrix was  $I - H_X \Sigma_M H_X^\mathsf{T}$ , which did not have the same guarantee. These simplifications enable using the Schur complement in formulating our constrained optimization problem, as detailed in Appendix  $\mathsf{F}$ .

### APPENDIX D THE APPROXIMATE DEFICIENCY IS WELL DEFINED

**Lemma 9.** For jointly Gaussian random vectors M, X and Y satisfying the assumption in Remark 3,  $\widehat{T}$  and  $\widehat{\Sigma}_T$  as defined by (19) and (18) yield an approximate deficiency  $\widehat{\delta}_G(M:Y\backslash X)$  that is well defined, i.e. the covariance matrix  $\widehat{\Sigma}_T + \widehat{T}\widehat{T}^T$  for the composite channel  $P_{Y'\mid X}\circ P_{X\mid M}$  is invertible.

*Proof.* We know that  $\widehat{\Sigma}_T \succcurlyeq 0$  by virtue of the constraint in (18) and thus  $\widehat{\Sigma}_T + \widehat{T}\widehat{T}^\mathsf{T} \succcurlyeq 0$  as well. For ease of notation, let  $A \coloneqq H_Y \Sigma_M H_Y^\mathsf{T}$  and  $B \coloneqq H_X \Sigma_M H_X^\mathsf{T}$ . Assume for a contradiction that  $\widehat{\Sigma}_T + \widehat{T}\widehat{T}^\mathsf{T}$  is rank deficient. This implies that there exists a vector  $v \ne \mathbf{0}$  such that:

$$v^{\mathsf{T}}(\widehat{\Sigma}_{T} + \widehat{T}\widehat{T}^{\mathsf{T}})v = v^{\mathsf{T}}(I + A - \widehat{T}B\widehat{T}^{\mathsf{T}})v = 0$$

$$\Rightarrow v^{\mathsf{T}}(I + A)v = v^{\mathsf{T}}(\widehat{T}B\widehat{T}^{\mathsf{T}})v$$

$$\stackrel{(a)}{\Rightarrow} (\widehat{T}^{\mathsf{T}}v)^{\mathsf{T}}B(\widehat{T}^{\mathsf{T}}v) > 0$$

$$\Rightarrow \widehat{T}^{\mathsf{T}}v \neq \mathbf{0}$$

where (a) follows from  $A = (H_Y \Sigma_M^{-\frac{1}{2}})(H_Y \Sigma_M^{-\frac{1}{2}})^{\mathsf{T}} \Rightarrow A \geq 0$ . But since  $\widehat{\Sigma}_T \geq 0$ , we have:

$$v^{\mathsf{T}}\widehat{\Sigma}_{T}v \geq 0$$

$$\Rightarrow v^{\mathsf{T}}(\widehat{\Sigma}_{T} + \widehat{T}\widehat{T}^{\mathsf{T}})v - v^{\mathsf{T}}(\widehat{T}\widehat{T}^{\mathsf{T}})v \geq 0$$

$$\Rightarrow v^{\mathsf{T}}\widehat{T}\widehat{T}^{\mathsf{T}}v = \|\widehat{T}^{\mathsf{T}}v\|_{2}^{2} \leq 0.$$

which is a contradiction since  $\widehat{T}^{\mathsf{T}}v \neq \mathbf{0} \Rightarrow \|\widehat{T}^{\mathsf{T}}v\|_2^2 > 0$ .

### APPENDIX E PROOF OF PROPOSITION 4

Proof of Proposition 4. For ease of notation, we omit the function arguments  $(M:Y\setminus X)$  and refer simply to  $\widehat{\delta}_G$ ,  $\delta_G$ , and  $\delta$ .  $(\delta=0\Rightarrow\widehat{\delta}_G=0)$  It was shown by Torgersen [24, Theorem 8.2.13] that  $\delta=0\Rightarrow\delta_G=0$ , thus it suffices to show that  $\delta_G=0\Rightarrow\widehat{\delta}_G=0$ . When  $\delta_G$  is well-defined, we know that  $\Sigma_T+TT^{\mathsf{T}}\succcurlyeq 0$  is invertible and thus  $\Sigma_T+TT^{\mathsf{T}},(\Sigma_T+TT^{\mathsf{T}})^{-1}\succ 0$ . This implies that the first term of (17) is greater than zero unless  $(TH_X-H_Y)M=0$ . Thus  $\delta_G=0$  implies that  $(TH_X-H_Y)M=0$  almost everywhere in M, i.e. that there exists a  $T^*$  such that  $T^*H_X=H_Y$ . Thus, we also know that the objective function in (18) is minimized by  $T=T^*$ . To show that  $T^*$  is in the feasible set, we note that  $\delta_G=0$  implies that there exists a  $\Sigma_T^*\succcurlyeq 0$  such that  $\Sigma_T^*+T^*T^*=I\Rightarrow I-T^*T^*T^*\succcurlyeq 0$ . As such, when  $T=T^*$  we have that  $\Sigma_T=I+H_Y\Sigma_MH_Y^\mathsf{T}-T^*(I+H_X\Sigma_MH_X^\mathsf{T})T^{*\mathsf{T}}=I-T^*T^{*\mathsf{T}}=\Sigma_T^*$ .

 $(\delta=0 \Leftarrow \widehat{\delta}_G=0)$  This follows from  $\widehat{\delta}_G \geq \delta \geq 0$ .

 $(\delta = I(M;Y) \Rightarrow \widehat{\delta}_G = I(M;Y))$  Note that if  $\widehat{T} = \mathbf{0}$ , we have

$$\widehat{\Sigma}_{T} = I + H_{Y} \Sigma_{M} H_{Y}^{\mathsf{T}} 
\Rightarrow \widehat{P}_{Y'|X} \circ P_{X|M} = P_{Y} 
\Rightarrow \widehat{\delta}_{G} = I(M; Y).$$
(117)

As such, it suffices to show that  $\delta = I(M;Y)$  implies that the objective function in (18) is minimized at T = 0. Suppose for a contradiction that there exists a  $\widetilde{T}$  such that:

$$\mathbb{E}_{P_M} \left[ \| (\widetilde{T}H_X - H_Y)M \|_A^2 \right] < \mathbb{E}_{P_M} \left[ \| H_Y M \|_A^2 \right]$$
 (118)

with  $A := I + H_Y \Sigma_M H_Y^\mathsf{T}$  giving the marginal covariance matrix for Y (i.e.  $P_Y = \mathcal{N}(\mathbf{0}, A)$ ). This implies that

$$\mathbb{E}_{P_M} \left[ \| (\lambda \widetilde{T} H_X - H_Y) M \|_A^2 \right] < \mathbb{E}_{P_M} \left[ \| H_Y M \|_A^2 \right]$$
(119)

for any  $\lambda \in (0,1)$ . The implication follows from the convexity of the Mahalanobis distance, noting that  $\lambda \widetilde{T} = \lambda \widetilde{T} + (1-\lambda)\mathbf{0}$ . In other words, we can keep making  $\widetilde{T}$  "smaller" (by multiplying it by smaller values of  $\lambda$ ), until  $\widetilde{\Sigma}_T \coloneqq A - \widetilde{T}\widetilde{T}^\mathsf{T}$  is PSD, while still making sure that (118) holds. Defining  $\widetilde{P}_{Y'|X} \coloneqq \mathcal{N}(\widetilde{T}X,\widetilde{\Sigma}_T)$ , we note that  $\widetilde{P}_{Y'|X} \circ P_{X|M} = \mathcal{N}(\widetilde{T}H_XM,A)$ . As such:

$$\mathbb{E}_{P_{M}} \left[ D(P_{Y|M} \| \widetilde{P}_{Y'|X} \circ P_{X|M}) \right] - I(M;Y)$$

$$= \mathbb{E}_{P_{M}} \left[ D(P_{Y|M} \| \widetilde{P}_{Y'|X} \circ P_{X|M}) - D(P_{Y|M} \| P_{Y}) \right]$$

$$= \mathbb{E}_{P_{M}} \left[ \| (\widetilde{T}H_{X} - H_{Y})M \|_{A}^{2} \right] - \mathbb{E}_{P_{M}} \left[ \| H_{Y}M \|_{A}^{2} \right] < 0.$$

But since  $\widetilde{P}_{Y'\mid X}\in\mathcal{C}_G(Y\mid X)$ , we have:

$$\delta_G \le \mathbb{E}_{P_M} \left[ D(P_{Y|M} \| \widetilde{P}_{Y'|X} \circ P_{X|M}) \right] < I(M;Y) \le \delta, \tag{120}$$

which is a contradiction.

### APPENDIX F IMPLEMENTATION DETAILS

We briefly discuss how to reformulate the optimization problem in (18) such that it satisfies the disciplined convex programming (DCP) rules and can be solved using the CVXPY software package [33, 34]. First we note that the objective function can be rewritten using the trace trick. Letting  $A = I + H_Y \Sigma_M H_Y^{\mathsf{T}}$  for ease of notation:

$$\mathbb{E}_{P_{M}} \left[ \| (TH_{X} - H_{Y})M \|_{A}^{2} \right]$$

$$= \mathbb{E}_{P_{M}} \left[ M^{\mathsf{T}} (TH_{X} - H_{Y})^{\mathsf{T}} A^{-1} (TH_{X} - H_{Y})M \right]$$

$$= \mathbb{E}_{P_{M}} \left[ \operatorname{Tr} \left( M^{\mathsf{T}} (TH_{X} - H_{Y})^{\mathsf{T}} A^{-1} (TH_{X} - H_{Y})M \right) \right]$$

$$= \mathbb{E}_{P_{M}} \left[ \operatorname{Tr} \left( MM^{\mathsf{T}} (TH_{X} - H_{Y})^{\mathsf{T}} A^{-1} (TH_{X} - H_{Y}) \right) \right]$$

$$= \operatorname{Tr} \left( \Sigma_{M} (TH_{X} - H_{Y})^{\mathsf{T}} A^{-1} (TH_{X} - H_{Y}) \right)$$

$$= \| A^{-\frac{1}{2}} TH_{X} \Sigma_{M}^{\frac{1}{2}} - A^{-\frac{1}{2}} H_{Y} \Sigma_{M}^{\frac{1}{2}} \|_{F}^{2}$$

where  $\|\cdot\|_F^2$  is the squared Frobenius norm. Next, the constraint can be rewritten using the Schur complement [35]:

$$I + H_{Y} \Sigma_{M} H_{Y}^{\mathsf{T}} - T (I + H_{X} \Sigma_{M} H_{X}^{\mathsf{T}}) T^{\mathsf{T}} \geq 0$$

$$\updownarrow$$

$$\begin{bmatrix} I + H_{Y} \Sigma_{M} H_{Y}^{\mathsf{T}} & T \\ T^{\mathsf{T}} & (I + H_{X} \Sigma_{M} H_{X}^{\mathsf{T}})^{-1} \end{bmatrix} \geq 0$$

Combining the two, we obtain the problem in a form that can solved directly by CVX:

$$\widehat{T} = \underset{T}{\operatorname{argmin}} \quad \|A^{-\frac{1}{2}}TH_{X}\Sigma_{M}^{\frac{1}{2}} - A^{-\frac{1}{2}}H_{Y}\Sigma_{M}^{\frac{1}{2}}\|_{F}^{2}$$
s.t.
$$\begin{bmatrix} I + H_{Y}\Sigma_{M}H_{Y}^{\mathsf{T}} & T \\ T^{\mathsf{T}} & (I + H_{X}\Sigma_{M}H_{X}^{\mathsf{T}})^{-1} \end{bmatrix} \succcurlyeq 0$$
(121)

We solved the problem used the splitting conic solver (SCS) [36, 37] with relaxation parameter 1, maximum iteration number 5000, and convergence tolerance of 1e-10. The maximum iteration number and convergence tolerance were chosen to be conservatively large and small, respectively, as we found lower and higher values of these parameters to yield inferior results (i.e. larger estimated deficiencies) and computational time was not an issue. Due to issues of numerical imprecision, the estimated  $\widehat{\Sigma}_T$  was occasionally found to have very small negative eigenvalues (i.e. greater than -1e-6). To ensure that the estimated  $\widehat{\Sigma}_T$  was positive semidefinite, we replaced all negative eigenvalues with zero.

### $\begin{array}{c} \text{Appendix G} \\ \text{Step-By-Step Experimental Procedure} \end{array}$

Here, we describe the procedure used to generate the plots in Figure 1.

- 1) Sample  $d_M$ ,  $d_X$ ,  $d_Y$  according one of (S1)–(S4).
- 2) Sample a covariance matrix  $\Sigma \in \mathbb{R}^{d \times d}$  (where  $d = d_M + d_X + d_Y$ ) from a standard Wishart distribution.
- 3) Compute I(M; (X, Y)), I(M; X), and I(M; Y).
- 4) Compute conditional mean and covariances and whiten to obtain  $H_X$ ,  $H_Y$ , and  $\Sigma_{X|M} = \Sigma_{Y|M} = I$ .
- 5) Estimate the deficiencies  $\hat{\delta}_G(M:Y\setminus X)$  and  $\hat{\delta}_G(M:X\setminus Y)$ , using the Python CVX package to solve (121).
- 6) Compute the approximate  $\delta$ -PID atoms.
- 7) Check if  $\widehat{RI}$  and  $\widehat{SI}$  are non-negative.
- 8) If  $d_M = 1$ , check if either  $\widehat{UI}_X \approx 0$  or  $\widehat{UI}_Y \approx 0$ .

#### APPENDIX H

### Details of the Simulation Comparing the $\sim$ -PID and the $\widehat{\delta}_G$ -PID

#### A. Simulation setup

The results shown in Figure 2 are for a multivariate Poisson distribution, which is defined below. We used a small number of dimensions ( $d_M = 2$  and  $d_X = d_Y = 1$ ) in order to allow for computational tractability of the discrete  $\sim$ -PID estimator of Banerjee et al. [23].

We took  $M_i \sim \text{i.i.d.}$  Poisson $(\lambda = 2)$ , for both components of M (i.e, i = 1, 2). We took  $X = X_1 + X_2 + N_X$ , where  $X_i \sim \text{Binomial}(M_i, w_i^X)$  for some "weight"  $w_i^X$ , and  $N_X \sim \text{Poisson}(\lambda_X = 1)$ . Y was defined in the same way as X, with  $Y_i$ ,  $N_Y$ ,  $X_i$  and  $N_X$  all being independent of each other. The results shown in Figure 2 are for  $w_1^Y = w_2^Y = w_2^X = 0.5$ , while  $w_1^X$  is varied between 0.0 and 1.0 in increments of 0.1 on the x-axis.

The discrete  $\sim$ -PID was estimated by truncating the Poisson distributions, while ensuring >95% of probability was captured. For computing the  $\hat{\delta}_G$ -PID, the Poisson distribution was approximated as a Gaussian distribution by considering the sample

covariance matrix, estimated from  $N=10^6$  data points. This was observed to produce a stable covariance estimate, following which channel parameters such as  $H_X$ ,  $\Sigma_{X|M}$ , etc. were extracted from the estimated covariance matrix. The convex optimization problem in the definition of  $\hat{\delta}_G$ -PID was solved using CVXPY (see Appendix F for details).

#### B. Results and Limitations

It should be noted that this experiment has several intrinsic limitations:

- The Poisson distributions had to be truncated for reasons of finiteness and computational tractability, before estimating the
   ∼-PID. As mentioned above, we endeavoured to ensure that the distribution was captured well, but the truncation could
   nevertheless skew the discrete-PID estimates.
- 2) The estimation of the sample covariance matrix used to compute the  $\hat{\delta}_G$ -PID could also contribute to error.
- 3) Lastly and most importantly, the two PIDs being considered are different, i.e., the  $\sim$ -PID for the Poisson distribution, and the  $\delta$ -PID for the Gaussian approximation. These PIDs likely produce slightly different values: the  $\delta$ -PID is closer in spirit to the PID of Harder et al. [4] (see [5] for an explanation), which was shown to have different values from the  $\sim$ -PID by Bertschinger et al. [3].

These limitations suggest that we have no way of truly knowing how accurate either of the two estimates are. However, their degree of agreement despite the use of completely different estimation techniques cannot be purely coincidental, and argues in favor of the practical applicability of our method. In particular, these results provide evidence suggesting that:

- 1) Our approximate PID is able to differentiate between cases of zero- and non-zero unique information.
- 2) Our proposed method matches expected trends for every one of the four PID quantities.
- 3) As a fraction of total mutual information, each PID value is reasonably close to its expected value, suggesting our method can be used to assess relative differences between PID quantities in different settings.

## APPENDIX I 3-DIMENSIONAL SIMPLEX VIEWS

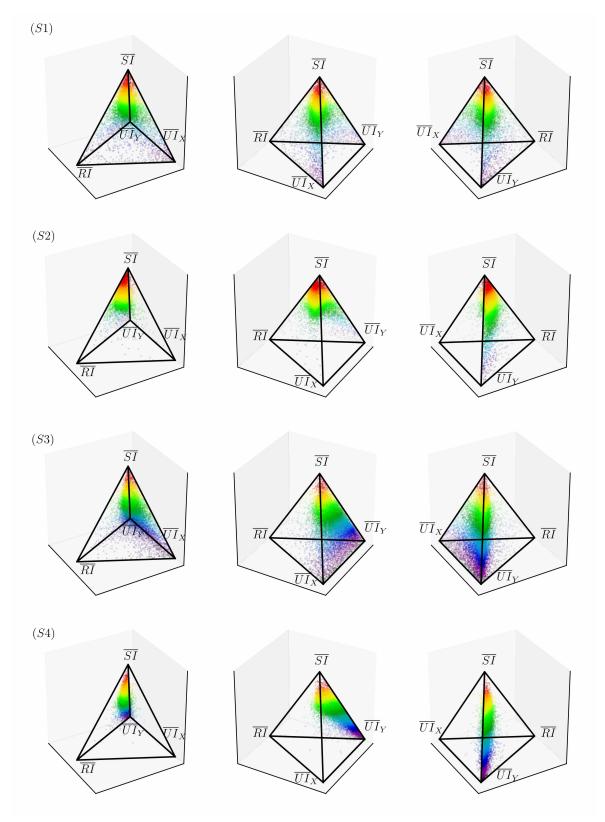


Fig. 3: Alternative views of Figure 1. Each row displays one of the four sampling schemes, and each column provides a rotated view of the simplex.