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► **To cite this version:**

Samir M. Perlaza, Xinying Zou. The Generalization Error of Machine Learning Algorithms. 2024. hal-04789606

HAL Id: hal-04789606

<https://inria.hal.science/hal-04789606v1>

Preprint submitted on 18 Nov 2024

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The Generalization Error of Machine Learning Algorithms

Samir M. Perlaza[Ⓛ] and Xinying Zou[Ⓛ]

Abstract—In this paper, the method of gaps, a technique for deriving closed-form expressions in terms of information measures for the generalization error of machine learning algorithms is introduced. The method relies on two central observations: (a) The generalization error is an average of the variation of the expected empirical risk with respect to changes on the probability measure (used for expectation); and (b) these variations, also referred to as gaps, exhibit closed-form expressions in terms of information measures. The expectation of the empirical risk can be either with respect to a measure on the models (with a fixed dataset) or with respect to a measure on the datasets (with a fixed model), which results in two variants of the method of gaps. The first variant, which focuses on the gaps of the expected empirical risk with respect to a measure on the models, appears to be the most general, as no assumptions are made on the distribution of the datasets. The second variant develops under the assumption that datasets are made of independent and identically distributed data points. All existing exact expressions for the generalization error of machine learning algorithms can be obtained with the proposed method. Also, this method allows obtaining numerous new exact expressions, which improves the understanding of the generalization error; establish connections with other areas in statistics, e.g., hypothesis testing; and potentially, might guide algorithm designs.

Index Terms—Supervised Learning, Worst-Case Data Generating Measure; Gibbs Algorithm, Generalization Error, and Sensitivity.

I. INTRODUCTION

The *generalization error* in statistical machine learning is the expectation (w.r.t. the joint probability distribution of datasets and models) of the difference between the population risk and the empirical risk [1]–[11]. The generalization error has become a key metric for assessing an algorithm’s performance and its ability to generalize beyond training data. Traditional approaches for analyzing the generalization error generally fall into two categories. The first category derives upper bounds on the generalization error based on properties of the hypothesis class, such as Rademacher complexity and VC dimension [12]–[16]. The second category examines the dependency between learning algorithms and data distributions through various information-theoretic metrics [17]–[25]. The initial exact characterizations of generalization error using

information measures were introduced for the Gibbs algorithm in [2] and further expanded in [26]. A more general result, which considers a σ -finite measure as the reference for the Gibbs algorithm, was presented in [9]. For learning algorithms beyond Gibbs, two main types of guarantees are provided under the information-theoretic framework. The first type is often referred to as *guarantees in probability*, which assert that with high probability over the probability measure of the datasets, the expected risk induced by the learning algorithm is bounded above by a certain threshold. This type of guarantees is referred to as PAC-Bayesian generalization bounds as in [27]–[33]. In parallel, *guarantees in expectation* provide bounds on the generalization error. To account for the dependence between the learning algorithm and the data distribution, mutual information is a common metric in these analyses. Such information measure was first introduced in [34] and later extended in [4]. Chaining techniques were incorporated in [20], [22] to derive upper bounds, with similar bounds appearing in [10], [35] and related studies. Alternative metrics such as Wasserstein distance [7], [18], [21], [25], maximal leakage [19], [36], mutual f -information [37], and Jensen-Shannon divergence [5] have also been used to derive generalization bounds. Comprehensive literature reviews of these guarantees can be found in [38] and, more recently, in [39]. Nonetheless, for any specific use, the tightness of many of these bounds cannot be guaranteed, as noted in [40] and [41]. Recently, exact characterizations of the generalization error, applicable to any statistical learning algorithm, were provided in [42] and [43]. These new expressions involve several information measures, e.g., relative entropy, mutual information and lautum information [44].

The present work is dedicated to deriving closed-form expressions for the generalization error of machine learning algorithms through the lens of information theory. The main contribution is a general method for such a purpose, which has been coined *the method of gaps*. Interestingly, all existing exact expressions for the generalization error of machine learning algorithms can be obtained with the proposed method.

A. Gaps and the Method of Gaps

In order to introduce the *method of gaps*, first the notion of *gap* is defined. A gap is the difference between two expectations of the empirical risk, each calculated using a different probability measure, both on the same measurable space. Hence, a gap can be understood as a measure of the variation of the expected empirical risk due to a change on the measure used to take such an expectation. The expectation of the empirical risk

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Parts of this work were submitted to The 39th Annual AAAI Conference on Artificial Intelligence, Philadelphia, Pennsylvania, 2025.

can be taken with respect to either (1) a probability measure over the set of models, keeping the dataset fixed; or (2) a probability measure over the set of datasets, keeping the model fixed. Variations in the first case are often called *algorithm-driven gaps*. This is because probability measures on the set of models correspond to different machine learning algorithms, meaning these variations reflect changes in the algorithm. Variations in the second case are known as *data-driven gaps*. These arise from changes in the probability measures over the datasets, which can be interpreted as changes in the statistical properties of the data. Certain algorithm-driven and data-driven gaps have been shown to have closed-form expressions in terms of relative entropies. The first closed-form expressions of an algorithm-driven gap were presented in [45, Theorem 1] to quantify the variation of the expected empirical risk due to a deviation from the Gibbs algorithm to an alternative algorithm. This foundational result serves as a key building block in this work for deriving closed-form expressions for algorithm-driven gaps due to transitions between arbitrary algorithms. See for instance, Theorem 37 in Section VII-D. The first-closed form expression for a data-driven gap due to a change from a worst-case data-generating (WCDG) probability measure to an arbitrary measure was presented in [46, Theorem 5.2]. This crucial result formed the basis for deriving the closed-form expressions for data-driven gaps due to changes from and to arbitrary probability measures in [42, Theorem 8]. In a nutshell, exact expressions for algorithm-driven gaps involve the Gibbs algorithm studied in [9], while exact expressions for data-driven gaps involve the WCDG probability measure introduced in [46]. In both cases, these expressions are surprisingly simple and flexible, as they contain free parameters that can be chosen subject to few constraints.

From this perspective, two variants of the method of gaps can be identified. The former, which is based on algorithm-driven gaps, involves two steps: (i) To express the generalization error as the expectation (with respect to a probability measure on the datasets) of a particular algorithm-driven gap (see Lemma 3 in Section IV-B); and (ii) To exploit the closed-form expressions for algorithm-driven gaps presented in Section VII-D to obtain expressions for the generalization error. The method of gaps via algorithm-driven gaps, was implicitly used to obtain the celebrated exact expression of the generalization error of the Gibbs algorithm in [9, Theorem 17]. Albeit no particular mention to a *method* is made therein, [9, Theorem 16] can be associated to *step one* of the method of gaps; and [9, Theorem 17] to *step two*. Unfortunately, the closed-form expressions for algorithm-driven gaps developed in [8], [9] are limited to transitions from the Gibbs algorithm to alternative algorithms. This limits such a theoretical framework to obtain exact expressions for the generalization error of arbitrary algorithms. Nonetheless, these findings are essential for obtaining the results presented in this work.

The second variant of the method of gaps, which is based on data-driven gaps consists also in two steps: (i) To express the generalization error as the expectation (with respect to a probability measure on the models) of a particular data-driven gap

(see [42, Equation (75)]); and (ii) To exploit the closed-form expressions for data-driven gaps presented in Section VIII to obtain expressions for the generalization error. This second variant was the method of proof used in [42] to obtain the first exact expression [42, Theorem 10] for the generalization error of arbitrary machine learning algorithms. Using the same method of proof, other closed-form expressions [43, Theorem 11 and Theorem 13] have been obtained. The expressions obtained via this second variant of the method of gaps are surprisingly flexible, as they depend on parameters that can be arbitrarily chosen subject to mild conditions. However, these expressions are developed under the assumption that datasets consist of data points that are independent and identically distributed. Interestingly, this assumption can be relaxed to identically distributed datapoints, but such a relaxation has not been explored in this work.

B. Contributions

The main contribution of this work consists in a novel method for developing closed-form expressions for the generalization error of machine learning algorithms. The technique features two distinct variants: One based on algorithm-driven gaps and another one based on data-driven gaps. While the variant based on data-driven gaps is established, having been used in [42], [46] and [43], the variant based on algorithm-driven gaps is original and yields innovative expressions for the generalization error. More importantly, this variant does not require the assumption that datasets are made of independent and identically distributed data points, which is the underlying assumption in the variant based on data-driven gaps.

Each variant of the method of gaps leads to different equivalent expressions for the generalization error of machine learning algorithms. Nonetheless, a common structure consisting of the addition of two terms can be identified. Independently of the variant, the first term, up to a constant factor, is either the mutual information or the lautum information between the models and the datasets. The second term is particular for each variant. Nonetheless, such terms appear to highlight some “geometric” duality between the two variants. From this perspective, another key contribution of this work is the establishment of parallels between the two variants of the method of gaps using simple connections to existing problems, for instance, mismatched hypothesis testing [47]. While these arguments illuminate interesting findings, many intriguing aspects of the expressions obtained with the method of gaps are left unexplored and open for future research.

C. Notation

Sets are denoted by calligraphic uppercase letters, except sets of probability measures. Given a set \mathcal{M} and a sigma-field \mathcal{F} on \mathcal{M} , the set of all probability measures that can be defined on the measurable space $(\mathcal{M}, \mathcal{F})$ is denoted by $\Delta(\mathcal{M}, \mathcal{F})$ or simply $\Delta(\mathcal{M})$, when the sigma-field is fixed in the analysis. If $\mathcal{M} \subseteq \mathbb{R}$, then the Borel sigma-field on \mathcal{M} is denoted by $\mathcal{B}(\mathcal{M})$. The subset of measures in $\Delta(\mathcal{M})$ that are absolutely continuous with a probability measure Q

is denoted by $\Delta_Q(\mathcal{M})$. Given a measure $P \in \Delta_Q(\mathcal{M})$, the Radon-Nikodym derivative of P with respect to Q is denoted by $\frac{dP}{dQ}$. Given a set \mathcal{N} , the set of all probability measures defined on $(\mathcal{M}, \mathcal{F})$ conditioned on an element of \mathcal{N} is denoted by $\Delta(\mathcal{M}|\mathcal{N})$. More specifically, given a measure $P_{M|N} \in \Delta(\mathcal{M}|\mathcal{N})$ and $n \in \mathcal{N}$, the measure $P_{M|N=n}$ is in $\Delta(\mathcal{M})$.

The *relative entropy* is defined below as the extension to σ -finite measures of the relative entropy usually defined for probability measures.

Definition 1 (Relative Entropy): Given two σ -finite measures P_1 and P_2 on the same measurable space, such that P_2 is absolutely continuous with respect to P_1 , the relative entropy of P_2 with respect to P_1 is

$$D(P_2||P_1) = \int \frac{dP_2}{dP_1}(x) \log\left(\frac{dP_2}{dP_1}(x)\right) dP_1(x), \quad (1)$$

where the function $\frac{dP_2}{dP_1}$ is the Radon-Nikodym derivative of P_2 with respect to P_1 .

Given a probability measure $P_N \in \Delta(\mathcal{N})$, the mutual information (see [48] and [49]) and lautum information (see [44]) induced by the measures $P_{M|N}$ and P_N are denoted respectively by

$$I(P_{M|N}; P_N) = \int D(P_{M|N=n}||P_M) dP_N(n), \quad \text{and} \quad (2)$$

$$L(P_{M|N}; P_N) = \int D(P_M||P_{M|N=n}) dP_N(n), \quad (3)$$

with $P_M \in \Delta(\mathcal{M})$ being the marginal measure induced by $P_{M|N}$ and P_N ; and $D(\cdot||\cdot)$ being the relative entropy in (1).

II. STATISTICAL SUPERVISED MACHINE LEARNING

Let \mathcal{M} , \mathcal{X} and \mathcal{Y} , with $\mathcal{M} \subseteq \mathbb{R}^d$, be sets of *models*, *patterns*, and *labels*, respectively. A pair $(x, y) \in \mathcal{X} \times \mathcal{Y}$ is referred to as a *labeled pattern* or as a *data point*. A training dataset $\mathbf{z} \in (\mathcal{X} \times \mathcal{Y})^n$ is a tuple of n data points of the form:

$$\mathbf{z} = ((x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)) \in (\mathcal{X} \times \mathcal{Y})^n. \quad (4)$$

Let the function $f : \mathcal{M} \times \mathcal{X} \rightarrow \mathcal{Y}$ be such that the label assigned to the pattern x according to the model $\theta \in \mathcal{M}$ is $f(\theta, x)$. The function $f(\theta, \cdot) : \mathcal{X} \rightarrow \mathcal{Y}$ might for instance represent a neural network whose weights are vectorized into θ . Let the function

$$\hat{\ell} : \mathcal{Y} \times \mathcal{Y} \rightarrow [0, +\infty], \quad (5)$$

be the risk or loss function. Such a function is often of the form $\hat{\ell}(\mu, \nu) = |\mu - \nu|^p$, with $p \geq 1$; or $\hat{\ell}(\mu, \nu) = \mathbb{1}_{\{\mu \neq \nu\}}$. In the following, the risk function $\hat{\ell}$ is assumed to be a nonnegative function and for all $y \in \mathcal{Y}$, $\hat{\ell}(y, y) = 0$.

In general, given a labelled pattern $(x, y) \in \mathcal{X} \times \mathcal{Y}$, the risk induced by a model $\theta \in \mathcal{M}$ is $\hat{\ell}(f(\theta, x), y)$. For the ease of notation, consider the function $\ell : \mathcal{X} \times \mathcal{Y} \times \mathcal{M} \rightarrow [0, +\infty]$ such that

$$\ell(x, y, \theta) = \hat{\ell}(f(\theta, x), y). \quad (6)$$

The problem of supervised machine learning boils down to devising an algorithm that takes as input a training dataset, as \mathbf{z} in (4), and outputs a model θ , with certain probability to satisfy some performance metric. The notion of *machine learning algorithm* is formally introduced hereunder.

Definition 2 (Algorithm): A conditional probability measure $P_{\Theta|\mathbf{Z}} \in \Delta(\mathcal{M}|(\mathcal{X} \times \mathcal{Y})^n)$ is said to represent a supervised machine learning algorithm.

Let $P_{\Theta|\mathbf{Z}} \in \Delta(\mathcal{M}|(\mathcal{X} \times \mathcal{Y})^n)$ be an algorithm. Hence, the instance of such an algorithm trained upon the dataset \mathbf{z} in (4) is denoted by $P_{\Theta|\mathbf{Z}=\mathbf{z}}$, which is simply a probability measure in $\Delta(\mathcal{M})$.

A central performance metric for a fixed model is the empirical risk it induces with respect to a given dataset. Such a metric is defined as follows.

Definition 3 (Empirical Risk): The *empirical risk* induced by a model $\theta \in \mathcal{M}$ with respect to the dataset \mathbf{z} in (4) is determined by the function $L : (\mathcal{X} \times \mathcal{Y})^n \times \mathcal{M} \rightarrow [0, +\infty]$, which satisfies

$$L(\mathbf{z}, \theta) = \frac{1}{n} \sum_{i=1}^n \ell(x_i, y_i, \theta). \quad (7)$$

The expectation of the empirical risk $L(\mathbf{z}, \theta)$ in (7) requires particular notations depending on whether such an expectation is with respect to a measure on the models or the datasets. More specifically, given a model θ , which is kept fixed, the expectation of $L(\mathbf{z}, \theta)$ under the assumption that the dataset \mathbf{z} is drawn from a probability measure $P \in \Delta((\mathcal{X} \times \mathcal{Y})^n)$ is denoted using the functional $R_\theta : \Delta((\mathcal{X} \times \mathcal{Y})^n) \rightarrow \mathbb{R}$, which satisfies

$$R_\theta(P) = \int L(\mathbf{z}, \theta) dP(\mathbf{z}). \quad (8)$$

Alternatively, given a dataset \mathbf{z} , which is kept fixed, the expectation of $L(\mathbf{z}, \theta)$ under the assumption that the model θ is drawn from a probability measure $P \in \Delta(\mathcal{M})$ is denoted using the functional $R_z : \Delta(\mathcal{M}) \rightarrow \mathbb{R}$, which satisfies

$$R_z(P) = \int L(\mathbf{z}, \theta) dP(\theta). \quad (9)$$

The following section introduces the generalization error. Later, it is shown that the generalization error of any machine learning algorithm can be characterized by studying the sensitivity of the functionals R_θ in (8) and R_z in (9).

III. GENERALIZATION ERROR

In a practical setting, the generalization capability of a machine learning algorithm is evaluated via *test datasets*, which are different to the *training dataset* [45].

In particular, given an algorithm $P_{\Theta|\mathbf{Z}} \in \Delta(\mathcal{M}|(\mathcal{X} \times \mathcal{Y})^n)$, a test dataset $\mathbf{u} \in (\mathcal{X} \times \mathcal{Y})^n$, and a training dataset $\mathbf{z} \in (\mathcal{X} \times \mathcal{Y})^n$, a typical evaluation of the generalization capability of the instance $P_{\Theta|\mathbf{Z}=\mathbf{z}}$ of such an algorithm consists in calculating the difference between the expected empirical risk

it induces on the test dataset \mathbf{u} and on the training dataset \mathbf{z} . That is, the difference

$$R_{\mathbf{u}}(P_{\Theta|Z=z}) - R_{\mathbf{z}}(P_{\Theta|Z=z}), \quad (10)$$

where the functionals $R_{\mathbf{u}}$ and $R_{\mathbf{z}}$ are both defined as in (9). In a nutshell, the evaluation consists in calculating the variation of the expected empirical risk induced by the algorithm $P_{\Theta|Z=z}$ with respect to a data set that changes from the training dataset \mathbf{z} to the test dataset \mathbf{u} . A small variation is interpreted as a good capability of the algorithm $P_{\Theta|Z}$ to generalize the training dataset \mathbf{z} into the test dataset \mathbf{u} . While the difference in (10) being smaller than certain threshold for certain test datasets is not a guarantee of good generalization into other test datasets, this is the most popular tool used by practitioners for evaluating machine learning algorithms. This is in part, because in most cases, test and training datasets are the only data actually available.

The analysis of the generalization capabilities of an algorithm $P_{\Theta|Z}$ can be deepened if further assumptions are adopted. For instance, it can be assumed that test and training datasets are both independently drawn from the same probability measure. This is indeed, one of the most popular assumptions, and the one adopted to define the *generalization error*. In a nutshell, the generalization error induced by an algorithm $P_{\Theta|Z}$ is the expectation of the variation in (10) under the assumption that both test and training datasets are independently sampled from the same probability measure in $\Delta((\mathcal{X} \times \mathcal{Y})^n)$.

Definition 4 (Generalization Error): The generalization error induced by the algorithm $P_{\Theta|Z} \in \Delta(\mathcal{M} | (\mathcal{X} \times \mathcal{Y})^n)$ under the assumption that training and test datasets are independently sampled from a probability measure $P_Z \in \Delta((\mathcal{X} \times \mathcal{Y})^n)$, which is denoted by $\overline{\overline{G}}(P_{\Theta|Z}, P_Z)$, is

$$\begin{aligned} & \overline{\overline{G}}(P_{\Theta|Z}, P_Z) \\ & \triangleq \int \int (R_{\mathbf{u}}(P_{\Theta|Z=z}) - R_{\mathbf{z}}(P_{\Theta|Z=z})) dP_Z(\mathbf{u}) dP_Z(\mathbf{z}). \end{aligned} \quad (11)$$

Often, the generalization error $\overline{\overline{G}}(P_{\Theta|Z}, P_Z)$ is defined as the expectation of the difference between the *population error* and the *empirical risk*. The population error, induced by a model $\theta \in \mathcal{M}$ under the assumption that datasets are drawn from the probability measure P_Z , is $R_{\theta}(P_Z)$, where the functional R_{θ} is defined in (8). Alternatively, the training error induced by the model θ with respect to a training dataset $\mathbf{z} \in (\mathcal{X} \times \mathcal{Y})^n$ is $L(\mathbf{z}, \theta)$, where the function L is defined in (7). Using these elements, the following lemma introduces an alternative expression for the generalization error $\overline{\overline{G}}(P_{\Theta|Z}, P_Z)$ in terms of the *population error* and the *empirical risk*, cf., [2, Equation 2] and [4, Equation 4].

Lemma 1: The generalization error $\overline{\overline{G}}(P_{\Theta|Z}, P_Z)$ in (11) satisfies

$$\begin{aligned} & \overline{\overline{G}}(P_{\Theta|Z}, P_Z) \\ & = \int \int (R_{\theta}(P_Z) - L(\mathbf{z}, \theta)) dP_{\Theta|Z=z}(\theta) dP_Z(\mathbf{z}), \end{aligned} \quad (12)$$

where the functional R_{θ} is defined in (8) and the function L is defined in (7).

Proof: The proof follows from (11) by observing the following equalities:

$$\begin{aligned} & \int \int R_{\mathbf{u}}(P_{\Theta|Z=z}) dP_Z(\mathbf{u}) dP_Z(\mathbf{z}) \\ & = \int \int \int L(\mathbf{u}, \theta) dP_{\Theta|Z=z}(\theta) dP_Z(\mathbf{u}) dP_Z(\mathbf{z}) \end{aligned} \quad (13)$$

$$= \int \int \left(\int L(\mathbf{u}, \theta) dP_Z(\mathbf{u}) \right) dP_{\Theta|Z=z}(\theta) dP_Z(\mathbf{z}) \quad (14)$$

$$= \int \int R_{\theta}(P_Z) dP_{\Theta|Z=z}(\theta) dP_Z(\mathbf{z}), \quad (15)$$

where the equality in (13) follows from (9); the equality in (14) follows from [50, Theorem 2.6.6]; and the equality in (15) follows from (8). The proof follows by observing that

$$\begin{aligned} & \int \int R_{\mathbf{z}}(P_{\Theta|Z=z}) dP_Z(\mathbf{u}) dP_Z(\mathbf{z}) \\ & = \int \int L(\mathbf{z}, \theta) dP_{\Theta|Z=z}(\theta) dP_Z(\mathbf{z}), \end{aligned} \quad (16)$$

where the equality in (16) follows from (9). Finally, using (15) and (16) in (11) leads to

$$\begin{aligned} & \overline{\overline{G}}(P_{\Theta|Z}, P_Z) \\ & = \int \int (R_{\theta}(P_Z) - L(\mathbf{z}, \theta)) dP_{\Theta|Z=z}(\theta) dP_Z(\mathbf{z}), \end{aligned} \quad (17)$$

which completes the proof. \blacksquare

The main contribution of this manuscript is a method that allows constructing explicit expressions for the generalization error in (11). In the following, such method is referred to as *the method of gaps* and is introduced in the next section.

IV. THE METHOD OF GAPS

The method of gaps is a two-step technique to construct explicit expressions for the generalization error $\overline{\overline{G}}(P_{\Theta|Z}, P_Z)$ in (11) in terms of information measures. The method is based on the analysis of the variations of the functionals R_{θ} in (8) and $R_{\mathbf{z}}$ in (9). More specifically, given two probability measures P_1 and P_2 in $\Delta(\mathcal{M})$ and two probability measures Q_1 and Q_2 in $\Delta((\mathcal{X} \times \mathcal{Y})^n)$, the differences $R_{\mathbf{z}}(P_1) - R_{\mathbf{z}}(P_2)$ and $R_{\theta}(Q_1) - R_{\theta}(Q_2)$ capture the variation of the functionals $R_{\mathbf{z}}$ and R_{θ} due to the change of measure from P_2 to P_1 , and from Q_2 to Q_1 , respectively. These differences are referred to as *gaps*. In a nutshell, the first step of the method of gaps consists in expressing the generalization error as either: (a) an expectation (with respect to some probability measure $Q \in \Delta((\mathcal{X} \times \mathcal{Y})^n)$) of the gap $R_{\mathbf{z}}(P_1) - R_{\mathbf{z}}(P_2)$, for some specific measures P_1 and P_2 ; or (b) an expectation (with respect to some probability measure $P \in \Delta(\mathcal{M})$) of the gap $R_{\theta}(Q_1) - R_{\theta}(Q_2)$, for some specific measures Q_1 and Q_2 . The second step consists in leveraging the properties of such gaps for expressing the expectations mentioned above in terms of information measures. To formalize the presentation of the method, the notion of gap is developed hereunder.

A. Gaps

The variations of the functional R_θ in (8), for some fixed model $\theta \in \mathcal{M}$; and those of the functional R_z in (9), for some fixed dataset $z \in (\mathcal{X} \times \mathcal{Y})^n$, due to changes in their arguments, are referred to as *gaps*. These gaps are studied via the following functionals:

$$G : (\mathcal{X} \times \mathcal{Y})^n \times \Delta(\mathcal{M}) \times \Delta(\mathcal{M}) \rightarrow \mathbb{R}; \text{ and} \quad (18)$$

$$G : \mathcal{M} \times \Delta(\mathcal{X} \times \mathcal{Y}) \times \Delta(\mathcal{X} \times \mathcal{Y}) \rightarrow \mathbb{R}, \quad (19)$$

where the former satisfies

$$G(z, P_1, P_2) = R_z(P_1) - R_z(P_2), \quad (20)$$

and the latter satisfies

$$\begin{aligned} & G(\theta, Q_1, Q_2) \\ &= \int \ell(x, y, \theta) dQ_1(x, y) - \int \ell(x, y, \theta) dQ_2(x, y), \end{aligned} \quad (21)$$

with the function ℓ defined in (6). Note that the measures P_1 and P_2 in (20) are in $\Delta(\mathcal{M})$, while the measures Q_1 and Q_2 in (21) are in $\Delta(\mathcal{X} \times \mathcal{Y})$. Despite the same notation G for the functionals in (20) and in (21), their distinction is immediate from their arguments, and thus, there is no ambiguity.

Given a fixed dataset z ; and two algorithms $P_{\Theta|Z} \in \Delta(\mathcal{M} | (\mathcal{X} \times \mathcal{Y})^n)$ and $Q_{\Theta|Z} \in \Delta(\mathcal{M} | (\mathcal{X} \times \mathcal{Y})^n)$ respectively trained upon some datasets z_1 and z_2 , the gap $G(z, P_{\Theta|Z=z_1}, Q_{\Theta|Z=z_2})$ characterizes the variation of the expected empirical risk R_z when the algorithm $Q_{\Theta|Z=z_1}$ changes to $P_{\Theta|Z=z_2}$. This justifies coining the gap $G(z, P_1, P_2)$ in (20) *algorithm-driven gap*, as P_1 and P_2 can be seen as instances of particular algorithms.

Similarly, the gap $G(\theta, Q_1, Q_2)$ in (21) characterizes the variation of the expected empirical risk R_θ in (8) when datasets are formed by n data points independently sampled from Q_1 instead of Q_2 . This observation becomes clearer by considering two product probability measures $P_Z \in \Delta((\mathcal{X} \times \mathcal{Y})^n)$ and $Q_Z \in \Delta((\mathcal{X} \times \mathcal{Y})^n)$ formed by the measures $P_Z \in \Delta(\mathcal{X} \times \mathcal{Y})$ and $Q_Z \in \Delta(\mathcal{X} \times \mathcal{Y})$. More specifically, for all measurable subsets of $(\mathcal{X} \times \mathcal{Y})^n$ of the form $\mathcal{A}_1 \times \mathcal{A}_2 \times \dots \times \mathcal{A}_n$, it holds that

$$P_Z(\mathcal{A}_1 \times \mathcal{A}_2 \times \dots \times \mathcal{A}_n) = \prod_{t=1}^n P_Z(\mathcal{A}_t), \text{ and} \quad (22)$$

$$Q_Z(\mathcal{A}_1 \times \mathcal{A}_2 \times \dots \times \mathcal{A}_n) = \prod_{t=1}^n Q_Z(\mathcal{A}_t). \quad (23)$$

Under this assumption, the following lemma presents an important property of the functional R_θ in (8).

Lemma 2: Consider a probability measure $P_Z \in \Delta((\mathcal{X} \times \mathcal{Y})^n)$ that satisfies (22) for some $P_Z \in \Delta(\mathcal{X} \times \mathcal{Y})$. Then, the functional R_θ in (8) satisfies

$$R_\theta(P_Z) = \int \ell(\theta, x, y) dP_Z(x, y), \quad (24)$$

where the function ℓ is defined in (6).

Proof: Note that from (8), it follows that

$$\begin{aligned} R_\theta(P_Z) &= \int L(z, \theta) dP_Z(z) \\ &= \int \frac{1}{n} \sum_{t=1}^n \ell(\theta, x_t, y_t) dP_Z(z) \end{aligned} \quad (25)$$

$$= \int \ell(\theta, x, y) dP_Z(x, y), \quad (26)$$

where the equality in (25) follows from (7); and the equality in (26) follows from [50, Theorem 1.6.3]. This completes the proof. \blacksquare

Lemma 2, given a fixed model $\theta \in \mathcal{M}$ and the probability measures P_Z and Q_Z that respectively satisfy (22) and (23), for some P_Z and Q_Z in $\Delta(\mathcal{X} \times \mathcal{Y})$, leads to the following equality:

$$G(\theta, P_Z, Q_Z) = R_\theta(P_Z) - R_\theta(Q_Z), \quad (27)$$

which is the variation of the functional R_θ when its argument changes from $Q_Z \in \Delta((\mathcal{X} \times \mathcal{Y})^n)$ to $P_Z \in \Delta((\mathcal{X} \times \mathcal{Y})^n)$. This justifies coining the gap $G(\theta, Q_1, Q_2)$ in (21) the *data-driven gap*, as P_Z and Q_Z are interpreted as statistical descriptions of the datasets. Note the limitation due to the fact that the analysis of the variations of the functional R_θ via the functional G in (21), implicitly assumes that datasets are formed by n independent and identically distributed data points (see (22)). This limitation is not present while studying the variation of the functional R_z via the functional G in (20). This induces two different variants of the method of gaps, the first one for the case of algorithm-driven gaps; and a more limited variant for the case of data-driven gaps.

B. Method of Algorithm-driven Gaps

1) Step One: The first step of the *method of algorithm-driven gaps* consists in writing the generalization error $\overline{G}(P_{\Theta|Z}, P_Z)$ in (11) in terms of the functional G in (20), as the expectation of an algorithm-driven gap. The following lemma formalizes this first step.

Lemma 3: Consider the generalization error $\overline{G}(P_{\Theta|Z}, P_Z)$ in (11) and assume that for all z , the probability measure $P_{\Theta|Z=z}$ is absolutely continuous with respect to the probability measure $P_\Theta \in \Delta(\mathcal{M})$, which satisfies for all measurable subsets C of \mathcal{M} ,

$$P_\Theta(C) = \int P_{\Theta|Z=z}(C) dP_Z(z). \quad (28)$$

Then,

$$\overline{G}(P_{\Theta|Z}, P_Z) = \int G(z, P_\Theta, P_{\Theta|Z=z}) dP_Z(z), \quad (29)$$

where the functional G is defined in (20).

Proof: The proof is presented in Appendix B. \blacksquare

Given a training dataset z , as the one in (4), a probability measure $P_{\Theta|Z=z}$ represents the specific instance of an algorithm $P_{\Theta|Z}$ obtained by training such an algorithm on the training dataset z . From this perspective, each dataset z

in $(\mathcal{X} \times \mathcal{Y})^n$ generates one instance of the algorithm $P_{\Theta|Z}$. From a Bayesian perspective, the instance $P_{\Theta|Z=z}$ of the algorithm $P_{\Theta|Z}$ can be understood as the posterior of the prior P_{Θ} in (28), after the observation of the training dataset z . From this perspective, Lemma 3 presents the generalization error $\bar{G}(P_{\Theta|Z}, P_Z)$ in (11) as the expectation (when z is assumed to be drawn from P_Z) of the variations of the empirical risk R_z in (9) when the measure on the models changes from the posterior $P_{\Theta|Z=z}$ to the prior P_{Θ} . From (28), note that P_{Θ} is a convex combination of all possible instances of the algorithm $P_{\Theta|Z}$. The coefficients of such a combination are determined by the probability measure on the datasets P_Z .

2) *Step Two*: The second step consists in exploiting the fact that algorithm-driven gaps exhibit closed form expressions involving the conditional Gibbs probability measure studied in [9], [51]–[54] and used in [55]–[59]. In order to formally describe this step, such a conditional Gibbs probability measure is introduced. Consider two parameters: (a) A σ -finite measure $Q \in \Delta(\mathcal{M})$; and (b) A positive real λ . These parameters are often referred to as the reference measure; and the temperature coefficient. A Gibbs probability measure, parametrized by Q and λ , and conditioned on a training dataset z in $(\mathcal{X} \times \mathcal{Y})^n$, is denoted by $P_{\Theta|Z=z}^{(Q,\lambda)} \in \Delta(\mathcal{M})$. This notation is chosen to explicitly highlight the parameters Q , λ , and the training dataset z . Before introducing an explicit expression for such a measure, two mathematical objects of central importance are introduced. First, let the function $K_{Q,z} : \mathbb{R} \rightarrow \mathbb{R} \cup \{+\infty\}$ be such that

$$K_{Q,z}(t) = \log \left(\int \exp(t L(z, \theta)) dQ(\theta) \right), \quad (30)$$

where the function L is defined in (7). The function $K_{Q,z}$, often referred to as the *log-partition function* of the measure $P_{\Theta|Z=z}^{(Q,\lambda)}$, is nondecreasing, convex, and differentiable infinitely many times [9, Lemma 15 and Lemma 16]. Let also the set $\mathcal{K}_{Q,z} \subset (0, +\infty)$ be

$$\mathcal{K}_{Q,z} \triangleq \left\{ s > 0 : K_{Q,z} \left(-\frac{1}{s} \right) < +\infty \right\}. \quad (31)$$

The set $\mathcal{K}_{Q,z}$ is either empty or a convex interval including the interval $(0, b)$, for some real $b \in (0, +\infty]$. See for instance, [9, Lemma 1]. Interestingly, when Q is a probability measure, it follows that $\mathcal{K}_{Q,z} = (0, +\infty)$. Let also the set \mathcal{K}_Q be

$$\mathcal{K}_Q \triangleq \bigcap_{z \in \text{supp } Q} \mathcal{K}_{Q,z}. \quad (32)$$

Using this notation, the Gibbs algorithm is defined as follows.

Definition 5 (Gibbs Algorithm): An algorithm, denoted by $P_{\Theta|Z}^{(Q,\lambda)} \in \Delta(\mathcal{M} | (\mathcal{X} \times \mathcal{Y})^n)$, is said to be a Gibbs algorithm with parameters $Q \in \Delta(\mathcal{M})$ and $\lambda \in \mathcal{K}_Q$, with \mathcal{K}_Q in (32), if the instance of such algorithm obtained by training it upon the dataset z in (4), denoted by $P_{\Theta|Z=z}^{(Q,\lambda)} \in \Delta(\mathcal{M})$, satisfies for all $\theta \in \text{supp } Q$,

$$\frac{dP_{\Theta|Z=z}^{(Q,\lambda)}}{dQ}(\theta) = \exp \left(-K_{Q,z} \left(-\frac{1}{\lambda} \right) - \frac{1}{\lambda} L(z, \theta) \right), \quad (33)$$

where the nonnegative function $\frac{dP_{\Theta|Z=z}^{(Q,\lambda)}}{dQ} : \mathcal{M} \rightarrow (0, +\infty)$ is the Radon-Nikodym derivative of the measure $P_{\Theta|Z=z}^{(Q,\lambda)}$ with respect to Q ; and the functions L and $K_{Q,z}$ are respectively defined in (7) and (30).

Using this notation, the second step of the method of gaps is formalized as follows.

Lemma 4: Consider the generalization error $\bar{G}(P_{\Theta|Z}, P_Z)$ in (11) and assume that for all $z \in (\mathcal{X} \times \mathcal{Y})^n$:

- (a) The probability measure $P_{\Theta|Z=z}$ is absolutely continuous with respect to the probability measure P_{Θ} in (28); and
- (b) The probability measures $P_{\Theta|Z=z}$ and P_{Θ} in (28) are absolutely continuous with respect to the σ -finite measure Q in (33).

Then,

$$\begin{aligned} \bar{G}(P_{\Theta|Z}, P_Z) &= \lambda \int \left(D(P_{\Theta} \| P_{\Theta|Z=z}^{(Q,\lambda)}) - D(P_{\Theta|Z=z} \| P_{\Theta|Z=z}^{(Q,\lambda)}) \right. \\ &\quad \left. + D(P_{\Theta|Z=z} \| Q) - D(P_{\Theta} \| Q) \right) dP_Z(z), \end{aligned} \quad (34)$$

where the measure $P_{\Theta|Z=z}^{(Q,\lambda)} \in \Delta(\mathcal{M})$ is defined in (33); and $\lambda \in \mathcal{K}_Q$, with \mathcal{K}_Q in (32).

Proof: The proof follows immediately from Lemma 3 and Theorem 37, which is introduced later in Section VII-D. \blacksquare

Note that while the right-hand side of the equality in (34) depends on the measure Q and a real λ , the left-hand side does not depend upon these parameters. This shows the paramount relevance of the equality in (34) as particular choices of Q and λ would yield different equivalent expressions for the generalization error $\bar{G}(P_{\Theta|Z}, P_Z)$ in (11). Section V explores some of these choices and presents some interesting explicit expressions for $\bar{G}(P_{\Theta|Z}, P_Z)$ emerging from (34).

C. Method of Data-driven Gaps

1) *Step One*: The first step of the *method of data-driven gaps* consists in writing the generalization error $\bar{G}(P_{\Theta|Z}, P_Z)$ in (11) in terms of the functional G in (21), as the expectation of a data-driven gap. To achieve such an objective, the central observation is that the joint probability measure $P_{\Theta|Z} \cdot P_Z \in \Delta(\mathcal{M} \times (\mathcal{X} \times \mathcal{Y})^n)$ shares common properties with the measure $P_{Z|\Theta} \cdot P_{\Theta} \in \Delta((\mathcal{X} \times \mathcal{Y})^n \times \mathcal{M})$, where P_{Θ} is in (28) and the conditional probability measure $P_{Z|\Theta} \in \Delta((\mathcal{X} \times \mathcal{Y})^n | \mathcal{M})$ satisfies for all measurable subsets \mathcal{B} of $(\mathcal{X} \times \mathcal{Y})^n$,

$$P_Z(\mathcal{B}) = \int P_{Z|\Theta=\theta}(\mathcal{B}) dP_{\Theta}(\theta). \quad (35)$$

These common properties are discussed in detail in Appendix A. In the following, it is assumed that the probability

measure P_Z in (35) is a product measure formed by the measure

$$P_Z \in \Delta(\mathcal{X} \times \mathcal{Y}). \quad (36)$$

That is, the probability measures P_Z and P_Z satisfy the equality in (22). For all $\theta \in \mathcal{M}$, the marginal measures of the probability measure $P_{Z|\Theta=\theta}$, denoted by $P_{Z_t|\Theta=\theta} \in \Delta(\mathcal{X} \times \mathcal{Y})$ with $t \in \{1, 2, \dots, n\}$, are probability measures satisfying the following conditions. For all $m \in \{1, 2, \dots, n\}$, let the set $\mathcal{B}_m \subset (\mathcal{X} \times \mathcal{Y})$ be

$$\mathcal{B}_m = \mathcal{A}_1 \times \mathcal{A}_2 \times \dots \times \mathcal{A}_n, \quad (37)$$

where for all $t \in \{1, 2, \dots, n\} \setminus \{m\}$, $\mathcal{A}_t = \mathcal{X} \times \mathcal{Y}$; and \mathcal{A}_m is any measurable subset \mathcal{A} of $\mathcal{X} \times \mathcal{Y}$. Hence, the marginal probability measure $P_{Z_m|\Theta=\theta}$ satisfies

$$P_{Z_m|\Theta=\theta}(\mathcal{A}) = P_{Z|\Theta=\theta}(\mathcal{B}_m). \quad (38)$$

Under the above assumptions on P_Z and P_Z , the marginal measures $P_{Z_1|\Theta=\theta}$, $P_{Z_2|\Theta=\theta}$, \dots , $P_{Z_n|\Theta=\theta}$ turn out to be identical to some $P_{Z|\Theta=\theta}$, as shown by the following lemma.

Lemma 5: Consider the conditional probability measure $P_{Z|\Theta} \in \Delta((\mathcal{X} \times \mathcal{Y})^n | \mathcal{M})$ and the probability measures P_Θ and P_Z in (35). If P_Z satisfies (22) for some probability measure $P_Z \in \Delta(\mathcal{X} \times \mathcal{Y})$, then, for all measurable sets \mathcal{A} of $(\mathcal{X} \times \mathcal{Y})$, for all $\theta \in \mathcal{M}$, and for all $t \in \{1, 2, \dots, n\}$, the measure $P_{Z_t|\Theta=\theta}$ in (38) satisfies,

$$P_{Z_t|\Theta=\theta}(\mathcal{A}) = P_{Z|\Theta=\theta}(\mathcal{A}), \quad (39)$$

for some probability measure $P_{Z|\Theta=\theta} \in \Delta(\mathcal{X} \times \mathcal{Y})$ that satisfies,

$$P_Z(\mathcal{A}) = \int P_{Z|\Theta=\theta}(\mathcal{A}) dP_\Theta(\theta). \quad (40)$$

Proof: From the assumptions on P_Z and P_Z , namely the equality in (22), the datasets are formed by data points that are independent and identically distributed with P_Z . Hence, for all $t \in \{1, 2, \dots, n\}$ and for all measurable sets \mathcal{A} of $\mathcal{X} \times \mathcal{Y}$,

$$P_Z(\mathcal{A}) = \int P_{Z_t|\Theta=\theta}(\mathcal{A}) dP_\Theta(\theta). \quad (41)$$

The proof is completed by [50, Theorem 5.3.1], which states the uniqueness of the measure $P_{Z_t|\Theta=\theta}$ (almost surely with respect to P_Θ), and thus, completes the proof of (39). ■

The following lemma formalizes the first step of the method of data-driven gaps.

Lemma 6: Consider the generalization error $\overline{\mathbb{G}}(P_{\Theta|Z}, P_Z)$ in (11) and assume that

- (a) The probability measure P_Z satisfies (22) for some $P_Z \in \Delta(\mathcal{X} \times \mathcal{Y})$;
- (b) For all $z \in (\mathcal{X} \times \mathcal{Y})^n$, the probability measures $P_{\Theta|Z=z}$ and P_Θ in (28) are mutually absolutely continuous; and
- (c) For all $\theta \in \mathcal{M}$, the probability measures $P_{Z|\Theta=\theta}$ and P_Z in (35) are mutually absolutely continuous.

Then,

$$\overline{\mathbb{G}}(P_{\Theta|Z}, P_Z) = \int \mathbb{G}(\theta, P_Z, P_{Z|\Theta=\theta}) dP_\Theta(\theta), \quad (42)$$

where the functional \mathbb{G} is defined in (21); and the probability measure $P_{Z|\Theta=\theta}$ satisfies (40).

Proof: The proof is presented in Appendix C. ■

From a Bayesian perspective, if the algorithm $P_{\Theta|Z=z}$ is understood as the posterior of the prior P_Θ after the observation of the training dataset z , then, the probability measure $P_{Z|\Theta=\theta}$ in (39) can be understood as the likelihood of the datasets after the observation of the model θ . From this perspective, Lemma 6 presents the generalization error $\overline{\mathbb{G}}(P_{\Theta|Z}, P_Z)$ in (11) as the expectation (when θ is assumed to be drawn from P_Θ in (28)) of the variations of the empirical risk R_θ in (8) when the measure on the data points changes from the likelihood $P_{Z|\Theta=\theta}$ to the ground-truth probability distribution P_Z , which is invariant with respect to the models.

2) *Step Two:* The second step consists in exploiting the fact that data-driven gaps exhibit closed-form expressions involving the WCDG probability measure introduced in [46] and further studied in [42]. The WCDG probability measure is conditioned on a model $\theta \in \mathcal{M}$; and parametrized by a real $\beta > 0$ and a probability measure P_S in $\Delta(\mathcal{X} \times \mathcal{Y})$. Such a WCDG probability measure is denoted by $P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)} \in \Delta_{P_S}(\mathcal{X} \times \mathcal{Y})$.

Defining an explicit expression for $P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}$, requires defining the following mathematical objects. Let $J_{P_S, \theta} : \mathbb{R} \rightarrow \mathbb{R}$ be the function

$$J_{P_S, \theta}(t) = \log \left(\int \exp(t\ell(\theta, x, y)) dP_S(x, y) \right), \quad (43)$$

where the function ℓ is defined in (6). The function $J_{P_S, \theta}$ in (43) is convex, nondecreasing, and differentiable infinitely many times in the interior of $\{t \in \mathbb{R} : J_{P_S, \theta}(t) < +\infty\}$ [42, Lemma 1]. Let also the sets $\mathcal{J}_{P_S, \theta} \subseteq (0, +\infty)$ and $\mathcal{J}_{P_S} \subseteq (0, +\infty)$ be

$$\mathcal{J}_{P_S, \theta} \triangleq \left\{ t \in (0, +\infty) : J_{P_S, \theta} \left(\frac{1}{t} \right) < +\infty \right\}, \quad (44)$$

and

$$\mathcal{J}_{P_S} \triangleq \bigcap_{\theta \in \text{supp } P_S} \mathcal{J}_{P_S, \theta}. \quad (45)$$

The set $\mathcal{J}_{P_S, \theta}$ is either empty or an interval including the interval $(b, +\infty)$, for some real $b \in (0, +\infty]$. See for instance, [42, Lemma 2]. Using this notation, the WCDG conditional probability measure is defined as follows.

Definition 6 (The WCDG conditional probability measure): A conditional probability measure, denoted by $P_{\hat{Z}|\Theta}^{(P_S, \beta)} \in \Delta(\mathcal{X} \times \mathcal{Y} | \mathcal{M})$, is said to be a WCDG conditional probability measure with parameters $P_S \in \Delta(\mathcal{X} \times \mathcal{Y})$ and $\beta \in \mathcal{J}_{P_S}$, with \mathcal{J}_{P_S} in (45), if for all $\theta \in \mathcal{M}$ and for all $(x, y) \in \text{supp } P_S$,

$$\frac{dP_{\hat{Z}|\Theta}^{(P_S, \beta)}}{dP_S}(x, y) = \exp \left(\frac{1}{\beta} \ell(\theta, x, y) - J_{P_S, \theta} \left(\frac{1}{\beta} \right) \right), \quad (46)$$

where the function $\frac{dP_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}}{dP_S} : \mathcal{X} \times \mathcal{Y} \rightarrow (0, +\infty)$ is the Radon-Nikodym derivative of the measure $P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}$ with respect to P_S ; and the functions ℓ and $J_{P_S, \theta}$ are defined in (6) and (43).

Using this notation, the second step of the method of data-driven gaps is formalized as follows.

Lemma 7: Consider the generalization error $\overline{\overline{G}}(P_{\Theta|Z}, P_Z)$ in (11) and assume that:

- (a) The probability measure P_Z satisfies (22) for some $P_Z \in \Delta(\mathcal{X} \times \mathcal{Y})$;
- (b) For all $z \in (\mathcal{X} \times \mathcal{Y})^n$, the probability measures $P_{\Theta|Z=z}$ and P_{Θ} in (28) are mutually absolutely continuous;
- (c) For all $\theta \in \mathcal{M}$, the probability measures $P_{Z|\Theta=\theta}$ and P_Z in (35) are mutually absolutely continuous; and
- (d) For all $\theta \in \mathcal{M}$, the probability measures $P_{Z|\Theta=\theta}$ and P_Z satisfy (40) and are both absolutely continuous with the probability measure $P_S \in \Delta(\mathcal{X} \times \mathcal{Y})$ in (46).

Then,

$$\begin{aligned} \overline{\overline{G}}(P_{\Theta|Z}, P_Z) = & \beta \int \left(D(P_{Z|\Theta=\theta} \| P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}) - D(P_Z \| P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}) \right. \\ & \left. - D(P_{Z|\Theta=\theta} \| P_S) + D(P_Z \| P_S) \right) dP_{\Theta}(\theta), \end{aligned} \quad (47)$$

where the probability measure $P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}$ is defined in (46); and $\beta \in \mathcal{J}_{P_S}$, with \mathcal{J}_{P_S} in (45).

Proof: Under Assumptions (a) and (c), Lemma 48 and Lemma 49 (in Appendix A) imply that for all $\theta \in \mathcal{M}$, the probability measures $P_{Z|\Theta=\theta}$ and P_Z are mutually absolutely continuous. Hence, the proof follows immediately from Lemma 6 and Theorem 43, which is introduced later in Section VIII. \blacksquare

Note that while the right-hand side of the equality in (47) depends on the probability measure P_S and β , the left-hand side does not depend upon these parameters. This shows the paramount relevance of the equality in (47) as particular choices of P_S and β would yield different equivalent expressions for the generalization error $\overline{\overline{G}}(P_{\Theta|Z}, P_Z)$ in (11). Section VI explores some of these choices and presents some interesting explicit expressions for $\overline{\overline{G}}(P_{\Theta|Z}, P_Z)$ emerging from (47).

V. EXPLICIT EXPRESSIONS OBTAINED VIA THE METHOD OF ALGORITHM-DRIVEN GAPS

This section focuses on constructing novel explicit expressions for the generalization error $\overline{\overline{G}}(P_{\Theta|Z}, P_Z)$ in (11) by exploring different choices of the parameters Q and λ in (34). It is important to highlight that in these expressions, the central building-block is the Gibbs algorithm $P_{\Theta|Z}^{(Q, \lambda)}$ (Definition 5). From this perspective, it can be admitted that the expressions for the generalization error $\overline{\overline{G}}(P_{\Theta|Z}, P_Z)$ presented in this

section are obtained by comparing the algorithm $P_{\Theta|Z}$ with the Gibbs algorithm $P_{\Theta|Z}^{(Q, \lambda)}$.

This section is divided in four subsections. The first three subsections provide explicit expressions for the generalization error $\overline{\overline{G}}(P_{\Theta|Z}, P_Z)$ aiming at establishing connections to existing results in statistics (statistical hypothesis testing), information theory (information measures), and Euclidian geometry (Pythagorean Theorems). The last subsection reviews the generalization error for the special case of the Gibbs algorithm.

A. Connections to Statistical Hypothesis Testing

The equality in (34) can be alternatively expressed as shown by the following theorem.

Theorem 8: Consider the generalization error $\overline{\overline{G}}(P_{\Theta|Z}, P_Z)$ in (11) and assume that: (a) For all $z \in (\mathcal{X} \times \mathcal{Y})^n$, the measure $P_{\Theta|Z=z}$ and the σ -finite measure Q in (33) are mutually absolutely continuous; and (b) The measures P_{Θ} in (28) and Q are mutually absolutely continuous. Then,

$$\begin{aligned} & \overline{\overline{G}}(P_{\Theta|Z}, P_Z) \\ &= \lambda \int \int \left(\log \frac{dP_{\Theta|Z=z}^{(Q, \lambda)}}{dQ}(\theta) \right) dP_{\Theta|Z=z}(\theta) P_Z(z) \\ & \quad - \lambda \int \int \left(\log \frac{dP_{\Theta|Z=z}^{(Q, \lambda)}}{dQ}(\theta) \right) dP_{\Theta}(\theta) dP_Z(z), \end{aligned} \quad (48)$$

where the Radon-Nikodym derivative $\frac{dP_{\Theta|Z=z}^{(Q, \lambda)}}{dQ}$ is defined in (33); and $\lambda \in \mathcal{K}_Q$, with \mathcal{K}_Q in (32).

Proof: Given the Assumptions (a) and (b), Lemma 4 holds. The proof follows by observing that the differences $D(P_{\Theta} \| P_{\Theta|Z=z}^{(Q, \lambda)}) - D(P_{\Theta} \| Q)$ and $D(P_{\Theta|Z=z} \| Q) - D(P_{\Theta|Z=z} \| P_{\Theta|Z=z}^{(Q, \lambda)})$ in (34) respectively satisfy the following equalities:

$$\begin{aligned} & D(P_{\Theta} \| P_{\Theta|Z=z}^{(Q, \lambda)}) - D(P_{\Theta} \| Q) \\ &= \int \left(\log \frac{dP_{\Theta}}{dP_{\Theta|Z=z}^{(Q, \lambda)}}(\theta) - \log \frac{dP_{\Theta}}{dQ}(\theta) \right) dP_{\Theta}(\theta) \\ &= - \int \left(\log \frac{dP_{\Theta|Z=z}^{(Q, \lambda)}}{dQ}(\theta) \right) dP_{\Theta}(\theta), \end{aligned} \quad (49)$$

where the equality in (50) holds from Assumption (b) and the fact that the measures $P_{\Theta|Z=z}^{(Q, \lambda)}$ and Q are mutually absolutely continuous [9, Lemma 3]. Using the same arguments,

$$\begin{aligned} & D(P_{\Theta|Z=z} \| Q) - D(P_{\Theta|Z=z} \| P_{\Theta|Z=z}^{(Q, \lambda)}) \\ &= \int \left(\log \frac{dP_{\Theta|Z=z}^{(Q, \lambda)}}{dQ}(\theta) \right) dP_{\Theta|Z=z}(\theta). \end{aligned} \quad (51)$$

Plugging both (50) and (51) into (34) yields (48), which completes the proof. \blacksquare

The relevance of Theorem 8 lies on the fact that it allows framing the generalization error $\overline{G}(P_{\Theta|Z}, P_Z)$ in (11) within the context of a mismatched hypothesis test (see [47] and [60]). More specifically, let the random variable $(\Theta, Z) \in \mathcal{M} \times (\mathcal{X} \times \mathcal{Y})^n$ follow the probability distribution associated to the probability measure $P_{\Theta|Z} \cdot P_Z \in \Delta(\mathcal{M} \times (\mathcal{X} \times \mathcal{Y})^n)$. Let (θ, z) be a realization of such a random variable. Consider a hypothesis test in which the objective is to determine whether such an realization (θ, z) is generated from either a probability distribution $P_{\Theta|Z}^{(Q, \lambda)} \cdot P_Z \in \Delta(\mathcal{M} \times (\mathcal{X} \times \mathcal{Y})^n)$ (null hypothesis) or from the alternative distribution $Q \cdot P_Z \in \Delta(\mathcal{M} \times (\mathcal{X} \times \mathcal{Y})^n)$ (alternative hypothesis). The resulting hypothesis test is said to be mismatched because neither the null hypothesis nor the alternative hypothesis matches the ground-truth probability measure $P_{\Theta|Z} \cdot P_Z$. In a nutshell, the null hypothesis presumes that the dataset z is obtained by sampling the probability measure P_Z , while the model θ is obtained by sampling the probability measure $P_{\Theta|Z=z}^{(Q, \lambda)}$. Conversely, the alternative hypothesis posits that the dataset z and the model θ are obtained by simultaneously sampling the probability measures P_Z and Q , implying independence between the random variables Z and Θ . From this perspective, the term $\log \frac{dP_{\Theta|Z=z}^{(Q, \lambda)}}{dQ}(\theta)$ in (51) appears to be the log-likelihood ratio to decide based upon the observation (θ, z) on the null or alternative hypothesis. Essentially, given a $\gamma \in \mathbb{R}$, if $\log \frac{dP_{\Theta|Z=z}^{(Q, \lambda)}}{dQ}(\theta) \geq \gamma$, then the null hypothesis is accepted. Alternatively, the null hypothesis is rejected if $\log \frac{dP_{\Theta|Z=z}^{(Q, \lambda)}}{dQ}(\theta) < \gamma$, which highlights the role of γ to trade-off between Type-I and Type-II errors in the context of such a mismatched hypothesis test [47]. From this perspective, the generalization error $\overline{G}(P_{\Theta|Z}, P_Z)$ in (11) can be interpreted as the variation of the expectation of the log-likelihood ratio of such a mismatched hypothesis test when the measure (used for expectation) changes from the product of the marginals of the ground truth, i.e., $P_{\Theta} \cdot P_Z$ to the ground truth probability measure $P_{\Theta|Z} \cdot P_Z$.

Variations in the expected log-likelihood ratio for mismatched hypothesis tests, due to changes in the measure used to compute the expectation, remain a shyly explored area in statistics and information theory. Nevertheless, it is crucial to emphasize that this concept might hold a pivotal role in the analysis of generalization error. Variations of the expected log-likelihood ratio of matched and mismatched hypothesis tests are found all along the remaining of this work.

B. Connections to Information Measures

Two particular choices for the reference measure Q in (34) are worth particular discussions as they lead to expressions involving either the mutual information or the lautum information. Those choices correspond to cases in which the gap $G(z, P_{\Theta}, P_{\Theta|Z=z})$ in (29) is calculated using either P_{Θ} or $P_{\Theta|Z=z}$ as reference measure. From Lemma 4, it follows that the case in which the reference measure is P_{Θ} leads to an expression involving the mutual information $I(P_{\Theta|Z}; P_Z)$, as shown by the following corollary.

Corollary 9: Consider the generalization error $\overline{G}(P_{\Theta|Z}, P_Z)$ in (11) and assume that for all $z \in (\mathcal{X} \times \mathcal{Y})^n$, the measure $P_{\Theta|Z=z}$ is absolutely continuous with respect to P_{Θ} in (28). Then,

$$\begin{aligned} \overline{G}(P_{\Theta|Z}, P_Z) &= \lambda I(P_{\Theta|Z}; P_Z) \\ &+ \lambda \int \left(D(P_{\Theta} \| P_{\Theta|Z=z}^{(P_{\Theta}, \lambda)}) - D(P_{\Theta|Z=z} \| P_{\Theta|Z=z}^{(P_{\Theta}, \lambda)}) \right) dP_Z(z), \end{aligned}$$

where $\lambda > 0$; and the measure $P_{\Theta|Z=z}^{(P_{\Theta}, \lambda)} \in \Delta(\mathcal{M})$ is defined as in (33).

Similarly, using Lemma 4, it is shown hereunder that the case in which the reference measure is $P_{\Theta|Z=z}$ leads to an expression involving the lautum information $L(P_{\Theta|Z}; P_Z)$.

Corollary 10: Consider the generalization error $\overline{G}(P_{\Theta|Z}, P_Z)$ in (11) and assume that for all $z \in (\mathcal{X} \times \mathcal{Y})^n$, the probability measures P_{Θ} in (28) and $P_{\Theta|Z=z}$ are mutually absolutely continuous. Then,

$$\begin{aligned} \overline{G}(P_{\Theta|Z}, P_Z) &= -\lambda L(P_{\Theta|Z}; P_Z) \\ &+ \lambda \int D(P_{\Theta} \| P_{\Theta|Z=z}^{(P_{\Theta|Z=z}, \lambda)}) dP_Z(z) \\ &- \lambda \int D(P_{\Theta|Z=z} \| P_{\Theta|Z=z}^{(P_{\Theta|Z=z}, \lambda)}) dP_Z(z), \end{aligned} \quad (52)$$

where $\lambda > 0$; and the measure $P_{\Theta|Z=z}^{(P_{\Theta|Z=z}, \lambda)} \in \Delta(\mathcal{M})$ is defined as in (33).

Independently of the choice of Q and λ in (34), the generalization error $\overline{G}(P_{\Theta|Z}, P_Z)$ in (11) can be written in terms of a mutual information $I(P_{\Theta|Z}; P_Z)$ as follows.

Theorem 11: Consider the generalization error $\overline{G}(P_{\Theta|Z}, P_Z)$ in (11) and assume that

- For all $z \in (\mathcal{X} \times \mathcal{Y})^n$, the probability measures P_{Θ} in (28) and $P_{\Theta|Z=z}$ are both absolutely continuous with respect to the σ -finite measure Q in (33); and
- The measure Q is absolutely continuous with respect to P_{Θ} .

Then,

$$\begin{aligned} \overline{G}(P_{\Theta|Z}, P_Z) &= \lambda I(P_{\Theta|Z}; P_Z) \\ &+ \lambda \int \left(D(P_{\Theta} \| P_{\Theta|Z=z}^{(Q, \lambda)}) - D(P_{\Theta|Z=z} \| P_{\Theta|Z=z}^{(Q, \lambda)}) \right) dP_Z(z), \end{aligned} \quad (53)$$

where the probability measure $P_{\Theta|Z=z}^{(Q, \lambda)}$ is defined in (33); and $\lambda \in \mathcal{K}_Q$, with \mathcal{K}_Q in (32).

Proof: The proof follows from Lemma 4, which holds under Assumption (a) and (b). The focus is on the differ-

ence $\int \left(D(P_{\Theta|Z=z} \| Q) - D(P_{\Theta} \| Q) \right) dP_Z(z)$ in (34), which satisfies the following equalities:

$$\begin{aligned} & \int \left(D(P_{\Theta|Z=z} \| Q) - D(P_{\Theta} \| Q) \right) dP_Z(z) \\ &= \int D(P_{\Theta|Z=z} \| Q) dP_Z(z) - D(P_{\Theta} \| Q) \end{aligned} \quad (54)$$

$$\begin{aligned} &= \int \left(\int \log \left(\frac{dP_{\Theta|Z=z}(\theta)}{dQ}(\theta) \right) dP_{\Theta|Z=z}(\theta) \right) P_Z(z) \\ &\quad - D(P_{\Theta} \| Q) \end{aligned} \quad (55)$$

$$\begin{aligned} &= \int \left(\int \log \left(\frac{dP_{\Theta|Z=z}(\theta)}{dQ}(\theta) \right) dP_{\Theta|Z=z}(\theta) \right) dP_Z(z) \\ &\quad - \int \log \left(\frac{dP_{\Theta}(\theta)}{dQ}(\theta) \right) dP_{\Theta}(\theta) \end{aligned} \quad (56)$$

$$\begin{aligned} &= \int \left(\int \log \left(\frac{dP_{\Theta|Z=z}(\theta)}{dQ}(\theta) \right) dP_{\Theta|Z=z}(\theta) \right) dP_Z(z) \\ &\quad - \int \left(\int \log \left(\frac{dP_{\Theta}(\theta)}{dQ}(\theta) \right) dP_{\Theta}(\theta) \right) dP_Z(z) \end{aligned} \quad (57)$$

$$= \int \left(\int \log \left(\frac{dP_{\Theta|Z=z}(\theta)}{dP_{\Theta}}(\theta) \right) dP_{\Theta|Z=z}(\theta) \right) dP_Z(z) \quad (58)$$

$$= I(P_{\Theta|Z}; P_Z), \quad (59)$$

where the equality in (58) relies on the Assumptions (a) and (b), which imply that the measures P_{Θ} and Q are mutually absolutely continuous, and thus, for all $\theta \in \mathcal{M}$, $\frac{dQ}{dP_{\Theta}}(\theta) = \left(\frac{dP_{\Theta}}{dQ}(\theta) \right)^{-1}$. This completes the proof. ■

It is important to highlight that the proof of Theorem 11 relies on the equality

$$\begin{aligned} & \int \log \left(\frac{dP_{\Theta}(\theta)}{dQ}(\theta) \right) dP_{\Theta}(\theta) \\ &= \int \left(\int \log \left(\frac{dP_{\Theta}(\theta)}{dQ}(\theta) \right) dP_{\Theta|Z=z}(\theta) \right) dP_Z(z), \end{aligned} \quad (60)$$

which holds under the assumption that the reference measure Q is independent of the datasets. More specifically, $Q \in \Delta(\mathcal{M})$ and $Q \notin \Delta(\mathcal{M} | (\mathcal{X} \times \mathcal{Y})^n)$. The equality in (60) is used to obtain the equality in (57).

The significance of Theorem 11 lies on the fact that it preserves the flexibility of selecting a reference measure Q within $\Delta(\mathcal{M})$, provided that conditions (a) and (b) are met. This freedom in choosing the reference measure is further explored in Section VII-E. Such a flexibility can also be preserved while using the lautum information $L(P_{\Theta|Z}; P_Z)$, as shown by the following theorem.

Theorem 12: Consider the generalization error $\overline{\mathbb{G}}(P_{\Theta|Z}, P_Z)$ in (11) and assume that for all $z \in (\mathcal{X} \times \mathcal{Y})^n$,

- (a) The measures P_{Θ} in (28) and $P_{\Theta|Z=z}$ are absolutely continuous with respect to a σ -finite measure $Q \in \Delta(\mathcal{M})$ (or a conditional σ -finite measure in $\Delta(\mathcal{M} | (\mathcal{X} \times \mathcal{Y})^n)$); and
- (b) The measures P_{Θ} and $P_{\Theta|Z=z}$ are mutually absolutely continuous.

Then,

$$\begin{aligned} & \overline{\mathbb{G}}(P_{\Theta|Z}, P_Z) \\ &= -\lambda L(P_{\Theta|Z}; P_Z) + \lambda \int \left(D(P_{\Theta} \| P_{\Theta|Z=z}^{(Q,\lambda)}) \right. \\ &\quad \left. - D(P_{\Theta|Z=z} \| P_{\Theta|Z=z}^{(Q,\lambda)}) + D(P_{\Theta|Z=z} \| Q) \right. \\ &\quad \left. - \int \log \frac{dP_{\Theta|Z=z}(\theta)}{dQ}(\theta) dP_{\Theta}(\theta) \right) dP_Z(z), \end{aligned} \quad (61)$$

where the probability measure $P_{\Theta|Z=z}^{(Q,\lambda)}$ is defined in (33); and $\lambda \in \mathcal{K}_Q$, with \mathcal{K}_Q in (32).

Proof: The proof follows from Lemma 4, which holds under Assumptions (a) and (b). Hence, in (34), under Assumptions (a) and (b), the following holds:

$$\begin{aligned} & \int D(P_{\Theta} \| Q) dP_Z(z) \\ &= \int \int \log \frac{dP_{\Theta}(\theta)}{dQ}(\theta) dP_{\Theta}(\theta) dP_Z(z) \end{aligned} \quad (62)$$

$$\begin{aligned} &= \int \int \log \frac{dP_{\Theta}}{dP_{\Theta|Z=z}}(\theta) dP_{\Theta}(\theta) dP_Z(z) \\ &\quad + \int \int \log \frac{dP_{\Theta|Z=z}}{dQ}(\theta) dP_{\Theta}(\theta) dP_Z(z) \end{aligned} \quad (63)$$

$$= L(P_{\Theta|Z}; P_Z) + \int \int \log \frac{dP_{\Theta|Z=z}(\theta)}{dQ}(\theta) dP_{\Theta}(\theta) dP_Z(z). \quad (64)$$

Plugging (64) into (34) yields (61), which completes the proof. ■

Subtracting (61) from (53) yields the following equality, which unveils a connection between hypothesis testing and the sum of the mutual information $I(P_{\Theta|Z}; P_Z)$ and the lautum information $L(P_{\Theta|Z}; P_Z)$.

Corollary 13: Given a conditional probability measure $P_{\Theta|Z} \in \Delta(\mathcal{M} | (\mathcal{X} \times \mathcal{Y})^n)$ and a probability measure $P_Z \in \Delta((\mathcal{X} \times \mathcal{Y})^n)$, assume that for all $z \in (\mathcal{X} \times \mathcal{Y})^n$:

- (a) The probability measures P_{Θ} in (28) and $P_{\Theta|Z=z}$ are both absolutely continuous with respect to some σ -finite measure $Q \in \Delta(\mathcal{M})$;
- (b) The measure Q is absolutely continuous with respect to P_{Θ} ; and
- (c) The measure P_{Θ} is absolutely continuous with respect to $P_{\Theta|Z=z}$.

Then,

$$\begin{aligned} & I(P_{\Theta|Z}; P_Z) + L(P_{\Theta|Z}; P_Z) \\ &= \int \int \log \left(\frac{dP_{\Theta|Z=z}(\theta)}{dQ}(\theta) \right) dP_{\Theta|Z=z}(\theta) dP_Z(z) \\ &\quad - \int \int \log \left(\frac{dP_{\Theta}(\theta)}{dQ}(\theta) \right) dP_{\Theta}(\theta) dP_Z(z). \end{aligned} \quad (65)$$

The equality in (65) holds significant interest as it expresses the sum of the mutual information $I(P_{\Theta|Z}; P_Z)$ and the lautum information $L(P_{\Theta|Z}; P_Z)$ in terms of a free parameter Q ,

which can be chosen subject to conditions (a) and (b). However, what truly elevates this equality is its profound connection to the realm of hypothesis testing [61]. More specifically, let the random variable $(\Theta, \mathbf{Z}) \in \mathcal{M} \times (\mathcal{X} \times \mathcal{Y})^n$ induce the probability measure $P_{\Theta|\mathbf{Z}} \cdot P_{\mathbf{Z}} \in \Delta(\mathcal{M} \times (\mathcal{X} \times \mathcal{Y})^n)$. Consider a hypothesis test in which the objective is to determine whether an observation $(\theta, \mathbf{z}) \in \mathcal{M} \times (\mathcal{X} \times \mathcal{Y})^n$ of such a random variable (Θ, \mathbf{Z}) is obtained by sampling the (ground-truth) probability measure $P_{\Theta|\mathbf{Z}} \cdot P_{\mathbf{Z}}$ (null hypothesis) or by sampling the alternative probability measure $Q \cdot P_{\mathbf{Z}} \in \Delta(\mathcal{M} \times (\mathcal{X} \times \mathcal{Y})^n)$ (alternative hypothesis). From this perspective, the term $\log \frac{dP_{\Theta|\mathbf{Z}=\mathbf{z}}}{dQ}(\theta)$ in (65) can be interpreted as the log-likelihood ratio used to decide between the null and alternative hypotheses based on the observation (θ, \mathbf{z}) . Essentially, for a given threshold $\gamma \in \mathbb{R}$, if $\log \frac{dP_{\Theta|\mathbf{Z}=\mathbf{z}}}{dQ}(\theta) \geq \gamma$, the null hypothesis is accepted, and the alternative hypothesis is rejected; otherwise, the opposite decision is made. The sum of the mutual information $I(P_{\Theta|\mathbf{Z}}; P_{\mathbf{Z}})$ and the lautum information $L(P_{\Theta|\mathbf{Z}}; P_{\mathbf{Z}})$ in (65) can be interpreted as the variation of the expectation of the log-likelihood ratio of such a hypothesis test when the measure (used for expectation) changes from the product of the marginals of the ground truth, i.e., $P_{\Theta} \cdot P_{\mathbf{Z}}$, to the ground-truth joint probability measure $P_{\Theta|\mathbf{Z}} \cdot P_{\mathbf{Z}}$.

An important observation is that the left-hand side of the equality in (65) is independent of the parameter Q . Hence, from the perspective of the hypothesis testing problem formulated earlier, it appears that the measure Q in the alternative hypothesis does not impact the variation of the expectation of the log-likelihood ratio when the measure (used for expectation) shifts from the product of the marginals of the ground truth to the ground-truth probability measure. Note also that such a variation is nonnegative. That is,

$$0 < \int \int \log \left(\frac{dP_{\Theta|\mathbf{Z}=\mathbf{z}}}{dQ}(\theta) \right) dP_{\Theta|\mathbf{Z}=\mathbf{z}}(\theta) dP_{\mathbf{Z}}(\mathbf{z}) - \int \int \log \left(\frac{dP_{\Theta|\mathbf{Z}=\mathbf{z}}}{dQ}(\theta) \right) dP_{\Theta}(\theta) dP_{\mathbf{Z}}(\mathbf{z}), \quad (66)$$

which follows from the fact that both mutual and lautum information are nonnegative. Finally, note for instance that if for all $\mathbf{z} \in (\mathcal{X} \times \mathcal{Y})^n$, the probability measures $P_{\Theta|\mathbf{Z}=\mathbf{z}}$ and P_{Θ} are mutually absolutely continuous, then Q can be set to be equal to P_{Θ} , which implies that the hypothesis test discussed earlier includes the test for independence.

The sum of the mutual information $I(P_{\Theta|\mathbf{Z}}; P_{\mathbf{Z}})$ and the lautum information $L(P_{\Theta|\mathbf{Z}}; P_{\mathbf{Z}})$ can be found on several equivalent expressions for the generalization error $\bar{G}(P_{\Theta|\mathbf{Z}}, P_{\mathbf{Z}})$ in (11), as shown by the following theorems.

Theorem 14: Consider the generalization error $\bar{G}(P_{\Theta|\mathbf{Z}}, P_{\mathbf{Z}})$ in (11) and assume that for all $\mathbf{z} \in (\mathcal{X} \times \mathcal{Y})^n$:

- (a) The probability measures P_{Θ} in (28) and $P_{\Theta|\mathbf{Z}=\mathbf{z}}$ are both absolutely continuous with respect to some σ -finite measure $Q \in \Delta(\mathcal{M})$;
- (b) The measure Q is absolutely continuous with respect to P_{Θ} ; and

- (c) The measure P_{Θ} is absolutely continuous with respect to $P_{\Theta|\mathbf{Z}=\mathbf{z}}$.

Then,

$$\begin{aligned} \bar{G}(P_{\Theta|\mathbf{Z}}, P_{\mathbf{Z}}) &= \lambda (I(P_{\Theta|\mathbf{Z}}; P_{\mathbf{Z}}) + L(P_{\Theta|\mathbf{Z}}; P_{\mathbf{Z}})) \\ &+ \lambda \int \int \log \frac{dP_{\Theta|\mathbf{Z}=\mathbf{z}}}{dP_{\Theta|\mathbf{Z}=\mathbf{z}}^{(Q,\lambda)}}(\theta) dP_{\Theta}(\theta) dP_{\mathbf{Z}}(\mathbf{z}) \\ &- \lambda \int \int \log \frac{dP_{\Theta|\mathbf{Z}=\mathbf{z}}}{dP_{\Theta|\mathbf{Z}=\mathbf{z}}^{(Q,\lambda)}}(\theta) dP_{\Theta|\mathbf{Z}=\mathbf{z}}(\theta) dP_{\mathbf{Z}}(\mathbf{z}), \quad (67) \end{aligned}$$

where the probability measure $P_{\Theta|\mathbf{Z}=\mathbf{z}}^{(Q,\lambda)}$ is defined in (33); and $\lambda \in \mathcal{K}_Q$, with \mathcal{K}_Q in (32).

Proof: The proof follows from Theorem 11, which holds under Assumptions (a) and (b). Note that the term $D(P_{\Theta} \| P_{\Theta|\mathbf{Z}=\mathbf{z}}^{(Q,\lambda)})$ within the integral in (53), can be re-written as follows:

$$\begin{aligned} &\int D(P_{\Theta} \| P_{\Theta|\mathbf{Z}=\mathbf{z}}^{(Q,\lambda)}) dP_{\mathbf{Z}}(\mathbf{z}) \\ &= \int \int \log \frac{dP_{\Theta}}{dP_{\Theta|\mathbf{Z}=\mathbf{z}}^{(Q,\lambda)}}(\theta) dP_{\Theta}(\theta) dP_{\mathbf{Z}}(\mathbf{z}) \quad (68) \end{aligned}$$

$$= \int \int \log \left(\frac{dP_{\Theta}}{dP_{\Theta|\mathbf{Z}=\mathbf{z}}^{(Q,\lambda)}}(\theta) \frac{dP_{\Theta|\mathbf{Z}=\mathbf{z}}}{dP_{\Theta|\mathbf{Z}=\mathbf{z}}}(\theta) \right) dP_{\Theta}(\theta) dP_{\mathbf{Z}}(\mathbf{z}) \quad (69)$$

$$\begin{aligned} &= \int \int \log \frac{dP_{\Theta|\mathbf{Z}=\mathbf{z}}}{dP_{\Theta|\mathbf{Z}=\mathbf{z}}^{(Q,\lambda)}}(\theta) dP_{\Theta}(\theta) dP_{\mathbf{Z}}(\mathbf{z}) \\ &+ \int \int \log \frac{dP_{\Theta}}{dP_{\Theta|\mathbf{Z}=\mathbf{z}}}(\theta) dP_{\Theta}(\theta) dP_{\mathbf{Z}}(\mathbf{z}) \quad (70) \end{aligned}$$

$$= \int \int \log \frac{dP_{\Theta|\mathbf{Z}=\mathbf{z}}}{dP_{\Theta|\mathbf{Z}=\mathbf{z}}^{(Q,\lambda)}}(\theta) dP_{\Theta}(\theta) dP_{\mathbf{Z}}(\mathbf{z}) + L(P_{\Theta|\mathbf{Z}}; P_{\mathbf{Z}}), \quad (71)$$

where the equality in (70) holds from Assumptions (a), (c) and [9, Lemma 3]. Plugging (71) into (53) completes the proof. \blacksquare

In Theorem 14, the term

$$\begin{aligned} &\int \int \log \frac{dP_{\Theta|\mathbf{Z}=\mathbf{z}}}{dP_{\Theta|\mathbf{Z}=\mathbf{z}}^{(Q,\lambda)}}(\theta) dP_{\Theta}(\theta) dP_{\mathbf{Z}}(\mathbf{z}) \\ &- \lambda \int \int \log \frac{dP_{\Theta|\mathbf{Z}=\mathbf{z}}}{dP_{\Theta|\mathbf{Z}=\mathbf{z}}^{(Q,\lambda)}}(\theta) dP_{\Theta|\mathbf{Z}=\mathbf{z}}(\theta) dP_{\mathbf{Z}}(\mathbf{z}), \quad (72) \end{aligned}$$

can be interpreted in the context of the following hypothesis test. Consider the training dataset \mathbf{z} in (4), which is obtained by sampling from the measure $P_{\mathbf{Z}}$. Assume that both the algorithm $P_{\Theta|\mathbf{Z}}$ and the Gibbs algorithm $P_{\Theta|\mathbf{Z}}^{(Q,\lambda)}$ are trained upon the same dataset \mathbf{z} . Hence, the hypothesis test consists in determining whether a model θ , obtained by sampling from the probability measure $P_{\Theta|\mathbf{Z}=\mathbf{z}}$, has been obtained from the ground-truth probability measure $P_{\Theta|\mathbf{Z}=\mathbf{z}}$ (null hypothesis); or from the probability measure $P_{\Theta|\mathbf{Z}=\mathbf{z}}^{(Q,\lambda)}$ (alternative hypothesis). In essence, the null hypothesis claims that the model θ is the result of the original algorithm under study, while the alternative hypothesis suggests it is the output of a Gibbs algorithm. The resulting log-likelihood ratio to distinguish between these two hypothesis, based on the observation of

the model θ , is $\log \frac{dP_{\Theta|Z=z}}{dP_{\Theta|Z=z}^{(Q,\lambda)}}(\theta)$. Hence, the term in (72) can be interpreted as the variation of the expectation of the log-likelihood ratio of such a hypothesis test when the measure (used for expectation) changes from the ground-truth joint probability measure $P_{\Theta|Z} \cdot P_Z$ to the product of the marginals of the ground truth, i.e., $P_{\Theta} \cdot P_Z$.

The following theorem leads to alternative equivalent expressions generalization error $\bar{G}(P_{\Theta|Z}, P_Z)$ in (11), which might also be interpreted within the context of a similar hypothesis test.

Theorem 15: Consider the generalization error $\bar{G}(P_{\Theta|Z}, P_Z)$ in (11) and assume that for all $z \in (\mathcal{X} \times \mathcal{Y})^n$:

- (a) The measures P_{Θ} in (28) and $P_{\Theta|Z=z}$ are absolutely continuous with respect to a σ -finite measure Q (or a conditional σ -finite measure in $\Delta(\mathcal{M} | (\mathcal{X} \times \mathcal{Y})^n)$); and
- (b) The measures P_{Θ} and $P_{\Theta|Z=z}$ are mutually absolutely continuous.

Then,

$$\begin{aligned} \bar{G}(P_{\Theta|Z}, P_Z) &= -\lambda (I(P_{\Theta|Z}; P_Z) + L(P_{\Theta|Z}; P_Z)) \\ &+ \lambda \int \int \log \frac{dP_{\Theta}}{dP_{\Theta|Z=z}^{(Q,\lambda)}}(\theta) dP_{\Theta}(\theta) dP_Z(z) \\ &- \lambda \int \int \log \frac{dP_{\Theta}}{dP_{\Theta|Z=z}^{(Q,\lambda)}}(\theta) dP_{\Theta|Z=z}(\theta) dP_Z(z) \\ &+ \lambda \int \int \log \frac{dP_{\Theta|Z=z}}{dQ}(\theta) dP_{\Theta|Z=z}(z) dP_Z(z) \\ &- \lambda \int \int \log \frac{dP_{\Theta|Z=z}}{dQ}(\theta) dP_{\Theta}(\theta) dP_Z(z), \end{aligned} \quad (73)$$

where the probability measure $P_{\Theta|Z=z}^{(Q,\lambda)}$ is defined in (33); and $\lambda \in \mathcal{K}_Q$, with \mathcal{K}_Q in (32).

Proof: The proof follows from Theorem 12, which holds under Assumptions (a) and (b). Note that the term $D(P_{\Theta|Z=z} \| P_{\Theta|Z=z}^{(Q,\lambda)})$ within the integral in (61), can be re-written as follows:

$$\begin{aligned} &D(P_{\Theta|Z=z} \| P_{\Theta|Z=z}^{(Q,\lambda)}) \\ &= \int \log \frac{dP_{\Theta|Z=z}}{dP_{\Theta|Z=z}^{(Q,\lambda)}}(\theta) dP_{\Theta|Z=z}(\theta) \end{aligned} \quad (74)$$

$$= \int \log \left(\frac{dP_{\Theta|Z=z}}{dP_{\Theta|Z=z}^{(Q,\lambda)}}(\theta) \frac{dP_{\Theta}}{dP_{\Theta}}(\theta) \right) dP_{\Theta|Z=z}(\theta) \quad (75)$$

$$= \int \log \frac{dP_{\Theta}}{dP_{\Theta|Z=z}^{(Q,\lambda)}}(\theta) dP_{\Theta|Z=z}(\theta) \quad (76)$$

$$+ \int \log \frac{dP_{\Theta|Z=z}}{dP_{\Theta}}(\theta) dP_{\Theta|Z=z}(\theta), \quad (77)$$

where the equality in (77) follows from Assumption (b) and [9, Lemma 3]. Plugging (77) into (61) yields (73), which completes the proof. \blacksquare

Although the expression presented in Theorem 15 may initially seem more intricate compared to the one in Theorem 14, it offers a distinct advantage: the flexibility to choose the reference

measure as a conditional measure. For example, by selecting Q as the conditional probability measure $P_{\Theta|Z}$, it significantly simplifies, as shown by the following corollary.

Corollary 16: Consider the generalization error $\bar{G}(P_{\Theta|Z}, P_Z)$ in (11) and assume that for all $z \in (\mathcal{X} \times \mathcal{Y})^n$, the measures P_{Θ} and $P_{\Theta|Z=z}$ are mutually absolutely continuous. Then,

$$\begin{aligned} \bar{G}(P_{\Theta|Z}, P_Z) &= -\lambda (I(P_{\Theta|Z}; P_Z) + L(P_{\Theta|Z}; P_Z)) \\ &+ \lambda \int \int \log \frac{dP_{\Theta}}{dP_{\Theta|Z=z}^{(P_{\Theta|Z=z}, \lambda)}}(\theta) dP_{\Theta}(\theta) dP_Z(z) \\ &- \lambda \int \int \log \frac{dP_{\Theta}}{dP_{\Theta|Z=z}^{(P_{\Theta|Z=z}, \lambda)}}(\theta) dP_{\Theta|Z=z}(\theta) dP_Z(z), \end{aligned} \quad (78)$$

where $\lambda > 0$; and the probability measure $P_{\Theta|Z=z}^{(P_{\Theta|Z=z}, \lambda)}$ is defined as in (33).

The interests of Corollary 16 lies on the fact that it is written in terms of the measure $P_{\Theta|Z=z}^{(P_{\Theta|Z=z}, \lambda)}$, which represents a Gibbs algorithm whose reference measure is dependent on the training dataset z . Interestingly, such a reference measure is precisely the algorithm under study $P_{\Theta|Z}$.

Another result from Theorem 15 and Corollary 13 follows by plugging the equality in (65) into (73).

Corollary 17: Consider the generalization error $\bar{G}(P_{\Theta|Z}, P_Z)$ in (11) and assume that for all $z \in (\mathcal{X} \times \mathcal{Y})^n$:

- (a) The probability measures P_{Θ} in (28) and $P_{\Theta|Z=z}$ are both absolutely continuous with respect to a σ -finite measure Q ;
- (b) The measures P_{Θ} and $P_{\Theta|Z=z}$ are mutually absolutely continuous; and
- (c) The measure Q is absolutely continuous with respect to P_{Θ} .

Then,

$$\begin{aligned} \bar{G}(P_{\Theta|Z}, P_Z) &= \lambda \int \int \log \frac{dP_{\Theta}}{dP_{\Theta|Z=z}^{(Q,\lambda)}}(\theta) dP_{\Theta}(\theta) dP_Z(z) \\ &- \lambda \int \int \log \frac{dP_{\Theta}}{dP_{\Theta|Z=z}^{(Q,\lambda)}}(\theta) dP_{\Theta|Z=z}(\theta) dP_Z(z), \end{aligned} \quad (79)$$

where the probability measure $P_{\Theta|Z=z}^{(Q,\lambda)}$ is defined in (33); and $\lambda \in \mathcal{K}_Q$, with \mathcal{K}_Q in (32).

Corollary 17 is reminiscent of Theorem 8 and thus, it has a similar interpretation.

C. Connections to Euclidian Geometry

Another expression for the generalization error $\bar{G}(P_{\Theta|Z}, P_Z)$ in (11), which leads to interesting connections to Euclidian geometry is presented hereunder.

Theorem 18: Consider the generalization error $\bar{G}(P_{\Theta|Z}, P_Z)$ in (11) and assume that for all $z \in (\mathcal{X} \times \mathcal{Y})^n$, the probability

measure $P_{\Theta|Z=z}$ is absolutely continuous with respect to some measure $Q \in \Delta(\mathcal{M})$. Then,

$$\begin{aligned} \overline{G}(P_{\Theta|Z}, P_Z) = & \lambda \int \int \left(D(P_{\Theta|Z=z} \| P_{\Theta|Z=u}^{(Q,\lambda)}) \right. \\ & \left. - D(P_{\Theta|Z=z} \| P_{\Theta|Z=z}^{(Q,\lambda)}) \right) dP_Z(u) dP_Z(z), \end{aligned} \quad (80)$$

where the probability measure $P_{\Theta|Z=z}^{(Q,\lambda)}$ satisfies (33); and $\lambda \in \mathcal{K}_Q$, with \mathcal{K}_Q in (32).

Proof: The proof consists in re-writing the difference $R_u(P_{\Theta|Z=z}) - R_z(P_{\Theta|Z=z})$ in (10) in terms of an algorithm-driven gap, i.e., using the functional G in (20). More specifically, consider the equalities

$$R_u(P_{\Theta|Z=z}) = G(u, P_{\Theta|Z=z}, P_{\Theta|Z=u}^{(Q,\lambda)}) + R_u(P_{\Theta|Z=u}^{(Q,\lambda)}) \quad (81)$$

and

$$R_z(P_{\Theta|Z=z}) = G(z, P_{\Theta|Z=z}, P_{\Theta|Z=z}^{(Q,\lambda)}) + R_z(P_{\Theta|Z=z}^{(Q,\lambda)}), \quad (82)$$

that implies,

$$\begin{aligned} & R_u(P_{\Theta|Z=z}) - R_z(P_{\Theta|Z=z}) \\ = & G(u, P_{\Theta|Z=z}, P_{\Theta|Z=u}^{(Q,\lambda)}) + R_u(P_{\Theta|Z=u}^{(Q,\lambda)}) \\ & - G(z, P_{\Theta|Z=z}, P_{\Theta|Z=z}^{(Q,\lambda)}) - R_z(P_{\Theta|Z=z}^{(Q,\lambda)}) \end{aligned} \quad (83)$$

$$\begin{aligned} = & R_u(P_{\Theta|Z=u}^{(Q,\lambda)}) + \lambda D(P_{\Theta|Z=u}^{(Q,\lambda)} \| Q) \\ & - R_z(P_{\Theta|Z=z}^{(Q,\lambda)}) - \lambda D(P_{\Theta|Z=z}^{(Q,\lambda)} \| Q) \\ & + \lambda \left(D(P_{\Theta|Z=z} \| P_{\Theta|Z=u}^{(Q,\lambda)}) - D(P_{\Theta|Z=z} \| P_{\Theta|Z=z}^{(Q,\lambda)}) \right) \end{aligned} \quad (84)$$

$$\begin{aligned} = & R_u(Q) - \lambda D(Q \| P_{\Theta|Z=u}^{(Q,\lambda)}) \\ & - R_z(Q) + \lambda D(Q \| P_{\Theta|Z=z}^{(Q,\lambda)}) \\ & + \lambda \left(D(P_{\Theta|Z=z} \| P_{\Theta|Z=u}^{(Q,\lambda)}) - D(P_{\Theta|Z=z} \| P_{\Theta|Z=z}^{(Q,\lambda)}) \right), \end{aligned} \quad (85)$$

where the equality in (84) follows from [45, Theorem 1], which holds under the assumption of the theorem and [9, Lemma 3]; and the equality in (85) follows from [9, Lemma 20]. Finally, from (85) and Definition 4, it follows that

$$\begin{aligned} & \overline{G}(P_{\Theta|Z}, P_Z) \\ = & \int \int (R_u(P_{\Theta|Z=z}) - R_z(P_{\Theta|Z=z})) dP_Z(u) dP_Z(z) \end{aligned} \quad (86)$$

$$\begin{aligned} = & \int \int (R_u(Q) - \lambda D(Q \| P_{\Theta|Z=u}^{(Q,\lambda)})) dP_Z(u) dP_Z(z) \\ & - \int \int (R_z(Q) - \lambda D(Q \| P_{\Theta|Z=z}^{(Q,\lambda)})) dP_Z(u) dP_Z(z) \\ & + \lambda \int \int \left(D(P_{\Theta|Z=z} \| P_{\Theta|Z=u}^{(Q,\lambda)}) \right. \\ & \left. - D(P_{\Theta|Z=z} \| P_{\Theta|Z=z}^{(Q,\lambda)}) \right) dP_Z(u) dP_Z(z) \end{aligned} \quad (87)$$

$$= \lambda \int \int \left(D(P_{\Theta|Z=z} \| P_{\Theta|Z=u}^{(Q,\lambda)}) \right. \\ \left. - D(P_{\Theta|Z=z} \| P_{\Theta|Z=z}^{(Q,\lambda)}) \right) dP_Z(u) dP_Z(z), \quad (88)$$

$$- D(P_{\Theta|Z=z} \| P_{\Theta|Z=z}^{(Q,\lambda)}) \Big) dP_Z(u) dP_Z(z), \quad (89)$$

which completes the proof. \blacksquare

Theorem 18 expresses the generalization error $\overline{G}(P_{\Theta|Z}, P_Z)$ in (11) as the difference between the expectations of two relative entropies. The first relative entropy compares the algorithm $P_{\Theta|Z}$ to the Gibbs algorithm $P_{\Theta|Z}^{(Q,\lambda)}$, under the assumption that such algorithms are trained on independent datasets drawn from the same probability distribution P_Z . The second relative entropy compares these algorithms under the assumption that they are trained on the same dataset drawn from P_Z . In particular, the first relative entropy satisfies the following property.

Lemma 19: Consider a probability measure $P_Z \in \Delta((\mathcal{X} \times \mathcal{Y})^n)$ and a conditional probability measure $P_{\Theta|Z} \in \Delta(\mathcal{M} | (\mathcal{X} \times \mathcal{Y})^n)$ and assume that for all $z \in (\mathcal{X} \times \mathcal{Y})^n$,

- The measures $P_{\Theta|Z=z}$ and P_{Θ} in (28) are absolutely continuous with respect to some measure $Q \in \Delta(\mathcal{M})$;
- The measure $P_{\Theta|Z=z}$ is absolutely continuous with respect to P_{Θ} .

Then,

$$\begin{aligned} & \int \int D(P_{\Theta|Z=u} \| P_{\Theta|Z=z}^{(Q,\lambda)}) dP_Z(u) dP_Z(z) \\ = & \int \left(D(P_{\Theta} \| P_{\Theta|Z=z}^{(Q,\lambda)}) + D(P_{\Theta|Z=z} \| P_{\Theta}) \right) dP_Z(z), \end{aligned} \quad (90)$$

where the probability measure $P_{\Theta|Z=z}^{(Q,\lambda)}$ satisfies (33); and $\lambda \in \mathcal{K}_Q$, with \mathcal{K}_Q in (32).

Proof: The proof follows by noticing that

$$\int \int D(P_{\Theta|Z=u} \| P_{\Theta|Z=z}^{(Q,\lambda)}) dP_Z(u) dP_Z(z)$$

$$= \int \int \int \log \left(\frac{dP_{\Theta|Z=u}(\theta)}{dP_{\Theta|Z=z}^{(Q,\lambda)}(\theta)} \right) dP_{\Theta|Z=u}(\theta) dP_Z(u) dP_Z(z)$$

$$= \int \int \int \log \left(\frac{dP_{\Theta}(\theta)}{dP_{\Theta|Z=z}^{(Q,\lambda)}(\theta)} \right) dP_{\Theta|Z=u}(\theta) dP_Z(u) dP_Z(z)$$

$$+ \int \int \int \log \left(\frac{dP_{\Theta|Z=u}(\theta)}{dP_{\Theta}(\theta)} \right) dP_{\Theta|Z=u}(\theta) dP_Z(u) dP_Z(z)$$

$$= \int \int \log \left(\frac{dP_{\Theta}(\theta)}{dP_{\Theta|Z=z}^{(Q,\lambda)}(\theta)} \right) dP_{\Theta}(\theta) dP_Z(z)$$

$$+ \int \int \log \left(\frac{dP_{\Theta|Z=u}(\theta)}{dP_{\Theta}(\theta)} \right) dP_{\Theta|Z=u}(\theta) dP_Z(u) \quad (91)$$

$$= \int \left(D(P_{\Theta} \| P_{\Theta|Z=z}^{(Q,\lambda)}) + D(P_{\Theta|Z=z} \| P_{\Theta}) \right) dP_Z(z), \quad (92)$$

which completes the proof. \blacksquare

The converse of the Pythagorean theorem [62, Book I, Proposition 48] together with Lemma 19, lead to the geometric construction shown in Figure 1. Such interpretation becomes

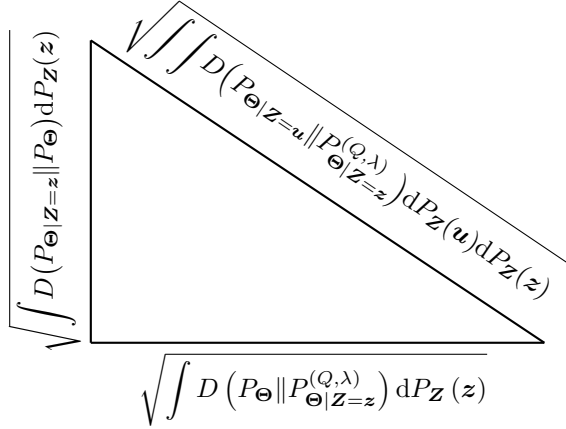


Fig. 1. Geometric interpretation of Lemma 19 involving only relative entropies. Note that $\int D(P_{\Theta|Z=z} || P_{\Theta}) dP_Z(z) = I(P_{\Theta|Z}; P_Z)$.

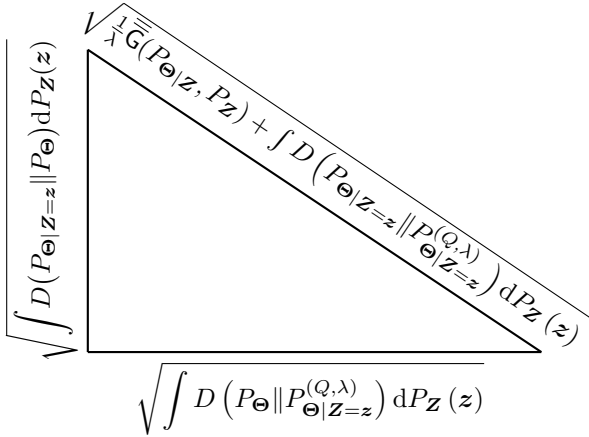


Fig. 2. Geometric interpretation of Lemma 19 involving the generalization error $\bar{G}(P_{\Theta|Z}, P_Z)$ in (11).

more interesting by noticing that, from Theorem 18, the square of the hypotenuse of the triangle in Figure 1 satisfies

$$\begin{aligned} & \int \int D(P_{\Theta|Z=u} || P_{\Theta|Z=z}^{(Q,\lambda)}) dP_Z(u) dP_Z(z) = \frac{1}{\lambda} \bar{G}(P_{\Theta|Z}, P_Z) \\ & + \int D(P_{\Theta|Z=z} || P_{\Theta|Z=z}^{(Q,\lambda)}) dP_Z(z), \end{aligned} \quad (93)$$

which involves the generalization error $\bar{G}(P_{\Theta|Z}, P_Z)$ in (11); and the length $\sqrt{\int D(P_{\Theta|Z=z} || P_{\Theta}) dP_Z(z)}$ is the square root of a mutual information, i.e., $\sqrt{I(P_{\Theta|Z}; P_Z)}$. This leads to the alternative interpretation shown in Figure 2.

D. Generalization Error of the Gibbs Algorithm

The generalization error of the Gibbs algorithm $P_{\Theta|Z}^{(Q,\lambda)}$ in (33), can be immediately obtained from Theorem 8 - Theorem 15; or Theorem 18. The following corollary formalizes this observation.

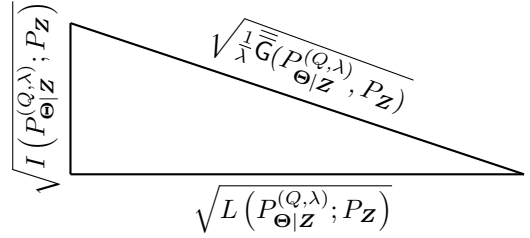


Fig. 3. Geometric interpretation of Lemma 19 for the Gibbs algorithm $P_{\Theta|Z}^{(Q,\lambda)}$ (Definition 5).

Corollary 20: The generalization error $\bar{G}(P_{\Theta|Z}^{(Q,\lambda)}, P_Z)$ in (11), with the measure $P_{\Theta|Z}^{(Q,\lambda)}$ in (33), is

$$\bar{G}(P_{\Theta|Z}^{(Q,\lambda)}, P_Z) = \lambda (I(P_{\Theta|Z}^{(Q,\lambda)}; P_Z) + L(P_{\Theta|Z}^{(Q,\lambda)}; P_Z)). \quad (94)$$

Corollary 20 has been proved numerous times before using several techniques. For instance, a proof for the case in which Q is a probability measure appears in [2]. The more general case in which Q is a σ -finite measure is proved in [9]. A proof for the particular case in which Q is a probability measure and datasets are formed by independent and identically distributed data points is presented in [46]. Figure 3 shows a geometric interpretation of Corollary 20, which is reminiscent of the Pythagorean theorem mentioned in the previous subsection.

Theorem 18 provides another expression for the generalization error of the Gibbs algorithm $P_{\Theta|Z}^{(Q,\lambda)}$ in (33), as shown by the following corollary.

Corollary 21: The generalization error $\bar{G}(P_{\Theta|Z}^{(Q,\lambda)}, P_Z)$ in (11), with the measure $P_{\Theta|Z}^{(Q,\lambda)}$ in (33), is

$$\bar{G}(P_{\Theta|Z}^{(Q,\lambda)}, P_Z) = \lambda \int \int D(P_{\Theta|Z=u} || P_{\Theta|Z=z}^{(Q,\lambda)}) dP_Z(u) dP_Z(z). \quad (95)$$

Corollary 21 shows that the generalization error of the Gibbs algorithm $P_{\Theta|Z}^{(Q,\lambda)}$ in (33) is equal to the average (expectation with respect to $P_Z \cdot P_Z$) of a pair-wise comparison via relative entropy of all the instances of such an algorithm.

VI. EXPLICIT EXPRESSIONS OBTAINED VIA THE METHOD OF DATA-DRIVEN GAPS

This section focuses on constructing novel explicit expressions for the generalization error $\bar{G}(P_{\Theta|Z}, P_Z)$ in (11) by exploring different choices of the parameters P_S and β in (47). It is important to highlight that in these expressions, the central building-block is the conditional WCDG probability measure $P_{\hat{Z}|\Theta}^{(P_S, \beta)} \in \Delta(\mathcal{X} \times \mathcal{Y} | \mathcal{M})$ in (46) (Definition 6). The first three subsections provide explicit expressions for the generalization error $\bar{G}(P_{\Theta|Z}, P_Z)$ aiming at establishing connections to existing results in statistics (statistical hypothesis testing), information theory (information measures), and Euclidian geometry (Pythagorean Theorems). The last section

focuses on the algorithm resulting from the WCDG probability measure.

A. Connections to Hypothesis Testing

A first connection to statistical hypothesis testing is made by the following theorem.

Theorem 22: Consider the generalization error $\overline{\overline{G}}(P_{\Theta|Z}, P_Z)$ in (11) and assume that:

- (a) The probability measure P_Z satisfies (22) for some $P_Z \in \Delta(\mathcal{X} \times \mathcal{Y})$;
- (b) For all $z \in (\mathcal{X} \times \mathcal{Y})^n$, the probability measures $P_{\Theta|Z=z}$ and P_{Θ} in (28) are mutually absolutely continuous;
- (c) For all $\theta \in \mathcal{M}$, the probability measures $P_{Z|\Theta=\theta}$ and P_Z in (35) are mutually absolutely continuous; and
- (d) For all $\theta \in \mathcal{M}$, the probability measures $P_{Z|\Theta=\theta}$ and P_Z satisfy (40) and are both mutually absolutely continuous with the probability measure $P_S \in \Delta(\mathcal{X} \times \mathcal{Y})$ in (46).

Then,

$$\begin{aligned} & \overline{\overline{G}}(P_{\Theta|Z}, P_Z) \\ &= \beta \left(\int \int \log \left(\frac{dP_S}{dP_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}}(z) \right) dP_{Z|\Theta=\theta}(z) dP_{\Theta}(\theta) \right. \\ & \quad \left. - \int \int \log \left(\frac{dP_S}{dP_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}}(z) \right) dP_Z(z) dP_{\Theta}(\theta) \right), \quad (96) \end{aligned}$$

where the probability measure $P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}$ is the WCDG probability measure in (46); and $\beta \in \mathcal{J}_{P_S}$, with \mathcal{J}_{P_S} in (45).

Proof: Under Assumptions (a), (b), (c), and (d), Lemma 7 holds. Then, the proof follows by observing that the difference $D(P_{Z|\Theta=\theta} \| P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}) - D(P_{Z|\Theta=\theta} \| P_S)$ and $D(P_Z \| P_S) - D(P_Z \| P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)})$ in (47) respectively satisfy the following equalities:

$$\begin{aligned} & D(P_{Z|\Theta=\theta} \| P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}) - D(P_{Z|\Theta=\theta} \| P_S) \\ &= \int \left(\log \frac{dP_{Z|\Theta=\theta}}{dP_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}}(z) - \log \frac{dP_{Z|\Theta=\theta}}{dP_S}(z) \right) dP_{Z|\Theta=\theta}(z) \quad (97) \\ &= \int \log \frac{dP_S}{dP_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}}(z) dP_{Z|\Theta=\theta}(z), \quad (98) \end{aligned}$$

where the equality in (98) follows from the Assumption (d). Similarly,

$$\begin{aligned} & D(P_Z \| P_S) - D(P_Z \| P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}) \\ &= \int \left(\log \frac{dP_Z}{dP_S}(z) - \log \frac{dP_Z}{dP_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}}(z) \right) dP_Z(z) \quad (99) \\ &= - \int \log \frac{dP_S}{dP_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}}(z) dP_Z(z), \quad (100) \end{aligned}$$

where the equality in (100) follows from Assumption (d). Plugging both (98) and (100) into (47) yields (96), which completes the proof. \blacksquare

Theorem 22 is reminiscent of Theorem 8, and thus, its relevance lies on the fact that it allows framing the generalization error $\overline{\overline{G}}(P_{\Theta|Z}, P_Z)$ in (11) within the context of mismatched hypothesis testing [47], [60]. Let the random variable $(Z, \Theta) \in (\mathcal{X} \times \mathcal{Y} \times \mathcal{M})$ follow the probability measure $P_{Z|\Theta} \cdot P_{\Theta} \in \Delta(\mathcal{X} \times \mathcal{Y} \times \mathcal{M})$, with P_{Θ} and $P_{Z|\Theta}$ satisfying (28) and (40). Let $(z, \theta) \in (\mathcal{X} \times \mathcal{Y}) \times \mathcal{M}$ be a realization of such a random variable. Consider a hypothesis test to decide whether the realization $(z, \theta) \in (\mathcal{X} \times \mathcal{Y}) \times \mathcal{M}$ has been generated by the product measure $P_S \cdot P_{\Theta}$ (*null hypothesis*) or the joint measure $P_{\hat{Z}|\Theta}^{(P_S, \beta)} \cdot P_{\Theta}$ (*alternative hypothesis*). The hypothesis testing is said to be mismatched because neither the null hypothesis nor the alternative hypothesis matches the ground-truth probability measure $P_{Z|\Theta} \cdot P_{\Theta}$. From this perspective, the term $\frac{dP_S}{dP_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}}(z)$, which satisfies for all $z \in \text{supp } P_Z$ and for all $\theta \in \text{supp } P_{\Theta}$,

$$\frac{dP_S}{dP_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}}(z) = \frac{dP_S \cdot P_{\Theta}}{dP_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)} \cdot P_{\Theta}}(z, \theta), \quad (101)$$

appears to be the log-likelihood ratio for deciding upon the observation (z, θ) between the null and alternative hypothesis.

Given an $\eta \in \mathbb{R}$, if $\log \left(\frac{dP_S}{dP_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}}(z) \right) \geq \eta$, then the null hypothesis is accepted. Alternatively, the null hypothesis is rejected and the alternative hypothesis is accepted if $\log \left(\frac{dP_S}{dP_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}}(z) \right) < \eta$. From this perspective, the expression in (96) can be interpreted as the variation of the expectation of the log-likelihood ratio of such a hypothesis testing problem, when the measure that generates the observations varies from the product of the marginal measures P_Z and P_{Θ} to the joint measure $P_{Z|\Theta} \cdot P_{\Theta}$.

The following theorem is reminiscent of Corollary 17 and might also be interpreted in the context of a statistical hypothesis test.

Theorem 23: Consider the generalization error $\overline{\overline{G}}(P_{\Theta|Z}, P_Z)$ in (11) and assume that:

- (a) The probability measure P_Z satisfies (22) for some $P_Z \in \Delta(\mathcal{X} \times \mathcal{Y})$;
- (b) For all $z \in (\mathcal{X} \times \mathcal{Y})^n$, the probability measures $P_{\Theta|Z=z}$ and P_{Θ} in (28) are mutually absolutely continuous;
- (c) For all $\theta \in \mathcal{M}$, the probability measures $P_{Z|\Theta=\theta}$ and P_Z in (35) are mutually absolutely continuous; and
- (d) For all $\theta \in \mathcal{M}$, the probability measures $P_{Z|\Theta=\theta}$ and P_Z satisfy (40) and are both mutually absolutely continuous with the probability measure $P_S \in \Delta(\mathcal{X} \times \mathcal{Y})$ in (46).

Then,

$$\begin{aligned} & \overline{\mathbb{G}}(P_{\Theta|Z}, P_Z) \\ &= \beta \left(\int \int \log \left(\frac{dP_Z}{dP_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}}(z) \right) dP_{Z|\Theta=\theta}(z) dP_{\Theta}(\theta) \right. \\ & \quad \left. - \int \int \log \left(\frac{dP_Z}{dP_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}}(z) \right) dP_Z(z) dP_{\Theta}(\theta) \right), \quad (102) \end{aligned}$$

where the measure $P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}$ is the WCDG probability measure in (46); and $\beta \in \mathcal{J}_{P_S}$, with \mathcal{J}_{P_S} in (45).

Proof: Under Assumptions (a), (b), (c), and (d), Lemma 7 holds. Also, under Assumptions (a) and (c), Lemma 48 holds. Then, the proof follows from the equality in (47) by noticing that

$$\begin{aligned} & \int (D(P_{Z|\Theta=\theta} \| P_S) - D(P_Z \| P_S)) dP_{\Theta}(\theta) \\ &= \int \int \log \left(\frac{dP_{Z|\Theta=\theta}}{dP_S}(z) \right) dP_{Z|\Theta=\theta}(z) dP_{\Theta}(\theta) \\ & \quad - D(P_Z \| P_S) \quad (103) \end{aligned}$$

$$\begin{aligned} &= \int \int \log \left(\frac{dP_{Z|\Theta=\theta}}{dP_S}(z) \frac{dP_Z}{dP_Z}(z) \right) dP_{Z|\Theta=\theta}(z) dP_{\Theta}(\theta) \\ & \quad - D(P_Z \| P_S) \quad (104) \end{aligned}$$

$$\begin{aligned} &= \int \int \log \left(\frac{dP_{Z|\Theta=\theta}}{dP_Z}(z) \frac{dP_Z}{dP_S}(z) \right) dP_{Z|\Theta=\theta}(z) dP_{\Theta}(\theta) \\ & \quad - D(P_Z \| P_S) \quad (105) \end{aligned}$$

$$\begin{aligned} &= \int \int \log \left(\frac{dP_{Z|\Theta=\theta}}{dP_Z}(z) \right) dP_{Z|\Theta=\theta}(z) dP_{\Theta}(\theta) \\ & \quad + \int \int \log \left(\frac{dP_Z}{dP_S}(z) \right) dP_{Z|\Theta=\theta}(z) dP_{\Theta}(\theta) \\ & \quad - D(P_Z \| P_S) \quad (106) \end{aligned}$$

$$\begin{aligned} &= \int \int \log \left(\frac{dP_{Z|\Theta=\theta}}{dP_Z}(z) \right) dP_{Z|\Theta=\theta}(z) dP_{\Theta}(\theta) \\ & \quad + \int \log \left(\frac{dP_Z}{dP_S}(z) \right) dP_Z(z) - D(P_Z \| P_S) \quad (107) \end{aligned}$$

$$\begin{aligned} &= \int \int \log \left(\frac{dP_{Z|\Theta=\theta}}{dP_Z}(z) \right) dP_{Z|\Theta=\theta}(z) dP_{\Theta}(\theta), \quad (108) \end{aligned}$$

where the equality in (105) follows from Assumptions (a), (c), and (d), together with Lemma 48 (in Appendix A). Plugging (108) in (47) yields

$$\begin{aligned} \overline{\mathbb{G}}(P_{\Theta|Z}, P_Z) &= \beta \int \left(D(P_{Z|\Theta=\theta} \| P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}) - D(P_Z \| P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}) \right) \\ & \quad - \int \log \left(\frac{dP_{Z|\Theta=\theta}}{dP_Z}(z) \right) dP_{Z|\Theta=\theta}(z) dP_{\Theta}(\theta). \quad (109) \end{aligned}$$

Note also that from Assumptions (a) and (c), together with

Lemma 48 (in Appendix A), it holds that

$$\begin{aligned} & \int D(P_{Z|\Theta=\theta} \| P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}) dP_{\Theta}(\theta) \\ & - \int \int \log \left(\frac{dP_{Z|\Theta=\theta}}{dP_Z}(z) \right) dP_{Z|\Theta=\theta}(z) dP_{\Theta}(\theta) \quad (110) \end{aligned}$$

$$= \int \int \log \left(\frac{dP_Z}{dP_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}}(z) \right) dP_{Z|\Theta=\theta}(z) dP_{\Theta}(\theta). \quad (111)$$

By substituting (111) in (109) leads to (102), which completes the proof. \blacksquare

The right-hand side of (102) shows a connection to a mismatched hypothesis test. In this case, the goal is to decide whether the observation $(z, \theta) \in (\mathcal{X} \times \mathcal{Y}) \times \mathcal{M}$, sampled from $P_{Z|\Theta} \cdot P_{\Theta}$, is generated from $P_Z \cdot P_{\Theta}$ (null hypothesis) or the probability measure $P_{\hat{Z}|\Theta}^{(P_S, \beta)} \cdot P_{\Theta}$ (alternative hypothesis). Then, the term $\frac{dP_Z}{dP_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}}(z)$ appears to be the likelihood ratio

for deciding based upon the observation (z, θ) on the null or the alternative hypothesis. From this perspective, the generalization error $\overline{\mathbb{G}}(P_{\Theta|Z}, P_Z)$ in (11) can be interpreted as the variation of the expectation of the log-likelihood ratio of such a hypothesis testing problem, when the measure that generates the observations varies from the product of the marginal measures P_Z and P_{Θ} to the joint measure $P_{Z|\Theta} \cdot P_{\Theta}$.

B. Connections to Information Measures

Two particular choices for the reference measure P_S in (47) lead to closed-form expressions for the generalization error $\overline{\mathbb{G}}(P_{\Theta|Z}, P_Z)$ in (11) involving either the mutual information $I(P_{Z|\Theta}; P_{\Theta})$ or the lautum information $L(P_{Z|\Theta}; P_{\Theta})$. These choices correspond to cases in which the gap $\mathbb{G}(\theta, P_Z, P_{Z|\Theta=\theta})$ in (42) is calculated using either P_Z or $P_{Z|\Theta=\theta}$ instead of the reference measure P_S . From Lemma 7, it follows that the case in which the reference measure is P_Z leads to an expression involving the mutual information $I(P_{Z|\Theta}; P_{\Theta})$.

Corollary 24: Consider the generalization error $\overline{\mathbb{G}}(P_{\Theta|Z}, P_Z)$ in (11) and assume that:

- (a) The probability measure P_Z satisfies (22) for some $P_Z \in \Delta(\mathcal{X} \times \mathcal{Y})$;
- (b) For all $z \in (\mathcal{X} \times \mathcal{Y})^n$, the probability measures $P_{\Theta|Z=z}$ and P_{Θ} in (28) are mutually absolutely continuous; and
- (c) For all $\theta \in \mathcal{M}$, the probability measures $P_{Z|\Theta=\theta}$ and P_Z in (35) are mutually absolutely continuous.

Then,

$$\begin{aligned} \overline{\mathbb{G}}(P_{\Theta|Z}, P_Z) &= -\beta I(P_{Z|\Theta}; P_{\Theta}) \\ & \quad + \beta \int D(P_{Z|\Theta=\theta} \| P_{\hat{Z}|\Theta=\theta}^{(P_Z, \beta)}) dP_{\Theta}(\theta) \\ & \quad - \beta \int D(P_Z \| P_{\hat{Z}|\Theta=\theta}^{(P_Z, \beta)}) dP_{\Theta}(\theta), \quad (112) \end{aligned}$$

where the probability measure $P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}$ is defined in (46); and $\beta \in \mathcal{J}_{P_S}$ with \mathcal{J}_{P_S} in (45).

Alternatively, from Lemma 7, it follows that the case in which the reference measure is $P_{Z|\Theta=\theta}$ leads to an expression involving the lautum information $L(P_{Z|\Theta}; P_{\Theta})$.

Corollary 25: Consider the generalization error $\overline{\overline{G}}(P_{\Theta|Z}, P_Z)$ in (11) and assume that:

- (a) The probability measure P_Z satisfies (22) for some $P_Z \in \Delta(\mathcal{X} \times \mathcal{Y})$;
- (b) For all $z \in (\mathcal{X} \times \mathcal{Y})^n$, the probability measures $P_{\Theta|Z=z}$ and P_{Θ} in (28) are mutually absolutely continuous; and
- (c) For all $\theta \in \mathcal{M}$, the probability measures $P_{Z|\Theta=\theta}$ and P_Z in (35) are mutually absolutely continuous.

Then,

$$\begin{aligned} \overline{\overline{G}}(P_{\Theta|Z}, P_Z) &= \beta L(P_{Z|\Theta}; P_{\Theta}) \\ &+ \beta \int D\left(P_{Z|\Theta=\theta} \| P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}\right) dP_{\Theta}(\theta) \\ &- \beta \int D\left(P_Z \| P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}\right) dP_{\Theta}(\theta), \end{aligned} \quad (113)$$

where the probability measure $P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}$ is defined in (46); and $\beta \in \mathcal{J}_{P_S}$, with \mathcal{J}_{P_S} in (45).

Independently of the choice of P_S in (47), under the condition that $P_S \in \Delta(\mathcal{X} \times \mathcal{Y})$ (and not in $\Delta((\mathcal{X} \times \mathcal{Y})|\mathcal{M})$), the generalization error $\overline{\overline{G}}(P_{\Theta|Z}, P_Z)$ in (11) can be written in terms of a mutual information as follows.

Theorem 26: Consider the generalization error $\overline{\overline{G}}(P_{\Theta|Z}, P_Z)$ in (11) and assume that:

- (a) The probability measure P_Z satisfies (22) for some $P_Z \in \Delta(\mathcal{X} \times \mathcal{Y})$;
- (b) For all $z \in (\mathcal{X} \times \mathcal{Y})^n$, the probability measures $P_{\Theta|Z=z}$ and P_{Θ} in (28) are mutually absolutely continuous;
- (c) For all $\theta \in \mathcal{M}$, the probability measures $P_{Z|\Theta=\theta}$ and P_Z in (35) are mutually absolutely continuous; and
- (d) For all $\theta \in \mathcal{M}$, the probability measures $P_{Z|\Theta=\theta}$ and P_Z satisfy (40) and are both mutually absolutely continuous with the probability measure $P_S \in \Delta(\mathcal{X} \times \mathcal{Y})$ in (46).

Then,

$$\begin{aligned} \overline{\overline{G}}(P_{\Theta|Z}, P_Z) &= -\beta I(P_{Z|\Theta}; P_{\Theta}) \\ &+ \beta \int D\left(P_{Z|\Theta=\theta} \| P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}\right) dP_{\Theta}(\theta) \\ &- \beta \int D\left(P_Z \| P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}\right) dP_{\Theta}(\theta), \end{aligned} \quad (114)$$

where the probability measure $P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}$ is defined in (46); and $\beta \in \mathcal{J}_{P_S}$ with \mathcal{J}_{P_S} in (45).

Proof: Under Assumptions (a), (b), (c), and (d), Lemma 7 holds. Under Assumptions (a) and (c), Lemma 48 and Lemma 49 (in Appendix A) imply that for all $\theta \in \mathcal{M}$, the probability measures $P_{Z|\Theta=\theta}$ and P_Z are mutually absolutely continuous. Hence, the proof follows from the equality in (47)

by noticing that if $P_S \in \Delta(\mathcal{X} \times \mathcal{Y})$, under Assumption (d), then

$$\begin{aligned} &\int (D(P_{Z|\Theta=\theta} \| P_S) - D(P_Z \| P_S)) dP_{\Theta}(\theta) \\ &= I(P_{Z|\Theta}; P_{\Theta}), \end{aligned} \quad (115)$$

which completes the proof. \blacksquare

The importance of Theorem 26 lies on the fact that it allows the flexibility of choosing a reference measure P_S within $\Delta(\mathcal{X} \times \mathcal{Y})$, provided that Assumption (d) is met. Such a flexibility can also be preserved while using the lautum information $L(P_{Z|\Theta}; P_{\Theta})$, as shown by the following theorem.

Theorem 27: Consider the generalization error $\overline{\overline{G}}(P_{\Theta|Z}, P_Z)$ in (11) and assume that:

- (a) The probability measure P_Z satisfies (22) for some $P_Z \in \Delta(\mathcal{X} \times \mathcal{Y})$;
- (b) For all $z \in (\mathcal{X} \times \mathcal{Y})^n$, the probability measures $P_{\Theta|Z=z}$ and P_{Θ} in (28) are mutually absolutely continuous;
- (c) For all $\theta \in \mathcal{M}$, the probability measures $P_{Z|\Theta=\theta}$ and P_Z in (35) are mutually absolutely continuous; and
- (d) For all $\theta \in \mathcal{M}$, the probability measures $P_{Z|\Theta=\theta}$ and P_Z satisfy (40) and are both absolutely continuous with the probability measure $P_S \in \Delta(\mathcal{X} \times \mathcal{Y})$ in (46).

Then,

$$\begin{aligned} &\overline{\overline{G}}(P_{\Theta|Z}, P_Z) \\ &= \beta L(P_{Z|\Theta}; P_{\Theta}) + \beta \int \left(D\left(P_{Z|\Theta=\theta} \| P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}\right) \right. \\ &\quad \left. - D\left(P_Z \| P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}\right) - D(P_{Z|\Theta=\theta} \| P_S) \right. \\ &\quad \left. + \int \log \frac{dP_{Z|\Theta=\theta}}{dP_S}(z) dP_Z(z) \right) dP_{\Theta}(\theta), \end{aligned} \quad (116)$$

where the probability measure $P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}$ is defined in (46); and $\beta \in \mathcal{J}_{P_S}$, with \mathcal{J}_{P_S} in (45).

Proof: Under Assumptions (a), (b), (c), and (d), Lemma 7 holds. Under Assumptions (a) and (c), Lemma 48 and Lemma 49 (in Appendix A) imply that for all $\theta \in \mathcal{M}$, the probability measures $P_{Z|\Theta=\theta}$ and P_Z are mutually absolutely continuous. Hence, the proof follows from the equality in (47)

by noticing that

$$\begin{aligned} & \int D(P_Z \| P_S) dP_{\Theta}(\theta) \\ &= \int \int \log \left(\frac{dP_Z}{dP_{Z|\Theta=\theta}}(z) \frac{dP_{Z|\Theta=\theta}}{dP_S}(z) \right) dP_Z(z) dP_{\Theta}(\theta) \quad (117) \end{aligned}$$

$$\begin{aligned} &= \int \int \log \frac{dP_Z}{dP_{Z|\Theta=\theta}}(z) dP_Z(z) dP_{\Theta}(\theta) \\ &+ \int \int \log \frac{dP_{Z|\Theta=\theta}}{dP_S}(z) dP_Z(z) dP_{\Theta}(\theta) \quad (118) \end{aligned}$$

$$\begin{aligned} &= \int D(P_Z \| P_{Z|\Theta=\theta}) dP_{\Theta}(\theta) \\ &+ \int \int \log \frac{dP_{Z|\Theta=\theta}}{dP_S}(z) dP_Z(z) dP_{\Theta}(\theta) \quad (119) \end{aligned}$$

$$\begin{aligned} &= L(P_{Z|\Theta}; P_{\Theta}) \\ &+ \int \int \log \frac{dP_{Z|\Theta=\theta}}{dP_S}(z) dP_Z(z) dP_{\Theta}(\theta). \quad (120) \end{aligned}$$

The proof is completed by using (120) in (47), which leads to the equality in (116). \blacksquare

The following corollary of Theorem 26 and Theorem 27 is reminiscent of Corollary 13, as it provides an equivalent expression to the sum of the mutual information $I(P_{Z|\Theta}; P_{\Theta})$ and the lautum information $L(P_{Z|\Theta}; P_{\Theta})$ by substrating (116) from (114).

Corollary 28: Given a conditional probability measure $P_{\Theta|Z} \in \Delta(\mathcal{M} | (\mathcal{X} \times \mathcal{Y})^n)$ and a probability measure $P_Z \in \Delta((\mathcal{X} \times \mathcal{Y})^n)$, assume that:

- (a) The probability measure P_Z satisfies (22) for some $P_Z \in \Delta(\mathcal{X} \times \mathcal{Y})$;
- (b) For all $z \in (\mathcal{X} \times \mathcal{Y})^n$, the probability measures $P_{\Theta|Z=z}$ and P_{Θ} in (28) are mutually absolutely continuous;
- (c) For all $\theta \in \mathcal{M}$, the probability measures $P_{Z|\Theta=\theta}$ and P_Z in (35) are mutually absolutely continuous; and
- (d) For all $\theta \in \mathcal{M}$, the probability measures $P_{Z|\Theta=\theta}$ and P_Z satisfy (40) and are both mutually absolutely continuous with the probability measure $P_S \in \Delta(\mathcal{X} \times \mathcal{Y})$ in (46).

Then,

$$\begin{aligned} & I(P_{Z|\Theta}; P_{\Theta}) + L(P_{Z|\Theta}; P_{\Theta}) \\ &= \int \int \log \frac{dP_{Z|\Theta=\theta}}{dP_S}(z) dP_{Z|\Theta=\theta}(z) dP_{\Theta}(\theta) \\ &- \int \int \log \frac{dP_{Z|\Theta=\theta}}{dP_S}(z) dP_Z(z) dP_{\Theta}(\theta). \quad (121) \end{aligned}$$

Similar to Corollary 13, this alternative expression for the sum of the mutual information and the lautum information is interesting as it is formulated in terms of a free parameter P_S , which can be chosen subject to condition (b). This equality also shows a connection to hypothesis testing. More specifically, the goal is to decide whether the observation $(z, \theta) \in (\mathcal{X} \times \mathcal{Y}) \times \mathcal{M}$ has been generated by the joint measure $P_{Z|\Theta} \cdot P_{\Theta}$ (*null hypothesis*) or the product measure $P_S \cdot P_{\Theta}$ (*alternative hypothesis*). Then, the term $\frac{dP_{Z|\Theta=\theta}}{dP_S}$ appears to represent the likelihood ratio for this

matched hypothesis testing. From this perspective, the sum of the mutual information and the lautum information can be interpreted as the variation of the expectation of the log-likelihood ratio of such a hypothesis testing problem, when the measure that generates the observations varies from the joint measure $P_{Z|\Theta} \cdot P_{\Theta}$ to the product measure $P_Z \cdot P_{\Theta}$.

The following theorem provides an expression for the generalization error $\bar{G}(P_{\Theta|Z}, P_Z)$ in (11) involving the sum of the mutual and the lautum information in Corollary 28.

Theorem 29: Consider the generalization error $\bar{G}(P_{\Theta|Z}, P_Z)$ in (11) and assume that:

- (a) The probability measure P_Z satisfies (22) for some $P_Z \in \Delta(\mathcal{X} \times \mathcal{Y})$;
- (b) For all $z \in (\mathcal{X} \times \mathcal{Y})^n$, the probability measures $P_{\Theta|Z=z}$ and P_{Θ} in (28) are mutually absolutely continuous;
- (c) For all $\theta \in \mathcal{M}$, the probability measures $P_{Z|\Theta=\theta}$ and P_Z in (35) are mutually absolutely continuous; and
- (d) For all $\theta \in \mathcal{M}$, the probability measures $P_{Z|\Theta=\theta}$ and P_Z satisfy (40) and are both mutually absolutely continuous with the probability measure $P_S \in \Delta(\mathcal{X} \times \mathcal{Y})$ in (46).

Then,

$$\begin{aligned} \bar{G}(P_{\Theta|Z}, P_Z) &= -\beta (I(P_{Z|\Theta}; P_{\Theta}) + L(P_{Z|\Theta}; P_{\Theta})) \\ &+ \beta \int \int \log \left(\frac{dP_{Z|\Theta=\theta}}{dP_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}}(z) \right) dP_{Z|\Theta=\theta}(z) dP_{\Theta}(\theta) \\ &- \beta \int \int \log \left(\frac{dP_{Z|\Theta=\theta}}{dP_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}}(z) \right) dP_Z(z) dP_{\Theta}(\theta), \quad (122) \end{aligned}$$

where the probability measure $P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}$ is defined in (46); $\beta \in \mathcal{J}_{P_S}$ with \mathcal{J}_{P_S} in (45).

Proof: The proof follows from Theorem 26, which holds under Assumptions (a), (b), (c), and (d). Note that in (114), the following holds:

$$\begin{aligned} & - \int D(P_Z \| P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}) dP_{\Theta}(\theta) \\ &= - \int \int \log \left(\frac{dP_Z}{dP_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}}(z) \frac{dP_{\hat{Z}|\Theta=\theta}}{dP_{Z|\Theta=\theta}}(z) \right) dP_Z(z) dP_{\Theta}(\theta) \quad (123) \end{aligned}$$

$$\begin{aligned} &= \int \left(- \int \log \left(\frac{dP_Z}{dP_{Z|\Theta=\theta}}(z) \right) dP_Z(z) \right. \\ &\quad \left. - \int \log \left(\frac{dP_{\hat{Z}|\Theta=\theta}}{dP_{Z|\Theta=\theta}^{(P_S, \beta)}}(z) \right) dP_Z(z) \right) dP_{\Theta}(\theta) \quad (124) \end{aligned}$$

$$\begin{aligned} &= -L(P_{Z|\Theta}; P_{\Theta}) \\ &- \int \int \log \left(\frac{dP_{\hat{Z}|\Theta=\theta}}{dP_{Z|\Theta=\theta}^{(P_S, \beta)}}(z) \right) dP_Z(z) dP_{\Theta}(\theta), \quad (125) \end{aligned}$$

where the equality in (124) follows from Assumptions (a) and (d) and Lemma 49 (in Appendix A), which imply that for all $\theta \in \mathcal{M}$, the probability measures $P_{Z|\Theta=\theta}$ and P_Z are

mutually absolutely continuous. The proof ends by using the equality (125) into (114), which yields (122). \blacksquare

Note that the integrals on the right-hand side of (122) show a connection to a matched hypothesis testing [63]. More specifically, the goal is to decide whether an observation $(z, \theta) \in (\mathcal{X} \times \mathcal{Y}) \times \mathcal{M}$, sampled from $P_{Z|\Theta} \cdot P_{\Theta}$, is generated from $P_{Z|\Theta=\theta} \cdot P_{\Theta}$ (*null hypothesis*) or the probability measure $P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)} \cdot P_{\Theta}$ (*alternative hypothesis*). In this context, for all $z \in \text{supp } P_Z$ and for all $\theta \in \text{supp } P_{\Theta}$,

$$\frac{dP_{Z|\Theta=\theta}}{dP_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}}(z) = \frac{dP_{Z|\Theta=\theta} \cdot P_{\Theta}}{dP_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)} \cdot P_{\Theta}}(z, \theta), \quad (126)$$

appears to be the log-likelihood ratio for deciding upon the observation (z, θ) between the null and alternative hypothesis. The hypothesis test is said to be matched because $P_{Z|\Theta} \cdot P_{\Theta}$ (null hypothesis) is the ground-truth probability measure. From this perspective, the generalization error $\bar{G}(P_{\Theta|Z}, P_Z)$ in (11) can be interpreted as the variation of the expectation of the log-likelihood ratio of such a hypothesis testing problem, when the measure that generates the observations varies from the product of the marginal measures P_Z and P_{Θ} to the joint measure $P_{Z|\Theta} \cdot P_{\Theta}$.

C. Connections to Euclidian Geometry

The following lemma presents an alternative expression for the generalization error $\bar{G}(P_{\Theta|Z}, P_Z)$ in (11), in terms of the variation of the functional R_{θ} in (8) due to changes of the parameter $\theta \in \mathcal{M}$.

Lemma 30: Consider the generalization error $\bar{G}(P_{\Theta|Z}, P_Z)$ in (11) and assume that for all $\theta \in \mathcal{M}$

- (a) The probability measures P_{Θ} in (28) and the probability measure $P_{Z|\Theta=\theta}$ satisfy (35);
- (b) for all $\theta \in \mathcal{M}$, the probability measures $P_{Z|\Theta=\theta}$ and P_Z are mutually absolutely continuous; and
- (c) For all $z \in (\mathcal{X} \times \mathcal{Y})^n$, the probability measures $P_{\Theta|Z=z}$ and P_{Θ} in (28) are mutually absolutely continuous;

Then,

$$\bar{G}(P_{\Theta|Z}, P_Z) = \int \int \left(R_{\nu}(P_{Z|\Theta=\theta}) - R_{\theta}(P_{Z|\Theta=\theta}) \right) dP_{\Theta}(\nu) dP_{\Theta}(\theta), \quad (127)$$

where the functional R_{θ} is defined in (8).

Proof: The proof follows from observing two series of equal-

ities. The first equalities are:

$$\begin{aligned} & \int \int R_{\nu}(P_{Z|\Theta=\theta}) dP_{\Theta}(\nu) dP_{\Theta}(\theta) \\ &= \int \int \left(\int L(z, \nu) dP_{Z|\Theta=\theta}(z) \right) dP_{\Theta}(\nu) dP_{\Theta}(\theta) \quad (128) \end{aligned}$$

$$= \int \int \left(\int L(z, \nu) dP_{\Theta}(\nu) \right) dP_{Z|\Theta=\theta}(z) dP_{\Theta}(\theta) \quad (129)$$

$$= \int \int R_z(P_{\Theta}) dP_{Z|\Theta=\theta}(z) dP_{\Theta}(\theta) \quad (130)$$

$$= \int \int R_z(P_{\Theta}) \frac{dP_{Z|\Theta=\theta}}{dP_Z}(z) dP_Z(z) dP_{\Theta}(\theta) \quad (131)$$

$$= \int R_z(P_{\Theta}) \left(\int \frac{dP_{Z|\Theta=\theta}}{dP_Z}(z) dP_{\Theta}(\theta) \right) dP_Z(z) \quad (132)$$

$$= \int R_z(P_{\Theta}) dP_Z(z), \quad (133)$$

where the equality in (128) follows from (8); the equality in (129) follows by exchanging the order of the integrals [50, Theorem 2.6.6]; the equality in (130) follows from (9); the equality in (131) follows from Assumption (b) and [61, Theorem 2.2.3]; the equality in (132) follows from [50, Theorem 2.6.3]; and the equality in (133) follows from the fact that [50, Theorem 4.5.2]:

$$\int \frac{dP_{Z|\Theta=\theta}}{dP_Z}(z) dP_{\Theta}(\theta) = 1. \quad (134)$$

The second equalities are:

$$\begin{aligned} & \int \int R_{\theta}(P_{Z|\Theta=\theta}) dP_{\Theta}(\nu) dP_{\Theta}(\theta) \\ &= \int R_{\theta}(P_{Z|\Theta=\theta}) dP_{\Theta}(\theta) \quad (135) \end{aligned}$$

$$= \int \int L(z, \theta) dP_{Z|\Theta=\theta}(z) dP_{\Theta}(\theta) \quad (136)$$

$$= \int \int L(z, \theta) \frac{dP_{Z|\Theta=\theta}}{dP_Z}(z) dP_Z(z) dP_{\Theta}(\theta) \quad (137)$$

$$= \int \int L(z, \theta) \frac{dP_{Z|\Theta=\theta}}{dP_Z}(z) dP_{\Theta}(\theta) dP_Z(z) \quad (138)$$

$$= \int \int L(z, \theta) \frac{dP_{Z|\Theta=\theta}}{dP_Z}(z) \frac{dP_{\Theta}}{dP_{\Theta|Z=z}}(\theta) dP_{\Theta|Z=z}(\theta) dP_Z(z) \quad (139)$$

$$= \int \int L(z, \theta) dP_{\Theta|Z=z}(\theta) dP_Z(z) \quad (140)$$

$$= \int R_z(P_{\Theta|Z=z}) dP_Z(z), \quad (141)$$

where the equality in (136) follows from (8); the equality in (137) follows from Assumption (b) and [61, Theorem 2.2.3]; the equality in (138) follows from [50, Theorem 2.6.6]; the equality in (139) follows from Assumption (c) and [61, Theorem 2.2.3]; the equality in (140) follows from Assumption (b), which together with Lemma 46 and Lemma 47 (in Appendix A) imply that for all $(z, \theta) \in (\mathcal{X} \times \mathcal{Y})^n \times \mathcal{M}$,

$$\frac{dP_{Z|\Theta=\theta}}{dP_Z}(z) \frac{dP_{\Theta}}{dP_{\Theta|Z=z}}(\theta) = 1; \quad (142)$$

and the equality in (141) follows from (9).

From (133) and (141), it follows that

$$\int \int \left(R_\nu(P_{Z|\Theta=\theta}) - R_\theta(P_{Z|\Theta=\theta}) \right) dP_\Theta(\nu) dP_\Theta(\theta) \quad (143)$$

$$= \int R_z(P_\Theta) dP_Z(z) - \int R_z(P_{\Theta|Z=z}) dP_Z(z) \quad (144)$$

$$= \int G(z, P_\Theta, P_{\Theta|Z=z}) dP_Z(z) \quad (145)$$

$$= \bar{G}(P_{\Theta|Z}, P_Z), \quad (146)$$

where the equality in (145) follows from (20); and the equality in (146) follows from Lemma 3. This completes the proof. \blacksquare

Lemma 30 introduces an alternative expression for the generalization error $\bar{G}(P_{\Theta|Z}, P_Z)$ that is reminiscent of the expression in (11). More specifically, Lemma 30 presents $\bar{G}(P_{\Theta|Z}, P_Z)$ as the expectation of the variation

$$R_\nu(P_{Z|\Theta=\theta}) - R_\theta(P_{Z|\Theta=\theta}),$$

under the assumption that models ν and θ are independently sampled from the same probability measure $P_\Theta \in \Delta(\mathcal{M})$ in (28). The following theorem leverages this observation to obtain an equivalent expression for the the generalization error $\bar{G}(P_{\Theta|Z}, P_Z)$ that is of a similar form to the one introduced by Theorem 18.

Theorem 31: Consider the generalization error $\bar{G}(P_{\Theta|Z}, P_Z)$ in (11) and assume that:

- (a) The probability measure P_Z satisfies (22) for some $P_Z \in \Delta(\mathcal{X} \times \mathcal{Y})$;
- (b) The probability measures P_Θ in (28) and the probability measure $P_{Z|\Theta=\theta}$ satisfy (35);
- (c) For all $\theta \in \mathcal{M}$, the probability measures $P_{Z|\Theta=\theta}$ and P_Z are mutually absolutely continuous;
- (d) For all $z \in (\mathcal{X} \times \mathcal{Y})^n$, the probability measures $P_{\Theta|Z=z}$ and P_Θ in (28) are mutually absolutely continuous; and
- (e) For all $\theta \in \mathcal{M}$, the probability measures $P_{Z|\Theta=\theta}$ and P_Z satisfy (40) and are both mutually absolutely continuous with the probability measure $P_S \in \Delta(\mathcal{X} \times \mathcal{Y})$ in (46).

Then,

$$\bar{G}(P_{\Theta|Z}, P_Z) = \beta \int \int \left(D(P_{Z|\Theta=\mu} \| P_{\hat{Z}|\Theta=\mu}^{(P_S, \beta)}) - D(P_{Z|\Theta=\mu} \| P_{\hat{Z}|\Theta=\nu}^{(P_S, \beta)}) \right) dP_\Theta(\nu) dP_\Theta(\mu), \quad (147)$$

where the measure $P_{\hat{Z}|\Theta=\mu}^{(P_S, \beta)}$ is the WCDG probability measure in (46); and $\beta \in \mathcal{J}_{P_S}$, with \mathcal{J}_{P_S} in (45).

Proof: The proof follows from Lemma 30, which holds under Assumptions (b), (c), and (d). More specifically, the proof consists of re-writing the difference $R_\nu(P_{Z|\Theta=\mu}) - R_\mu(P_{Z|\Theta=\mu})$ in (127) using the functional G in (21). Under Assumption (a) and Lemma 5, note that for all $(\nu, \mu) \in \mathcal{M} \times \mathcal{M}$,

$$R_\nu(P_{Z|\Theta=\mu}) = \int \ell(\nu, x, y) dP_{Z|\Theta=\mu}(x, y), \quad (148)$$

where the conditional probability measure $P_{Z|\Theta}$ satisfies (40). Hence, the following holds for all $(\mu, \nu) \in \mathcal{M} \times \mathcal{M}$,

$$\begin{aligned} & R_\nu(P_{Z|\Theta=\mu}) \\ &= G(\nu, P_{Z|\Theta=\mu}, P_{\hat{Z}|\Theta=\nu}^{(P_S, \beta)}) + \int \ell(\nu, x, y) dP_{\hat{Z}|\Theta=\nu}^{(P_S, \beta)}(x, y), \end{aligned} \quad (149)$$

and

$$\begin{aligned} & R_\mu(P_{Z|\Theta=\mu}) \\ &= G(\mu, P_{Z|\Theta=\mu}, P_{\hat{Z}|\Theta=\mu}^{(P_S, \beta)}) + \int \ell(\mu, x, y) dP_{\hat{Z}|\Theta=\mu}^{(P_S, \beta)}(x, y), \end{aligned} \quad (150)$$

where the functional G is defined in (21). From Assumption (e) and Lemma 42 (in Section VIII), it holds that

$$\begin{aligned} & G(\nu, P_{Z|\Theta=\mu}, P_{\hat{Z}|\Theta=\nu}^{(P_S, \beta)}) \\ &= \beta \left(D(P_{Z|\Theta=\mu} \| P_S) - D(P_{Z|\Theta=\mu} \| P_{\hat{Z}|\Theta=\nu}^{(P_S, \beta)}) \right. \\ & \quad \left. - D(P_{\hat{Z}|\Theta=\nu}^{(P_S, \beta)} \| P_S) \right), \end{aligned} \quad (151)$$

and

$$\begin{aligned} & G(\mu, P_{Z|\Theta=\mu}, P_{\hat{Z}|\Theta=\mu}^{(P_S, \beta)}) \\ &= \beta \left(D(P_{Z|\Theta=\mu} \| P_S) - D(P_{Z|\Theta=\mu} \| P_{\hat{Z}|\Theta=\mu}^{(P_S, \beta)}) \right. \\ & \quad \left. - D(P_{\hat{Z}|\Theta=\mu}^{(P_S, \beta)} \| P_S) \right). \end{aligned} \quad (152)$$

Using these equalities, it follows from (149) and (150) that

$$\begin{aligned} & R_\nu(P_{Z|\Theta=\mu}) - R_\mu(P_{Z|\Theta=\mu}) \\ &= G(\nu, P_{Z|\Theta=\mu}, P_{\hat{Z}|\Theta=\nu}^{(P_S, \beta)}) + \int \ell(\nu, x, y) dP_{\hat{Z}|\Theta=\nu}^{(P_S, \beta)}(x, y) \\ & \quad - G(\mu, P_{Z|\Theta=\mu}, P_{\hat{Z}|\Theta=\mu}^{(P_S, \beta)}) - \int \ell(\mu, x, y) dP_{\hat{Z}|\Theta=\mu}^{(P_S, \beta)}(x, y) \quad (153) \\ &= \beta \left(-D(P_{Z|\Theta=\mu} \| P_{\hat{Z}|\Theta=\nu}^{(P_S, \beta)}) - D(P_{\hat{Z}|\Theta=\nu}^{(P_S, \beta)} \| P_S) \right) \\ & \quad - \beta \left(-D(P_{Z|\Theta=\mu} \| P_{\hat{Z}|\Theta=\mu}^{(P_S, \beta)}) - D(P_{\hat{Z}|\Theta=\mu}^{(P_S, \beta)} \| P_S) \right) \\ & \quad + \int \ell(\nu, x, y) dP_{\hat{Z}|\Theta=\nu}^{(P_S, \beta)}(x, y) \\ & \quad - \int \ell(\mu, x, y) dP_{\hat{Z}|\Theta=\mu}^{(P_S, \beta)}(x, y) \end{aligned} \quad (154)$$

$$\begin{aligned} &= \beta D(P_{Z|\Theta=\mu} \| P_{\hat{Z}|\Theta=\mu}^{(P_S, \beta)}) - \beta D(P_{Z|\Theta=\mu} \| P_{\hat{Z}|\Theta=\nu}^{(P_S, \beta)}) \\ & \quad + \int \ell(\nu, x, y) dP_{\hat{Z}|\Theta=\nu}^{(P_S, \beta)}(x, y) - \beta D(P_{\hat{Z}|\Theta=\nu}^{(P_S, \beta)} \| P_S) \\ & \quad - \int \ell(\mu, x, y) dP_{\hat{Z}|\Theta=\mu}^{(P_S, \beta)}(x, y) + \beta D(P_{\hat{Z}|\Theta=\mu}^{(P_S, \beta)} \| P_S) \end{aligned} \quad (155)$$

where the equality in (154) follows from both (151) and (152).

Therefore, from Lemma 30, it follows that

$$\begin{aligned} & \overline{\mathbb{G}}(P_{\Theta|Z}, P_Z) \\ &= \int \int R_{\nu}(P_{Z|\Theta=\mu}) - R_{\mu}(P_{Z|\Theta=\mu}) dP_{\Theta}(\nu) dP_{\Theta}(\mu) \quad (156) \\ &= \beta \int \int \left(D(P_{Z|\Theta=\mu} \| P_{\hat{Z}|\Theta=\mu}^{(P_S, \beta)}) \right. \\ & \quad \left. - D(P_{Z|\Theta=\mu} \| P_{\hat{Z}|\Theta=\nu}^{(P_S, \beta)}) \right) dP_{\Theta}(\nu) dP_{\Theta}(\mu), \quad (157) \end{aligned}$$

which completes the proof. \blacksquare

Theorem 31 expresses the generalization error as the difference between the expectations of two relative entropies. The first relative entropy compares the likelihood $P_{Z|\Theta=\theta}$ to the WCDG probability measure $P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}$, under the observation of the same model θ , which is drawn from P_{Θ} in (28). The second relative entropy compares these two conditional probability measures under the case that the observed models are dawning independently from the same probability measure P_{Θ} . More interestingly, the second relative entropy satisfies the following property.

Lemma 32: Consider a probability measure $P_Z \in \Delta((\mathcal{X} \times \mathcal{Y})^n)$ and a conditional probability measure $P_{\Theta|Z} \in \Delta(\mathcal{M} | (\mathcal{X} \times \mathcal{Y})^n)$ and assume that:

- (a) The probability measure P_Z satisfies (22) for some $P_Z \in \Delta(\mathcal{X} \times \mathcal{Y})$;
- (b) The probability measures P_{Θ} in (28) and the probability measure $P_{Z|\Theta=\theta}$ satisfy (35);
- (c) For all $\theta \in \mathcal{M}$, the probability measure $P_{Z|\Theta=\theta}$ is absolutely continuous with respect to P_Z ; and
- (d) For all $\theta \in \mathcal{M}$, the probability measures $P_{Z|\Theta=\theta}$ and P_Z satisfy (40) and are both absolutely continuous with the probability measure $P_S \in \Delta(\mathcal{X} \times \mathcal{Y})$ in (46).

Then,

$$\begin{aligned} & \int \int D(P_{Z|\Theta=\theta} \| P_{\hat{Z}|\Theta=\nu}^{(P_S, \beta)}) dP_{\Theta}(\nu) dP_{\Theta}(\theta) \\ &= \int \left(D(P_{Z|\Theta=\theta} \| P_Z) + D(P_Z \| P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}) \right) dP_{\Theta}(\theta), \end{aligned}$$

where the probability measure $P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}$ is defined in (46); $\beta \in \mathcal{J}_{P_S}$, with \mathcal{J}_{P_S} in (45).

Proof: The proof follows by noticing that

$$\begin{aligned} & \int \int D(P_{Z|\Theta=\theta} \| P_{\hat{Z}|\Theta=\nu}^{(P_S, \beta)}) dP_{\Theta}(\nu) dP_{\Theta}(\theta) \\ &= \int \int \int \log \frac{dP_{Z|\Theta=\theta}}{dP_{\hat{Z}|\Theta=\nu}^{(P_S, \beta)}}(z) dP_{Z|\Theta=\theta}(z) dP_{\Theta}(\nu) dP_{\Theta}(\theta) \quad (158) \\ &= \int \int \int \log \frac{dP_{Z|\Theta=\theta}}{dP_Z}(z) dP_{Z|\Theta=\theta}(z) dP_{\Theta}(\theta) \\ & \quad + \int \int \int \log \frac{dP_Z}{dP_{\hat{Z}|\Theta=\nu}^{(P_S, \beta)}}(z) dP_{Z|\Theta=\theta}(z) dP_{\Theta}(\nu) dP_{\Theta}(\theta), \quad (159) \\ &= \int D(P_{Z|\Theta=\theta} \| P_Z) dP_{\Theta}(\theta) \\ & \quad + \int \int \int \log \frac{dP_Z}{dP_{\hat{Z}|\Theta=\nu}^{(P_S, \beta)}}(z) dP_{Z|\Theta=\theta}(z) dP_{\Theta}(\nu) dP_{\Theta}(\theta), \quad (160) \end{aligned}$$

where the equality in (159) follows from Assumptions (a) and (c) together with Lemma 48 (in Appendix A) and [61, Theorem 2.2.3].

The rest of the proof follows from (160) by noticing that

$$\begin{aligned} & \int \int \int \log \frac{dP_Z}{dP_{\hat{Z}|\Theta=\nu}^{(P_S, \beta)}}(z) dP_{Z|\Theta=\theta}(z) dP_{\Theta}(\nu) dP_{\Theta}(\theta) \\ &= \int \int \int \log \left(\frac{dP_Z}{dP_{\hat{Z}|\Theta=\nu}^{(P_S, \beta)}}(z) \right) \\ & \quad \frac{dP_{Z|\Theta=\theta}}{dP_Z}(z) dP_Z(z) dP_{\Theta}(\nu) dP_{\Theta}(\theta) \quad (161) \\ &= \int \int \log \left(\frac{dP_Z}{dP_{\hat{Z}|\Theta=\nu}^{(P_S, \beta)}}(z) \right) \\ & \quad \left(\int \frac{dP_{Z|\Theta=\theta}}{dP_Z}(z) dP_{\Theta}(\theta) \right) dP_Z(z) dP_{\Theta}(\nu) \quad (162) \\ &= \int \int \log \left(\frac{dP_Z}{dP_{\hat{Z}|\Theta=\nu}^{(P_S, \beta)}}(z) \right) dP_Z(z) dP_{\Theta}(\nu) \quad (163) \\ &= \int D(P_Z \| P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}) dP_{\Theta}(\theta), \quad (164) \end{aligned}$$

where the equality in (161) follows from Assumptions (a) and (c) together with Lemma 48 (in Appendix A) and [61, Theorem 2.2.3]; the equality in (162) follows by exchanging the order of the integrals [50, Theorem 2.6.6]; the equality in (163) follows from [50, Theorem 4.5.2], which implies that

$$\int \frac{dP_{Z|\Theta=\theta}}{dP_Z}(z) dP_{\Theta}(\theta) = 1. \quad (165)$$

The proof is completed by plugging (164) into (160). \blacksquare

The converse of the Pythagorean theorem [62, Book I, Proposition 48] together with Lemma 32, lead to the geometric con-

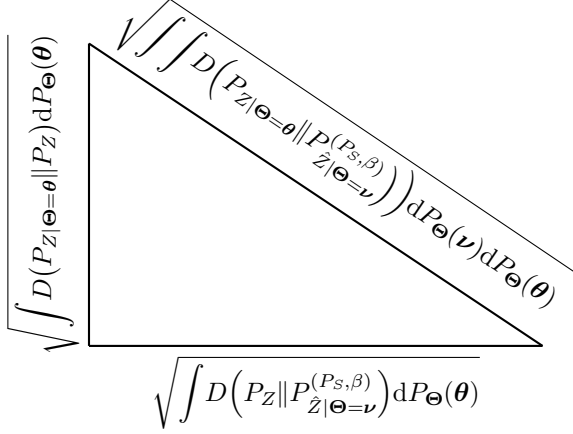


Fig. 4. Geometric interpretation of Lemma 32 involving only relative entropies. Note that $\int D(P_{Z|\Theta=\theta} || P_Z) dP_{\Theta}(\theta) = I(P_{Z|\Theta}; P_{\Theta})$.

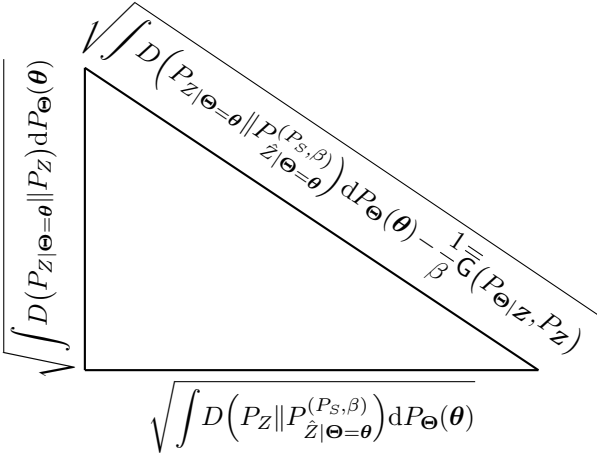


Fig. 5. Geometric interpretation of Lemma 32 involving only relative entropies. Note that $\int D(P_{Z|\Theta=\theta} || P_Z) dP_{\Theta}(\theta) = I(P_{Z|\Theta}; P_{\Theta})$.

struction shown in Figure 4. Note the duality between Figure 1 and Figure 4. From Theorem 31, it follows that

$$\begin{aligned} & \int \int D(P_{Z|\Theta=\mu} || P_{\hat{Z}|\Theta=\nu}^{(P_S, \beta)}) dP_{\Theta}(\nu) dP_{\Theta}(\mu) \\ &= \int D(P_{Z|\Theta=\mu} || P_{\hat{Z}|\Theta=\mu}^{(P_S, \beta)}) dP_{\Theta}(\mu) - \frac{1}{\beta} \overline{\overline{G}}(P_{\Theta|Z}, P_Z), \end{aligned} \quad (166)$$

which involves the generalization error $\overline{\overline{G}}(P_{\Theta|Z}, P_Z)$ in (11). This observation leads to the construction in Figure 5, which exhibits a duality with Figure 2.

VII. ALGORITHM-DRIVEN GAPS

The purpose of this section is to provide explicit expressions for the algorithm-driven gap $G(z, P_1, P_2)$ in (20) for an arbitrary dataset z and two arbitrary probability measures P_1 and P_2 in $\Delta(\mathcal{M})$. In particular, these expressions are in terms of the Gibbs probability measure $P_{\Theta|Z=z}^{(Q, \lambda)}$ in (33), which represents a Gibbs algorithm. For the ease of presentation, the analysis of $G(z, P_1, P_2)$ is performed using the fact that

$G(z, P_1, P_2) = G(z, P_1, P_{\Theta|Z=z}^{(Q, \lambda)}) - G(z, P_2, P_{\Theta|Z=z}^{(Q, \lambda)})$. Thus, the focus is on the gap $G(z, P, P_{\Theta|Z=z}^{(Q, \lambda)})$, for an arbitrary measure $P \in \Delta(\mathcal{M})$.

A. Deviations from the Gibbs Measure

The variation or *sensitivity* of the functional R_z in (9) to deviations from the probability measure $P_{\Theta|Z=z}^{(Q, \lambda)}$ in (33) to an alternative probability measure P is

$$G(z, P, P_{\Theta|Z=z}^{(Q, \lambda)}) = R_z(P) - R_z(P_{\Theta|Z=z}^{(Q, \lambda)}), \quad (167)$$

where the functional G is defined in (20). The following theorem introduces an explicit expression for $G(z, P, P_{\Theta|Z=z}^{(Q, \lambda)})$.

Lemma 33 (Theorem 1 in [45]): The probability measure $P_{\Theta|Z=z}^{(Q, \lambda)}$ in (33) satisfies for all $P \in \Delta_Q(\mathcal{M})$,

$$\begin{aligned} & G(z, P, P_{\Theta|Z=z}^{(Q, \lambda)}) \\ &= \lambda (D(P_{\Theta|Z=z}^{(Q, \lambda)} || Q) + D(P || P_{\Theta|Z=z}^{(Q, \lambda)}) - D(P || Q)), \end{aligned} \quad (168)$$

where the functional G is defined in (20).

An interesting observation from Lemma 33 is that when the reference measure Q is a probability measure, it holds that $D(P || Q) \geq 0$ [9, Theorem 1], which leads to the following corollary of Lemma 33.

Corollary 34: If Q is a probability measure, then the gap $G(z, P, P_{\Theta|Z=z}^{(Q, \lambda)})$ in (167) satisfies

$$G(z, P, P_{\Theta|Z=z}^{(Q, \lambda)}) \leq \lambda (D(P_{\Theta|Z=z}^{(Q, \lambda)} || Q) + D(P || P_{\Theta|Z=z}^{(Q, \lambda)})), \quad (169)$$

with equality if and only if $D(P || Q) = 0$.

The gap $G(z, P, P_{\Theta|Z=z}^{(Q, \lambda)})$ in (167) is nonnegative. This follows immediately from [9, Lemma 20] and Lemma 33, as suggested in the following corollary.

Corollary 35: The gap $G(z, P, P_{\Theta|Z=z}^{(Q, \lambda)})$ in (167) satisfies

$$G(z, P, P_{\Theta|Z=z}^{(Q, \lambda)}) \geq 0 \quad (170)$$

with equality if $D(P || P_{\Theta|Z=z}^{(Q, \lambda)}) = 0$.

B. Priors and Posteriors

From Lemma 33, under the assumption that Q is a probability measure, it follows that

$$R_z(Q) - R_z(P_{\Theta|Z=z}^{(Q, \lambda)}) = \lambda (D(Q || P_{\Theta|Z=z}^{(Q, \lambda)}) + D(P_{\Theta|Z=z}^{(Q, \lambda)} || Q)),$$

where the right-hand side is a symmetrized Kullback-Liebler divergence, also known as Jeffrey's divergence [64], between the measures Q and $P_{\Theta|Z=z}^{(Q, \lambda)}$. More importantly, when Q is a probability measure, it follows from [9, Theorem 1] that $D(P_{\Theta|Z=z}^{(Q, \lambda)} || Q) \geq 0$ and $D(Q || P_{\Theta|Z=z}^{(Q, \lambda)}) \geq 0$, which reveals the fact that the expected empirical risk induced by the Gibbs probability measure $P_{\Theta|Z=z}^{(Q, \lambda)}$ is smaller than or equal to the expected empirical risk induced by the reference measure Q . This observation is formalized by the following corollary of Lemma 33.

Corollary 36: If Q is a probability measure, then the probability measure $P_{\Theta|Z=z}^{(Q,\lambda)}$ in (33) satisfies

$$R_z \left(P_{\Theta|Z=z}^{(Q,\lambda)} \right) \leq R_z(Q), \quad (171)$$

where the function R_z is defined in (9).

Note that the reference measure Q in Corollary 36 can be chosen independently of the dataset z . From this perspective, the measure Q can be interpreted as a prior on the models, while the probability measure $P_{\Theta|Z=z}^{(Q,\lambda)}$ can be interpreted as a posterior once the prior Q is confronted with the training dataset z .

C. A Geometric Interpretation

In Lemma 33, note that if Q is a probability measure, then it holds from [9, Theorem 1] that $D(P\|Q) \geq 0$, $D(P\|P_{\Theta|Z=z}^{(Q,\lambda)}) \geq 0$, and $D(P_{\Theta|Z=z}^{(Q,\lambda)}\|Q) \geq 0$. Thus, from (167), it holds that

$$\begin{aligned} & G(z, P, P_{\Theta|Z=z}^{(Q,\lambda)}) + \lambda D(P\|Q) \\ &= R_z(P) + \lambda D(P\|Q) - R_z(P_{\Theta|Z=z}^{(Q,\lambda)}) \end{aligned} \quad (172)$$

$$\geq R_z(P_{\Theta|Z=z}^{(Q,\lambda)}) + \lambda D(P_{\Theta|Z=z}^{(Q,\lambda)}\|Q) - R_z(P_{\Theta|Z=z}^{(Q,\lambda)}) \quad (173)$$

$$= \lambda D(P_{\Theta|Z=z}^{(Q,\lambda)}\|Q), \quad (174)$$

and moreover,

$$\begin{aligned} & G(z, P, P_{\Theta|Z=z}^{(Q,\lambda)}) + \lambda D(P\|Q) \\ &= \lambda \left(D(P_{\Theta|Z=z}^{(Q,\lambda)}\|Q) + D(P\|P_{\Theta|Z=z}^{(Q,\lambda)}) \right) \end{aligned} \quad (175)$$

$$\geq \lambda D(P\|P_{\Theta|Z=z}^{(Q,\lambda)}), \quad (176)$$

where the inequality in (173) follows from (33); and the equality in (175) follows from Lemma 33.

Hence, under the assumption that the measure Q is a probability measure, the equality in (168) can be written as follows:

$$\begin{aligned} & \left(\sqrt{\frac{1}{\lambda} G(z, P, P_{\Theta|Z=z}^{(Q,\lambda)}) + D(P\|Q)} \right)^2 \\ &= \left(\sqrt{D(P_{\Theta|Z=z}^{(Q,\lambda)}\|Q)} \right)^2 + \left(\sqrt{D(P\|P_{\Theta|Z=z}^{(Q,\lambda)})} \right)^2, \end{aligned} \quad (177)$$

which together with (175) and (176) imply that a right-angled triangle can be constructed such that the hypotenuse exhibits length $\sqrt{\frac{1}{\lambda} G(z, P, P_{\Theta|Z=z}^{(Q,\lambda)}) + D(P\|Q)}$ and the short sides exhibit lengths $\sqrt{D(P_{\Theta|Z=z}^{(Q,\lambda)}\|Q)}$ and $\sqrt{D(P\|P_{\Theta|Z=z}^{(Q,\lambda)})}$, respectively. Figure 6 shows this interpretation of the gap $G(z, P, P_{\Theta|Z=z}^{(Q,\lambda)})$ in (167).

D. Sensitivity from/to Arbitrary Deviations

Given two probability measures P_1 and P_2 , both in $\Delta(\mathcal{M})$, and a dataset $z \in (\mathcal{X} \times \mathcal{Y})^n$, the focus is on the variation of the functional R_z in (9) from P_2 to P_1 . In terms of the functional G in (20), such a variation is $G(z, P_1, P_2)$. The following theorem provides an exact expression for such a variation.

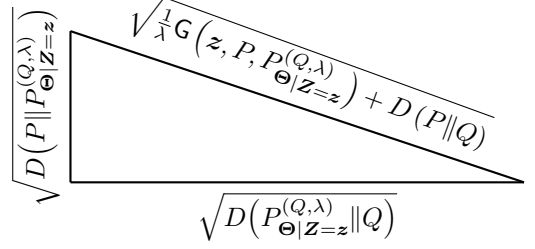


Fig. 6. Geometric interpretation of the gap $G(z, P, P_{\Theta|Z=z}^{(Q,\lambda)})$ in (167).

Theorem 37: If the probability measures P_1 and P_2 are both absolutely continuous with respect to the σ -finite measure Q in (33), then the gap $G(z, P_1, P_2)$ in (20) satisfies

$$\begin{aligned} G(z, P_1, P_2) &= \lambda \left(D(P_1\|P_{\Theta|Z=z}^{(Q,\lambda)}) - D(P_2\|P_{\Theta|Z=z}^{(Q,\lambda)}) \right. \\ &\quad \left. + D(P_2\|Q) - D(P_1\|Q) \right), \end{aligned} \quad (178)$$

where the probability measure $P_{\Theta|Z=z}^{(Q,\lambda)}$ is defined in (33).

Proof: The proof follows from Lemma 33 and by noticing that $G(z, P_1, P_2) = G(z, P_1, P_{\Theta|Z=z}^{(Q,\lambda)}) - G(z, P_2, P_{\Theta|Z=z}^{(Q,\lambda)})$. ■

In Theorem 37, as long as the probability measures P_1 and P_2 are both absolutely continuous with respect to the σ -finite measure Q , the reference measure Q can be arbitrarily chosen. Similarly, the parameter λ can be arbitrarily chosen within the set $\mathcal{K}_{Q,z}$ in (31). Some notions of optimality for the choice of λ have been studied in [65]. This flexibility in the choice of these parameters is essentially because only the right-hand side of (178) depends on them. Another interesting observation is that none of the terms in the right-hand side of (178) depends simultaneously on both P_1 and P_2 . These observations highlight the significant flexibility of the expression in (178) to construct closed-form expressions for the gap $G(z, P_1, P_2)$.

E. Choice of the Reference Measure

The choice of Q in (178) is subject to the constraint that both probability measures P_1 and P_2 must be absolutely continuous with respect to Q . From this perspective, the measure Q can be seen as a free parameter, which can be strategically chosen.

1) Probability Measures: Two choices of Q , as a probability measure, for which the expression in the right-hand side of (178) significantly simplifies are $Q = P_1$ and $Q = P_2$, which leads to the following corollary of Theorem 37.

Corollary 38: If P_1 is absolutely continuous with P_2 , then $G(z, P_1, P_2)$ in (178) satisfies:

$$\begin{aligned} & G(z, P_1, P_2) \\ &= \lambda \left(D(P_1\|P_{\Theta|Z=z}^{(P_2,\lambda)}) - D(P_1\|P_2) - D(P_2\|P_{\Theta|Z=z}^{(P_2,\lambda)}) \right). \end{aligned} \quad (179)$$

Alternatively, if P_2 is absolutely continuous with P_1 then

$$\begin{aligned} & \mathsf{G}(z, P_1, P_2) \\ &= \lambda \left(D(P_1 \| P_{\Theta|Z=z}^{(P_1, \lambda)}) + D(P_2 \| P_1) - D(P_2 \| P_{\Theta|Z=z}^{(P_1, \lambda)}) \right), \end{aligned} \quad (180)$$

where for all $i \in \{1, 2\}$, the probability measure $P_{\Theta|Z=z}^{(P_i, \lambda)}$ satisfies (33) under the assumption that $Q = P_i$.

In the case in which none of the measures is absolutely continuous with respect to its counterpart, choosing Q as a convex combination of P_1 and P_2 guarantees an explicit expression for $\mathsf{G}(z, P_1, P_2)$ in (178). The following corollary formalizes this observation.

Corollary 39: For all $\alpha \in (0, 1)$, $\mathsf{G}(z, P_1, P_2)$ in (178) satisfies

$$\begin{aligned} & \mathsf{G}(z, P_1, P_2) \\ &= \lambda \left(D(P_1 \| P_{\Theta|Z=z}^{(\alpha P_1 + (1-\alpha)P_2, \lambda)}) - D(P_2 \| P_{\Theta|Z=z}^{(\alpha P_1 + (1-\alpha)P_2, \lambda)}) \right. \\ & \quad \left. + D(P_2 \| \alpha P_1 + (1-\alpha)P_2) - D(P_1 \| \alpha P_1 + (1-\alpha)P_2) \right), \end{aligned} \quad (181)$$

where the probability measure $P_{\Theta|Z=z}^{(\alpha P_1 + (1-\alpha)P_2, \lambda)}$ satisfies (33) under the assumption that $Q = \alpha P_1 + (1-\alpha)P_2$.

The measure Q in (33) can also be chosen as a σ -finite measure, e.g., the counting measure or the Lebesgue measure.

2) *The Counting Measure:* Assume for instance that the set of models \mathcal{M} is countable and the reference measure Q is the counting measure. Under this assumption, any probability measure $P \in \Delta(\mathcal{M})$ is absolutely continuous with respect to the counting measure Q . The Radon-Nikodym derivative of P with respect to Q is the probability mass function of P , denoted by $p : \mathcal{M} \rightarrow [0, 1]$. Interestingly, under the current assumption, $D(P \| Q)$ is equal to negative Shannon's discrete entropy of P . That is, $D(P \| Q) = \sum_{\theta \in \mathcal{M}} p(\theta) \log(p(\theta)) \triangleq -H(P)$. This observation leads to the following corollary of Theorem 37.

Corollary 40: Let the set \mathcal{M} be countable and let Q in (33) be the corresponding counting measure. Then, the gap $\mathsf{G}(z, P_1, P_2)$ in (20) satisfies

$$\begin{aligned} & \mathsf{G}(z, P_1, P_2) \\ &= \lambda \left(D(P_1 \| P_{\Theta|Z=z}^{(Q, \lambda)}) - D(P_2 \| P_{\Theta|Z=z}^{(Q, \lambda)}) - H(P_2) + H(P_1) \right), \end{aligned} \quad (182)$$

where the probability measure $P_{\Theta|Z=z}^{(Q, \lambda)}$ is defined in (33); and the terms $H(P_1)$ and $H(P_2)$ represent Shannon's discrete entropy of the probability measures P_1 and P_2 , respectively.

From [9, Theorem 3], it follows that the probability mass function of the measure $P_{\Theta|Z=z}^{(Q, \lambda)}$ in (182), denoted $p_{\lambda, z} : \mathcal{M} \rightarrow [0, 1]$, satisfies

$$p_{\lambda, z}(\theta) = \frac{dP_{\Theta|Z=z}^{(Q, \lambda)}}{dQ}(\theta) \quad (183)$$

$$= \frac{\exp(-\frac{1}{\lambda}L(z, \theta))}{\sum_{\nu \in \mathcal{M}} \exp(-\frac{1}{\lambda}L(z, \nu))}, \quad (184)$$

where the function $\frac{dP_{\Theta|Z=z}^{(Q, \lambda)}}{dQ}$ is in (33).

An important observation from Corollary 40 is that for all $i \in \{1, 2\}$, while the term $D(P_i \| P_{\Theta|Z=z}^{(Q, \lambda)})$ is convex in P_i , the term $H(P_i)$ is concave in P_i [9, Theorem 2]. Interestingly, the term $H(P_i)$ is independent of the dataset z , the choice of the loss function ℓ in (6), and the regularization factor λ . Moreover, while the term $D(P_i \| P_{\Theta|Z=z}^{(Q, \lambda)})$ is minimized when $P_i = P_{\Theta|Z=z}^{(Q, \lambda)}$, the term $H(P_i)$ is minimized when P_i is concentrated on any singleton of \mathcal{M} . This shows the trade-off arising in model selection between randomly choosing the models by sampling the probability measure $P_{\Theta|Z=z}^{(Q, \lambda)}$ and choosing a model with probability one.

3) *The Lebesgue Measure:* Assume that the set \mathcal{M} is a subset of \mathbb{R}^d , and the reference measure Q is the corresponding Lebesgue measure. Under these assumptions, the Radon-Nikodym derivative of a given absolutely continuous probability measure P with respect to Q is the probability density function of P , denoted by $p : \mathcal{M} \rightarrow [0, 1]$. Under the current assumption, $D(P \| Q)$ is equal to negative Shannon's differential entropy of P . That is, $D(P \| Q) = \int p(\theta) \log(p(\theta)) d\theta \triangleq -h(P)$. This observation leads to the following corollary of Theorem 37.

Corollary 41: Let the set \mathcal{M} be a subset of \mathbb{R}^d , and let Q in (33) be the corresponding Lebesgue measure. Then, the gap $\mathsf{G}(z, P_1, P_2)$ in (20) satisfies

$$\begin{aligned} & \mathsf{G}(z, P_1, P_2) \\ &= \lambda \left(D(P_1 \| P_{\Theta|Z=z}^{(Q, \lambda)}) - D(P_2 \| P_{\Theta|Z=z}^{(Q, \lambda)}) - h(P_2) + h(P_1) \right), \end{aligned} \quad (185)$$

where the probability measure $P_{\Theta|Z=z}^{(Q, \lambda)}$ is defined in (33); and the terms $h(P_1)$ and $h(P_2)$ represent Shannon's differential entropy of the probability measures P_1 and P_2 , respectively.

From [9, Theorem 3], it follows that the probability density function of the measure $P_{\Theta|Z=z}^{(Q, \lambda)}$ in (185), denoted $p_{\lambda, z} : \mathcal{M} \rightarrow [0, 1]$, satisfies

$$p_{\lambda, z}(\theta) = \frac{dP_{\Theta|Z=z}^{(Q, \lambda)}}{dQ}(\theta) \quad (186)$$

$$= \frac{\exp(-\frac{1}{\lambda}L(z, \theta))}{\int \exp(-\frac{1}{\lambda}L(z, \nu)) d\nu}, \quad (187)$$

where the function $\frac{dP_{\Theta|Z=z}^{(Q, \lambda)}}{dQ}$ is in (33). Despite the fact that for all $i \in \{1, 2\}$, the convexity of $D(P_i \| P_{\Theta|Z=z}^{(Q, \lambda)})$ and the concavity of $h(P_i)$ with respect to P_i hold as in the previous case, these terms do not lead to useful interpretations as, for instance, the differential entropy $h(P_i)$ might be negative and unboundedly increase or decrease.

VIII. DATA-DRIVEN GAPS

The purpose of this section is to provide explicit expressions for the data-driven gap $\mathsf{G}(\theta, Q_1, Q_2)$ in (21) for an arbitrary model $\theta \in \mathcal{M}$ and two arbitrary probability measures Q_1 and Q_2 in $\Delta(\mathcal{X} \times \mathcal{Y})$. Interestingly, these expressions are in terms of the a WCDG probability measure $P_{Z|\Theta=\theta}^{(P_S, \beta)}$ in (46).

A. Deviations from the WCDG probability measure

The variation or *sensitivity* of the functional R_θ in (8) to deviations from the WCDG probability measure $P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}$ in (46) to an alternative probability measure $P \in \Delta(\mathcal{X} \times \mathcal{Y})$ is

$$G(\theta, P, P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}) = R_\theta(P) - R_\theta(P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}), \quad (188)$$

where the functional G is defined in (21). The following lemma introduces an explicit expression for $G(\theta, P, P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)})$.

Lemma 42 ([42, Theorem 6]): The probability measure $P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}$ in (46) satisfies, for all $P \in \Delta_{P_S}(\mathcal{X} \times \mathcal{Y})$,

$$G(\theta, P, P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}) = \beta \left(D(P\|P_S) - D(P\|P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}) - D(P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}\|P_S) \right), \quad (189)$$

where the functional G is defined in (21).

B. Sensitivity from/to Arbitrary Deviations

Given two probability measures P_1 and P_2 , both in $\Delta(\mathcal{X} \times \mathcal{Y})$, and a model $\theta \in \mathcal{M}$, the focus is on the variation of the function R_θ in (8) from P_2 to P_1 . In terms of the functional G in (21), such a variation is $G(\theta, P_1, P_2)$. The following theorem provides an exact expression for such a variation.

Theorem 43 ([42, Theorem 8]): For all $P_1 \in \Delta_{P_S}(\mathcal{X} \times \mathcal{Y})$ and $P_2 \in \Delta_{P_S}(\mathcal{X} \times \mathcal{Y})$, and for all $\theta \in \mathcal{M}$,

$$G(\theta, P_1, P_2) = \beta \left(D(P_2\|P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}) - D(P_1\|P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}) - D(P_2\|P_S) + D(P_1\|P_S) \right), \quad (190)$$

where the functional G is defined in (21); and the parameter β , the model θ , and the measures P_S and $P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}$ jointly satisfy (46).

C. Choice of the Reference Measure

The choice of the reference measure P_S in (190) is subject to the constraint that both probability measures P_1 and P_2 must be absolutely continuous with respect to P_S . Despite this constraint, the reference measure P_S can be seen as a free parameter, which can be strategically chosen. Two choices of P_S , for which the expression in the right-hand side of (190) significantly simplifies are $P_S = P_1$ and $P_S = P_2$, which leads to the following corollary of Theorem 43.

Corollary 44 ([46, Corollary 3]): If P_1 is absolutely continuous with P_2 , then the gap $G(\theta, P_1, P_2)$ in (21) satisfies:

$$G(\theta, P_1, P_2) = \beta \left(D(P_2\|P_{\hat{Z}|\Theta=\theta}^{(P_1, \beta)}) - D(P_1\|P_{\hat{Z}|\Theta=\theta}^{(P_1, \beta)}) + D(P_1\|P_2) \right). \quad (191)$$

Alternatively, if P_2 is absolutely continuous with P_1 then,

$$G(\theta, P_1, P_2) = \beta \left(D(P_2\|P_{\hat{Z}|\Theta=\theta}^{(P_1, \beta)}) - D(P_1\|P_{\hat{Z}|\Theta=\theta}^{(P_1, \beta)}) - D(P_2\|P_1) \right), \quad (192)$$

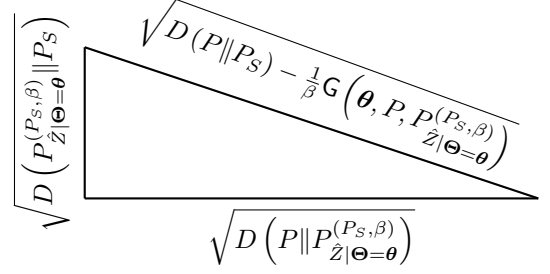


Fig. 7. Geometric interpretation of the gap $G(\theta, P, P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)})$ in (189).

where for all $i \in \{1, 2\}$, the probability measure $P_{\hat{Z}|\Theta=\theta}^{(P_i, \beta)}$ satisfies (46) under the assumption that $P_S = P_i$.

Interestingly, absolute continuity of P_1 with respect to P_2 or P_2 with respect to P_1 is not necessary for obtaining an expression for the gap $G(\theta, P_1, P_2)$ in (21). In the case in which none of the measures is absolutely continuous with respect to its counterpart, choosing P_S as a convex combination of P_1 and P_2 always guarantees an explicit expression for the gap $G(\theta, P_1, P_2)$. The following corollary formalizes this observation.

Corollary 45: For all $P_1 \in \Delta_{P_S}(\mathcal{X} \times \mathcal{Y})$ and $P_2 \in \Delta_{P_S}(\mathcal{X} \times \mathcal{Y})$, for all $\theta \in \mathcal{M}$, and for all $\alpha \in (0, 1)$,

$$G(\theta, P_1, P_2) = \beta \left(D(P_2\|P_{\hat{Z}|\Theta=\theta}^{(\alpha P_1 + (1-\alpha)P_2, \beta)}) - D(P_1\|P_{\hat{Z}|\Theta=\theta}^{(\alpha P_1 + (1-\alpha)P_2, \beta)}) - D(P_2\|\alpha P_1 + (1-\alpha)P_2) + D(P_1\|\alpha P_1 + (1-\alpha)P_2) \right), \quad (193)$$

where the functional G is defined in (21); and the parameter β , the model θ , and the measures $\alpha P_1 + (1-\alpha)P_2$ and $P_{\hat{Z}|\Theta=\theta}^{(\alpha P_1 + (1-\alpha)P_2, \beta)}$ jointly satisfy (46).

D. A Geometric Interpretation

In Lemma 42, the reference measure P_S is a probability measure. Then, from [9, Theorem 1], it follows that $D(P\|P_S) \geq 0$, $D(P\|P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}) \geq 0$ and $D(P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}\|P_S) \geq 0$. This observation together with (189) lead to the following inequality:

$$0 \leq D(P\|P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}) + D(P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}\|P_S) = D(P\|P_S) - \frac{1}{\beta} G(\theta, P, P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}). \quad (194)$$

Moreover,

$$\begin{aligned} & \beta D(P\|P_S) - G(\theta, P, P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}) \\ &= - (R_\theta(P) - \beta D(P\|P_S)) + R_\theta(P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}) \\ &\geq - (R_\theta(P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}) - \beta D(P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}\|P_S)) \\ &\quad + R_\theta(P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}) \end{aligned} \quad (195)$$

$$= \beta D(P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}\|P_S), \quad (196)$$

where the equality in (195) follows from [42, Lemma 3]. Similarly,

$$\begin{aligned} & \beta D(P\|P_S) - G\left(\theta, P, P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}\right) \\ &= \beta D\left(P\|P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}\right) + \beta D\left(P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}\|P_S\right) \quad (197) \\ &\geq \beta D\left(P\|P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}\right), \quad (198) \end{aligned}$$

where (197) follows from Lemma 42.

From these observations, the equality in (189) can be written as follows:

$$\begin{aligned} & \left(\sqrt{D(P\|P_S) - \frac{1}{\beta} G\left(\theta, P, P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}\right)}\right)^2 \\ &= \left(\sqrt{D\left(P\|P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}\right)}\right)^2 + \left(\sqrt{D\left(P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}\|P_S\right)}\right)^2. \quad (199) \end{aligned}$$

The equality in (199) together with the inequalities in (196) and (198) imply that a right-angled triangle can be constructed such that the hypotenuse exhibits length $\sqrt{D(P\|P_S) - \frac{1}{\beta} G\left(\theta, P, P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}\right)}$ and the short sides exhibit lengths $\sqrt{D\left(P\|P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}\right)}$ and $\sqrt{D\left(P_{\hat{Z}|\Theta=\theta}^{(P_S, \beta)}\|P_S\right)}$, respectively. Figure 7 shows this geometric interpretation.

IX. CONCLUSIONS AND FINAL REMARKS

In this work, closed-form expressions for the generalization error have been derived in terms of information-theoretic measures. Two distinct classes of expressions are identified. The first class encompasses formulations involving the Gibbs algorithm, as defined by the Gibbs probability measure in Definition 5. The second class pertains to expressions incorporating the WCDG probability measure, defined in Definition 6. While the former represents a more general framework, as it imposes no specific conditions on the probability distribution of datasets, both classes offer unique and complementary insights. These insights establish connections between the generalization error and concepts such as hypothesis testing, information measures, and Euclidean geometry. However, these connections have been only briefly explored in this work, and their full potential to enhance the understanding of generalization error remains an open avenue for further research.

It is important to note that the derived expressions do not significantly simplify the numerical computation of the generalization error. This is unsurprising, as the primary goal of this study is to provide a deeper conceptual understanding of the generalization error from an information-theoretic perspective. Specifically, the established connections between the generalization error, the Gibbs algorithm, and the WCDG probability measure represent a significant advancement in this goal. Concerning the connection to the Gibbs algorithm, probably, the expression that best unveils the relevance of these findings is the one in Theorem 18. Note that such expression implies that the generalization error of an arbitrary machine learning

algorithm can be understood as a comparison, via relative entropy, of all possible instances of the algorithm under study with all possible instances of the Gibbs algorithm in two scenarios: (a) Both algorithms are trained upon the same training datasets drawn from the same probability distribution; and (b) Both algorithms are trained upon training datasets independently drawn from the same probability distribution. Alternatively, concerning the connection to the WCDG probability measure, probably, the expression that best unveils the relevance of these findings is the one in Theorem 31. The expression therein implies that the generalization error of a given machine learning algorithm consists of a comparison, via relative entropy, of all possible likelihoods on the data-points induced by the algorithm under study; and the WCDG probability measure in two scenarios: (a) both probability measures, e.g., likelihood and WCDG probability measures, are conditioned on the same model drawn from the same probability distribution; and (b) both probability measures are respectively conditioned upon models independently drawn from the same probability distribution.

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APPENDIX A

STATISTICAL PROPERTIES OF ALGORITHMS

An algorithm $P_{\Theta|Z} \in \Delta(\mathcal{M} | (\mathcal{X} \times \mathcal{Y})^n)$ and a probability measure $P_Z \in \Delta((\mathcal{X} \times \mathcal{Y})^n)$ determine two unique probability measures in $\Delta((\mathcal{X} \times \mathcal{Y})^n \times \mathcal{M})$ and $\Delta(\mathcal{M} \times (\mathcal{X} \times \mathcal{Y})^n)$, respectively. Such probability measures are respectively denoted by $P_{Z,\Theta}$ and $P_{\Theta,Z}$ and for all measurable sets $\mathcal{A} \subset (\mathcal{X} \times \mathcal{Y})^n \times \mathcal{M}$, it follows that

$$P_{Z,\Theta}(\mathcal{A}) = \int P_{\Theta|Z=z}(\mathcal{A}_z) dP_Z(z), \quad (200)$$

where \mathcal{A}_z is the section of the set \mathcal{A} determined by z , namely,

$$\mathcal{A}_z \triangleq \{\theta \in \mathcal{M} : (z, \theta) \in \mathcal{A}\}. \quad (201)$$

Alternatively, for all measurable sets $\mathcal{B} \subset \mathcal{M} \times (\mathcal{X} \times \mathcal{Y})^n$, it follows that

$$P_{\Theta,Z}(\mathcal{B}) = \int P_{\Theta|Z=z}(\mathcal{B}_z) dP_Z(z), \quad (202)$$

where \mathcal{B}_z is the section of the set \mathcal{B} determined by z , namely,

$$\mathcal{B}_z \triangleq \{\theta \in \mathcal{M} : (\theta, z) \in \mathcal{B}\}. \quad (203)$$

If the sets \mathcal{A} and \mathcal{B} are of the form $\mathcal{A} = \mathcal{C} \times \mathcal{D}$ and $\mathcal{B} = \mathcal{D} \times \mathcal{C}$, for some $\mathcal{C} \subseteq (\mathcal{X} \times \mathcal{Y})^n$ and $\mathcal{D} \subseteq \mathcal{M}$, then, it holds that

$$P_{Z,\Theta}(\mathcal{C} \times \mathcal{D}) = \int_{\mathcal{C}} P_{\Theta|Z=z}(\mathcal{D}) dP_Z(z) = P_{\Theta,Z}(\mathcal{D} \times \mathcal{C}). \quad (204)$$

In particular, if $\mathcal{C} = (\mathcal{X} \times \mathcal{Y})^n$ in (204), then, it follows that

$$P_{Z,\Theta}((\mathcal{X} \times \mathcal{Y})^n \times \mathcal{D}) = P_{\Theta,Z}(\mathcal{D} \times (\mathcal{X} \times \mathcal{Y})^n) = P_{\Theta}(\mathcal{D}), \quad (205)$$

where the probability measure $P_{\Theta} \in \Delta(\mathcal{M})$ also satisfies (28).

Alternatively, if $\mathcal{D} = \mathcal{M}$ in (204), then, it holds that

$$P_{Z,\Theta}(\mathcal{C} \times \mathcal{M}) = P_{\Theta,Z}(\mathcal{M} \times \mathcal{C}) = P_Z(\mathcal{C}). \quad (206)$$

Hence, in the following, the measures P_{Θ} in (205) and P_Z in (206) are said to be the marginals of the joint probability measures $P_{Z,\Theta}$ in (200) and $P_{\Theta,Z}$ in (202).

The instance $P_{\Theta|Z=z}$ of the algorithm $P_{\Theta|Z}$, for some dataset $z \in (\mathcal{X} \times \mathcal{Y})^n$, can be interpreted as the posterior probability measure of the prior P_{Θ} after the observation of the dataset z . Let the conditional probability measure $P_{Z|\Theta} \in \Delta((\mathcal{X} \times \mathcal{Y})^n | \mathcal{M})$ be such that for all measurable sets $\mathcal{C} \subset (\mathcal{X} \times \mathcal{Y})^n$,

$$P_Z(\mathcal{C}) = \int P_{Z|\Theta=\theta}(\mathcal{C}) dP_{\Theta}(\theta), \quad (207)$$

with P_{Θ} in (205) and P_Z in (206). Such a conditional probability measure $P_{Z|\Theta}$ exists and is unique almost surely with respect to P_{Θ} [50, Theorem 5.3.1]. The probability measure $P_{Z|\Theta}$ can be interpreted as the likelihood (on the datasets) induced by the posterior $P_{\Theta|Z}$ and the ground-truth probability distribution of the datasets P_Z . The joint probability measures $P_{Z,\Theta}$ and $P_{\Theta,Z}$ can be described via the conditional probability measure $P_{\Theta|Z}$ and the probability measure P_Z as in (200) and in (202); or via the conditional probability measure $P_{Z|\Theta}$ and the probability measure P_{Θ} . More specifically, for all measurable sets $\mathcal{A} \in (\mathcal{X} \times \mathcal{Y})^n \times \mathcal{M}$, it follows that

$$P_{Z,\Theta}(\mathcal{A}) = \int P_{Z|\Theta=\theta}(\mathcal{A}_{\theta}) dP_{\Theta}(\theta), \quad (208)$$

where \mathcal{A}_{θ} is the section of the set \mathcal{A} determined by θ , namely,

$$\mathcal{A}_{\theta} = \{z \in (\mathcal{X} \times \mathcal{Y})^n : (z, \theta) \in \mathcal{A}\}. \quad (209)$$

Alternatively, for all measurable sets $\mathcal{B} \subset \mathcal{M} \times (\mathcal{X} \times \mathcal{Y})^n$, it follows that

$$P_{\Theta, Z}(\mathcal{B}) = \int P_{Z|\Theta=\theta}(\mathcal{B}_\theta) dP_\Theta(\theta), \quad (210)$$

where the section \mathcal{B}_θ of the set \mathcal{B} is

$$\mathcal{B}_\theta = \{z \in (\mathcal{X} \times \mathcal{Y})^n : (\theta, z) \in \mathcal{B}\}. \quad (211)$$

For all measurable sets $\mathcal{A} \in (\mathcal{X} \times \mathcal{Y})^n \times \mathcal{M}$, let the set $\hat{\mathcal{A}} \in \mathcal{M} \times (\mathcal{X} \times \mathcal{Y})^n$ be

$$\hat{\mathcal{A}} = \{(\theta, z) \in \mathcal{M} \times (\mathcal{X} \times \mathcal{Y})^n : (z, \theta) \in \mathcal{A}\}, \quad (212)$$

then, from (208) and (210), it holds that

$$P_{Z, \Theta}(\mathcal{A}) = P_{\Theta, Z}(\hat{\mathcal{A}}). \quad (213)$$

The following lemmas, Lemma 46 and Lemma 47, present some properties of the probability measures mentioned above, which are known, but given their central roles in this work, are presented and proved using the current notation.

Lemma 46: Consider the conditional probability measures $P_{\Theta|Z}$ and $P_{Z|\Theta}$; and the probability measures P_Θ and P_Z that jointly satisfy (28) and (207). Assume that:

- (a) For all $z \in (\mathcal{X} \times \mathcal{Y})^n$, the probability measure $P_{\Theta|Z=z}$ is absolutely continuous with respect to P_Θ ; and
- (b) For all $\theta \in \mathcal{M}$, the probability measure $P_{Z|\Theta=\theta}$ is absolutely continuous with respect to P_Z .

Then, for all $(z, \theta) \in (\mathcal{X} \times \mathcal{Y})^n \times \mathcal{M}$,

$$\frac{dP_{Z|\Theta=\theta}}{dP_Z}(z) = \frac{dP_{\Theta|Z=z}}{dP_\Theta}(\theta), \quad (214)$$

almost surely with respect to the product measure $P_Z P_\Theta \in \Delta((\mathcal{X} \times \mathcal{Y})^n \times \mathcal{M})$.

Proof: From (208), it holds that

$$P_{Z, \Theta}(\mathcal{A}) = \int \int_{\mathcal{A}_\theta} dP_{Z|\Theta=\theta}(z) dP_\Theta(\theta) \quad (215)$$

$$= \int \int_{\mathcal{A}_\theta} \frac{dP_{Z|\Theta=\theta}}{dP_Z}(z) dP_Z(z) dP_\Theta(\theta) \quad (216)$$

$$= \int \int \frac{dP_{Z|\Theta=\theta}}{dP_Z}(z) \mathbb{1}_{\{z \in \mathcal{A}_\theta\}} dP_Z(z) dP_\Theta(\theta) \quad (217)$$

$$= \int \frac{dP_{Z|\Theta=\theta}}{dP_Z}(z) \mathbb{1}_{\{z \in \mathcal{A}_\theta\}} dP_Z P_\Theta(z, \theta) \quad (218)$$

$$= \int_{\mathcal{A}} \frac{dP_{Z|\Theta=\theta}}{dP_Z}(z) dP_Z P_\Theta(z, \theta), \quad (219)$$

where, the set \mathcal{A}_θ is defined in (209). Moreover, the equality in (216) follows from Assumption (b) and [61, Theo-

rem 2.2.3]. Using similar arguments, from (200), it follows that

$$P_{Z, \Theta}(\mathcal{A}) = \int \int_{\mathcal{A}_z} dP_{\Theta|Z=z}(\theta) dP_Z(z) \quad (220)$$

$$= \int \int_{\mathcal{A}_z} \frac{dP_{\Theta|Z=z}}{dP_\Theta}(\theta) dP_\Theta(\theta) dP_Z(z) \quad (221)$$

$$= \int \int \frac{dP_{\Theta|Z=z}(\theta) \mathbb{1}_{\{\theta \in \mathcal{A}_z\}}}{dP_\Theta} dP_\Theta(\theta) dP_Z(z) \quad (222)$$

$$= \int \int \frac{dP_{\Theta|Z=z}(\theta) \mathbb{1}_{\{\theta \in \mathcal{A}_z\}}}{dP_\Theta} dP_Z(z) dP_\Theta(\theta) \quad (223)$$

$$= \int \frac{dP_{\Theta|Z=z}(\theta) \mathbb{1}_{\{\theta \in \mathcal{A}_z\}}}{dP_\Theta} dP_Z P_\Theta(z, \theta) \quad (224)$$

$$= \int_{\mathcal{A}} \frac{dP_{\Theta|Z=z}(\theta)}{dP_\Theta} dP_Z P_\Theta(z, \theta), \quad (225)$$

where, the set \mathcal{A}_z is defined in (201). Moreover, the equality in (221) follows from Assumption (a) and [61, Theorem 2.2.3]; and the equality in (223) follows by exchanging the order of the integrals [50, Theorem 2.6.6]. The proof is completed by noticing that from (219) and (225), the following equalities hold:

$$P_{Z, \Theta}(\mathcal{A}) = \int_{\mathcal{A}} \frac{dP_{Z|\Theta=\theta}}{dP_Z}(z) dP_Z P_\Theta(z, \theta) \quad (226)$$

$$= \int_{\mathcal{A}} \frac{dP_{\Theta|Z=z}}{dP_\Theta}(\theta) dP_Z P_\Theta(z, \theta), \quad (227)$$

which together with [61, Theorem 2.2.3] implies the equality in (214) almost surely with respect to the product measure $P_Z P_\Theta \in \Delta((\mathcal{X} \times \mathcal{Y})^n \times \mathcal{M})$. This completes the proof. \blacksquare

Lemma 47: Consider the conditional probability measures $P_{\Theta|Z}$ and $P_{Z|\Theta}$; and the probability measures P_Θ and P_Z that jointly satisfy (28) and (207). Assume that:

- (a) For all $z \in (\mathcal{X} \times \mathcal{Y})^n$, the probability measure P_Θ is absolutely continuous with respect to $P_{\Theta|Z=z}$; and
- (b) For all $\theta \in \mathcal{M}$, the probability measure P_Z is absolutely continuous with respect to $P_{Z|\Theta=\theta}$.

Then, for all $(z, \theta) \in (\mathcal{X} \times \mathcal{Y})^n \times \mathcal{M}$,

$$\frac{dP_Z}{dP_{Z|\Theta=\theta}}(z) = \frac{dP_\Theta}{dP_{\Theta|Z=z}}(\theta), \quad (228)$$

almost surely with respect to the measure $P_{Z, \Theta} \in \Delta((\mathcal{X} \times \mathcal{Y})^n \times \mathcal{M})$ in (200).

Proof: The proof follows by observing that for all measurable sets $\mathcal{A} \in (\mathcal{X} \times \mathcal{Y})^n \times \mathcal{M}$, the product measure $P_Z P_\Theta \in$

$\Delta((\mathcal{X} \times \mathcal{Y})^n \times \mathcal{M})$ satisfies

$$P_Z P_\Theta(\mathcal{A}) = \int_{\mathcal{A}} dP_Z P_\Theta(z, \theta) \quad (229)$$

$$= \int \int_{\mathcal{A}_\theta} dP_Z(z) dP_\Theta(\theta) \quad (230)$$

$$= \int \int_{\mathcal{A}_\theta} \frac{dP_Z}{dP_{Z|\Theta=\theta}}(z) dP_{Z|\Theta=\theta}(z) dP_\Theta(\theta) \quad (231)$$

$$= \int \int \frac{dP_Z}{dP_{Z|\Theta=\theta}}(z) \mathbb{1}_{\{z \in \mathcal{A}_\theta\}} dP_{Z|\Theta=\theta}(z) dP_\Theta(\theta) \quad (232)$$

$$= \int \frac{dP_Z}{dP_{Z|\Theta=\theta}}(z) \mathbb{1}_{\{z \in \mathcal{A}_\theta\}} dP_{Z,\Theta}(z, \theta) \quad (233)$$

$$= \int_{\mathcal{A}} \frac{dP_Z}{dP_{Z|\Theta=\theta}}(z) dP_{Z,\Theta}(z, \theta), \quad (234)$$

where the set \mathcal{A}_θ is defined in (209); the equality in (231) follows from Assumption (b) and [61, Theorem 2.2.3]; and the measure $P_{Z,\Theta}$ is defined in (208).

The proof proceeds by noticing that for all measurable sets $\mathcal{A} \in (\mathcal{X} \times \mathcal{Y})^n \times \mathcal{M}$, the product measure $P_Z P_\Theta \in \Delta((\mathcal{X} \times \mathcal{Y})^n \times \mathcal{M})$ also satisfies

$$P_Z P_\Theta(\mathcal{A}) = \int_{\mathcal{A}} dP_Z P_\Theta(z, \theta) \quad (235)$$

$$= \int \int_{\mathcal{A}_\theta} dP_Z(z) dP_\Theta(\theta) \quad (236)$$

$$= \int \int_{\mathcal{A}_z} dP_\Theta(\theta) dP_Z(z) \quad (237)$$

$$= \int \int_{\mathcal{A}_z} \frac{dP_\Theta}{dP_{\Theta|Z=z}}(\theta) dP_{\Theta|Z=z}(\theta) dP_Z(z) \quad (238)$$

$$= \int \int \frac{dP_\Theta}{dP_{\Theta|Z=z}}(\theta) \mathbb{1}_{\{\theta \in \mathcal{A}_z\}} dP_{\Theta|Z=z}(\theta) dP_Z(z) \quad (239)$$

$$= \int \frac{dP_\Theta}{dP_{\Theta|Z=z}}(\theta) \mathbb{1}_{\{\theta \in \mathcal{A}_z\}} dP_{\Theta,Z}(\theta, z) \quad (240)$$

$$= \int_{\hat{\mathcal{A}}} \frac{dP_\Theta}{dP_{\Theta|Z=z}}(\theta) dP_{\Theta,Z}(\theta, z) \quad (241)$$

$$= \int_{\mathcal{A}} \frac{dP_\Theta}{dP_{\Theta|Z=z}}(\theta) dP_{Z,\Theta}(z, \theta), \quad (242)$$

where the sets \mathcal{A}_z , \mathcal{A}_θ , and $\hat{\mathcal{A}}$ are defined in (201), (209), and (212); and the measure $P_{\Theta,Z}$ is defined in (202). The equality in (237) follows by exchanging the order of the integrals [50, Theorem 2.6.6]; the equality in (238) follows from Assumption (a) and [61, Theorem 2.2.3].

The proof is completed by noticing that from (234) and (242), the following equalities hold:

$$P_{Z,\Theta}(\mathcal{A}) = \int_{\mathcal{A}} \frac{dP_Z}{dP_{Z|\Theta=\theta}}(z) dP_{Z,\Theta}(z, \theta), \quad (243)$$

$$= \int_{\mathcal{A}} \frac{dP_\Theta}{dP_{\Theta|Z=z}}(\theta) dP_{Z,\Theta}(z, \theta), \quad (244)$$

which together with [61, Theorem 2.2.3] implies the equality in (228) almost surely with respect to the measure $P_{Z,\Theta} \in$

$\Delta((\mathcal{X} \times \mathcal{Y})^n \times \mathcal{M})$ in (200). This completes the proof. \blacksquare

The following lemmas, Lemma 48 and Lemma 49, introduce other properties for the particular case in which P_Z satisfies (22) for some $P_Z \in \Delta(\mathcal{X} \times \mathcal{Y})$.

Lemma 48: Consider the conditional probability measure $P_{Z|\Theta}$ and the probability measure P_Z , both in (207). Assume that:

- (a) The probability measure P_Z satisfies (22) for some $P_Z \in \Delta(\mathcal{X} \times \mathcal{Y})$; and
- (b) For all $\theta \in \mathcal{M}$, the probability measure $P_{Z|\Theta=\theta}$ is absolutely continuous with respect to P_Z .

Then, for all $\theta \in \mathcal{M}$, the probability measure $P_{Z|\Theta=\theta}$ in (40) is absolutely continuous with respect to P_Z .

Proof: For all measurable sets $\mathcal{A} \subset (\mathcal{X} \times \mathcal{Y})^n$ and for all $\theta \in \mathcal{M}$,

$$P_{Z|\Theta=\theta}(\mathcal{A}) = \int_{\mathcal{A}} dP_{Z|\Theta=\theta}(z) \quad (245)$$

$$= \int_{\mathcal{A}} \frac{dP_{Z|\Theta=\theta}}{P_Z}(z) dP_Z(z) \quad (246)$$

$$= \int \int_{\mathcal{A}_z} \frac{dP_{Z|\Theta=\theta}}{P_Z}(z, \nu) dP_{Z_{-1}}(\nu) dP_Z(z), \quad (247)$$

where the equality in (246) follows from Assumption (b) and [61, Theorem 2.2.3]; and the equality in (247) follows from Assumption (a), where the set \mathcal{A}_z is the section of the set \mathcal{A} determined by $z \in \mathcal{X} \times \mathcal{Y}$:

$$\mathcal{A}_z = \{\nu \in (\mathcal{X} \times \mathcal{Y})^{n-1} : (z, \nu) \in \mathcal{A}\}, \quad (248)$$

and the measure $P_{Z_{-1}}$ is a product distribution in $\Delta((\mathcal{X} \times \mathcal{Y})^{n-1})$ formed by P_Z . That is, the product measure $P_Z \cdot P_{Z_{-1}}$ is identical to the measure P_Z in (22).

Given a measurable set $\mathcal{B} \subset \mathcal{X} \times \mathcal{Y}$, consider the set \mathcal{A} that satisfies:

$$\mathcal{A} = \mathcal{B} \times \mathcal{A}^{(2)} \times \mathcal{A}^{(3)} \times \dots \times \mathcal{A}^{(n)}, \quad (249)$$

where

$$\mathcal{A}^{(2)} = \mathcal{A}^{(3)} = \dots = \mathcal{A}^{(n)} = \mathcal{X} \times \mathcal{Y}. \quad (250)$$

Hence, for all $z \in \mathcal{B}$, it follows that the section of the set \mathcal{A} in (249) determined by z is

$$\mathcal{A}_z = (\mathcal{X} \times \mathcal{Y})^{n-1}. \quad (251)$$

Using such a fact, it follows that for the sets \mathcal{A} and \mathcal{B} in (249), and for all $\theta \in \mathcal{M}$,

$$P_{Z|\Theta=\theta}(\mathcal{B}) = P_{Z|\Theta=\theta}(\mathcal{A}) \quad (252)$$

$$= \int \int_{\mathcal{A}_z} \frac{dP_{Z|\Theta=\theta}}{P_Z}(z, \nu) dP_{Z_{-1}}(\nu) dP_Z(z) \quad (253)$$

$$= \int \int \frac{dP_{Z|\Theta=\theta}}{P_Z}(z, \nu) dP_{Z_{-1}}(\nu) dP_Z(z), \quad (254)$$

where the equality in (252) follows from (38) and the observation that under Assumption (a), Lemma 5 holds; the equality in (253) follows from (247); and the equality in (254) follows from (251).

Hence, given that the set \mathcal{B} can be any measurable subset of $\mathcal{X} \times \mathcal{Y}$, the equality in (254), together with [61, Theorem 2.2.3], imply that the probability measure $P_{Z|\Theta=\theta}$ is absolutely continuous with respect to P_Z . Moreover, the Radon-Nikodym derivative of $P_{Z|\Theta=\theta}$ with respect to P_Z , denoted by $\frac{dP_{Z|\Theta=\theta}}{dP_Z}$, is

$$\frac{dP_{Z|\Theta=\theta}}{dP_Z}(z) = \int \frac{dP_{Z|\Theta=\theta}}{P_Z}(z, \nu) dP_{Z_{-1}}(\nu), \quad (255)$$

which completes the proof. \blacksquare

Lemma 49: Consider the probability measure P_Z and the conditional probability measure $P_{Z|\Theta}$, both in (207). Assume that:

- (a) The probability measure P_Z satisfies (22) for some $P_Z \in \Delta(\mathcal{X} \times \mathcal{Y})$; and
- (b) For all $\theta \in \mathcal{M}$, the probability measure P_Z is absolutely continuous with respect to $P_{Z|\Theta=\theta}$.

Then, for all $\theta \in \mathcal{M}$, the probability measure P_Z is absolutely continuous with respect to $P_{Z|\Theta=\theta}$ in (40).

Proof: The proof follows along the lines of the proof of Lemma 48. For all measurable sets $\mathcal{A} \subset (\mathcal{X} \times \mathcal{Y})^n$ and for all $\theta \in \mathcal{M}$,

$$P_Z(\mathcal{A}) = \int_{\mathcal{A}} dP_Z(z) \quad (256)$$

$$= \int_{\mathcal{A}} \frac{dP_Z}{dP_{Z|\Theta=\theta}}(z) dP_{Z|\Theta=\theta}(z) \quad (257)$$

$$= \int \int_{\mathcal{A}_z} \frac{dP_Z}{dP_{Z|\Theta=\theta}}(z, \nu) dP_{Z_{-1}|Z_1=z, \Theta=\theta}(\nu) dP_{Z|\Theta=\theta}(z) \quad (258)$$

$$= \int \int_{\mathcal{A}_z} \frac{dP_Z}{dP_{Z|\Theta=\theta}}(z, \nu) dP_{Z_{-1}|Z_1=z, \Theta=\theta}(\nu) dP_{Z|\Theta=\theta}(z), \quad (259)$$

where the equality in (257) follows from Assumption (b) and [61, Theorem 2.2.3]; and in the equality (258), the set \mathcal{A}_z is defined in (248) and the probability measure $P_{Z_{-1}|Z_1=z, \Theta=\theta} \in \Delta((\mathcal{X} \times \mathcal{Y})^{n-1})$ is the one that satisfies for all measurable subsets \mathcal{C} of $(\mathcal{X} \times \mathcal{Y})^{n-1}$,

$$P_{Z|\Theta=\theta}((\mathcal{X} \times \mathcal{Y}) \times \mathcal{C}) = \int P_{Z_{-1}|Z_1=z, \Theta=\theta}(\mathcal{C}) dP_{Z|\Theta=\theta}(z), \quad (260)$$

where the measure $P_{Z|\Theta=\theta}$ is the marginal defined in (38); and finally, the equality (259) follows from Assumption (a) and Lemma 5.

The proof continues by noticing that for a given measurable subset \mathcal{B} of $\mathcal{X} \times \mathcal{Y}$, the set \mathcal{A} in (249) satisfies for all $\theta \in \mathcal{M}$,

$$P_Z(\mathcal{B}) = P_Z(\mathcal{A}) \quad (261)$$

$$= \int \int_{\mathcal{A}_z} \frac{dP_Z}{dP_{Z|\Theta=\theta}}(z, \nu) dP_{Z_{-1}|Z_1=z, \Theta=\theta}(\nu) dP_{Z|\Theta=\theta}(z), \quad (262)$$

$$= \int \int_{\mathcal{A}_z} \frac{dP_Z}{dP_{Z|\Theta=\theta}}(z, \nu) dP_{Z_{-1}|Z_1=z, \Theta=\theta}(\nu) dP_{Z|\Theta=\theta}(z), \quad (263)$$

where the equality in (261) follows from Assumption (a); the equality in (262) follows from (259); and the equality in (263) follows from (251). Hence, given that the set \mathcal{B} can be any measurable subset of $\mathcal{X} \times \mathcal{Y}$, the equality in (263), together with [61, Theorem 2.2.3], imply that the probability measure P_Z is absolutely continuous with respect to $P_{Z|\Theta=\theta}$. Moreover, the Radon-Nikodym derivative of P_Z with respect to $P_{Z|\Theta=\theta}$, denoted by $\frac{dP_Z}{dP_{Z|\Theta=\theta}}$, is

$$\frac{dP_Z}{dP_{Z|\Theta=\theta}}(z) = \int \frac{dP_Z}{dP_{Z|\Theta=\theta}}(z, \nu) dP_{Z_{-1}|Z_1=z, \Theta=\theta}(\nu), \quad (264)$$

which completes the proof. \blacksquare

Lemma 48 and Lemma 49 lead to the following corollary.

Corollary 50: Consider the probability measure P_Z and the conditional probability measure $P_{Z|\Theta}$, both in (207). Assume that:

- (a) The probability measure P_Z satisfies (22) for some $P_Z \in \Delta(\mathcal{X} \times \mathcal{Y})$; and
- (b) For all $\theta \in \mathcal{M}$, the probability measures P_Z and $P_{Z|\Theta=\theta}$ are mutually absolutely continuous.

Then, for all $\theta \in \mathcal{M}$, the probability measures P_Z and $P_{Z|\Theta=\theta}$ in (40) are mutually absolutely continuous.

This appendix ends stating the following property of the functionals R_θ in (8) and R_z in (9).

Lemma 51: Consider the conditional probability measures $P_{\Theta|Z}$ and $P_{Z|\Theta}$; and the probability measures P_Θ and P_Z that jointly satisfy (28) and (207). Then, the functionals R_θ in (8) and R_z in (9), satisfy

$$\int R_z(P_\Theta) dP_Z(z) = \int R_\theta(P_Z) dP_\Theta(\theta). \quad (265)$$

Consider also the following assumptions:

- (a) For all $z \in (\mathcal{X} \times \mathcal{Y})^n$, the probability measure $P_{\Theta|Z=z}$ is absolutely continuous with respect to P_Θ ; and
- (b) For all $\theta \in \mathcal{M}$, the probability measure $P_{Z|\Theta=\theta}$ is absolutely continuous with respect to P_Z .

Then, the functionals R_θ and R_z also satisfy:

$$\int R_z(P_{\Theta|Z=z}) dP_Z(z) = \int R_\theta(P_{Z|\Theta=\theta}) dP_\Theta(\theta). \quad (266)$$

Proof: The proof of (265) follows from observing that

$$\int R_z(P_\Theta) dP_Z(z) = \int \int L(z, \theta) dP_\Theta(\theta) dP_Z(z) \quad (267)$$

$$= \int \int L(z, \theta) dP_Z(z) dP_\Theta(\theta) \quad (268)$$

$$= \int R_\theta(P_Z) dP_\Theta(\theta). \quad (269)$$

where the equality in (267) follows from (9); the equality in (268) follows by exchanging the order of the integrals [50, Theorem 2.6.6]; and finally, the equality in (269) follows from (8). This completes the proof of (266).

The proof of (266) follows from observing that

$$\begin{aligned} & \int R_z(P_{\Theta|Z=z}) dP_Z(z) \\ &= \int \int L(z, \theta) dP_{\Theta|Z=z}(\theta) dP_Z(z) \end{aligned} \quad (270)$$

$$= \int \int L(z, \theta) \frac{dP_{\Theta|Z=z}(\theta)}{dP_\Theta(\theta)} dP_\Theta(\theta) dP_Z(z) \quad (271)$$

$$= \int \int L(z, \theta) \frac{dP_{\Theta|Z=z}(\theta)}{dP_\Theta(\theta)} dP_Z(z) dP_\Theta(\theta) \quad (272)$$

$$= \int \int L(z, \theta) \frac{dP_{Z|\Theta=\theta}(z)}{dP_Z(z)} dP_Z(z) dP_\Theta(\theta) \quad (273)$$

$$= \int \int L(z, \theta) dP_{Z|\Theta=\theta}(z) dP_\Theta(\theta) \quad (274)$$

$$= \int R_\theta(P_{Z|\Theta=\theta}) dP_\Theta(\theta), \quad (275)$$

where the equality in (270) follows from (9); the equality in (271) follows from the assumption that $P_{\Theta|Z=z}$ is absolutely continuous with P_Θ and [61, Theorem 2.2.3]; the equality in (272) follows by exchanging the order of the integrals [50, Theorem 2.6.6]; the equality in (273) follows from Lemma 46; and finally, the equality in (275) follows from (8). This completes the proof of (266). ■

APPENDIX B PROOF OF LEMMA 3

The proof is essentially algebraic and follows from Definition 4. More specifically,

$$\begin{aligned} & \overline{\overline{G}}(P_{\Theta|Z}, P_Z) \\ &= \int \int (R_u(P_{\Theta|Z=z}) - R_z(P_{\Theta|Z=z})) dP_Z(u) dP_Z(z) \quad (276) \\ &= \int \int \int L(u, \theta) dP_{\Theta|Z=z}(\theta) dP_Z(u) dP_Z(z) \\ &\quad - \int R_z(P_{\Theta|Z=z}) dP_Z(z), \end{aligned} \quad (277)$$

where the equality in (277) follows from (9). The proof follows by noticing that

$$\begin{aligned} & \int \int \int L(u, \theta) dP_{\Theta|Z=z}(\theta) dP_Z(u) dP_Z(z) \\ &= \int \int \left(\int L(u, \theta) dP_Z(u) \right) dP_{\Theta|Z=z}(\theta) dP_Z(z) \end{aligned} \quad (278)$$

$$= \int \int R_\theta(P_Z) dP_{\Theta|Z=z}(\theta) dP_Z(z) \quad (279)$$

$$= \int \int R_\theta(P_Z) \frac{dP_{\Theta|Z=z}(\theta)}{dP_\Theta(\theta)} dP_\Theta(\theta) dP_Z(z) \quad (280)$$

$$= \int R_\theta(P_Z) \left(\int \frac{dP_{\Theta|Z=z}(\theta)}{dP_\Theta(\theta)} dP_Z(z) \right) dP_\Theta(\theta) \quad (281)$$

$$= \int R_\theta(P_Z) dP_\Theta(\theta) \quad (282)$$

$$= \int R_z(P_\Theta) dP_Z(z), \quad (283)$$

where the equalities in (278) and (281) follow by exchanging the order of the integrals [50, Theorem 2.6.6]; the equality in (279) follows from (8); the equality in (280) follows from the assumption that $P_{\Theta|Z=z}$ is absolutely continuous with P_Θ and [61, Theorem 2.2.3]; the equality in (282) follows from observing that

$$\int \frac{dP_{\Theta|Z=z}(\theta)}{dP_\Theta(\theta)} dP_Z(z) = 1; \quad (284)$$

and finally, the equality in (283) follows from Lemma 51 (in Appendix A).

Plugging the equality (283) in (277) yields

$$\begin{aligned} & \overline{\overline{G}}(P_{\Theta|Z}, P_Z) \\ &= \int R_z(P_\Theta) dP_Z(z) - \int R_z(P_{\Theta|Z=z}) dP_Z(z) \end{aligned} \quad (285)$$

$$= \int (R_z(P_\Theta) - R_z(P_{\Theta|Z=z})) dP_Z(z) \quad (286)$$

$$= \int G(z, P_\Theta, P_{\Theta|Z=z}) dP_Z(z), \quad (287)$$

which completes the proof.

APPENDIX C PROOF OF LEMMA 6

The proof is essentially algebraic and follows from Definition 4. More specifically,

$$\begin{aligned} & \overline{\overline{G}}(P_{\Theta|Z}, P_Z) \\ &= \int \int (R_u(P_{\Theta|Z=z}) - R_z(P_{\Theta|Z=z})) dP_Z(u) dP_Z(z) \end{aligned} \quad (288)$$

$$= \int \int \int (L(u, \theta) - L(z, \theta)) dP_{\Theta|Z=z}(\theta) dP_Z(u) dP_Z(z) \quad (289)$$

$$= \int \int \left(\int L(u, \theta) dP_Z(u) \right) dP_{\Theta|Z=z}(\theta) dP_Z(z) \quad (290)$$

$$- \int \int L(z, \theta) dP_{\Theta|Z=z}(\theta) dP_Z(z), \quad (291)$$

$$= \int \int (R_\theta(P_Z) - L(z, \theta)) dP_{\Theta|Z=z}(\theta) dP_Z(z), \quad (292)$$

where the equality in (289) follows from (9); the equality in (290) follows by exchanging the order of the integrals [50, Theorem 2.6.6]; and the equality in (292) follows from (8).

The proof continues by noticing that:

$$\begin{aligned} & \int \int \mathbb{R}_\theta(P_Z) dP_{\Theta|Z=z}(\theta) dP_Z(z) \\ &= \int \int \mathbb{R}_\theta(P_Z) \frac{dP_{\Theta|Z=z}(\theta)}{dP_\Theta}(\theta) dP_\Theta(\theta) dP_Z(z) \end{aligned} \quad (293)$$

$$= \int \mathbb{R}_\theta(P_Z) \left(\int \frac{dP_{\Theta|Z=z}(\theta)}{dP_\Theta}(\theta) dP_Z(z) \right) dP_\Theta(\theta) \quad (294)$$

$$= \int \mathbb{R}_\theta(P_Z) dP_\Theta(\theta) \quad (295)$$

$$= \int \int \left(\frac{1}{n} \sum_{t=1}^n \ell(x_t, y_t, \theta) \right) dP_Z(z) dP_\Theta(\theta) \quad (296)$$

$$= \frac{1}{n} \sum_{t=1}^n \int \int \ell(x, y, \theta) dP_Z(x, y) dP_\Theta(\theta) \quad (297)$$

$$= \int \int \ell(x, y, \theta) dP_Z(x, y) dP_\Theta(\theta), \quad (298)$$

where the equality (293) follows from Assumption (b) and [61, Theorem 2.2.3]; the equality in (294) follows by exchanging the order of the integrals [50, Theorem 2.6.6]; the equality in (295) follows from observing that

$$\int \frac{dP_{\Theta|Z=z}(\theta)}{dP_\Theta}(\theta) dP_Z(z) = 1; \quad (299)$$

the equality in (296) follows from (7) and (8); and finally, the equality in (297) follows from [50, Theorem 1.6.3].

Finally, note that

$$\begin{aligned} & \int \int \mathbb{L}(z, \theta) dP_{\Theta|Z=z}(\theta) dP_Z(z) \\ &= \int \int \mathbb{L}(z, \theta) \frac{dP_{\Theta|Z=z}(\theta)}{dP_\Theta}(\theta) dP_\Theta(\theta) dP_Z(z) \end{aligned} \quad (300)$$

$$= \int \int \mathbb{L}(z, \theta) \frac{dP_{\Theta|Z=z}(\theta)}{dP_\Theta}(\theta) dP_Z(z) dP_\Theta(\theta) \quad (301)$$

$$\begin{aligned} &= \int \int \mathbb{L}(z, \theta) \frac{dP_{\Theta|Z=z}(\theta)}{dP_\Theta}(\theta) \\ & \quad \frac{dP_Z}{dP_{Z|\Theta=\theta}}(z) dP_{Z|\Theta=\theta}(z) dP_\Theta(\theta) \end{aligned} \quad (302)$$

$$= \int \int \mathbb{L}(z, \theta) dP_{Z|\Theta=\theta}(z) dP_\Theta(\theta) \quad (303)$$

$$= \int \int \left(\frac{1}{n} \sum_{t=1}^n \ell(x_t, y_t, \theta) \right) dP_{Z|\Theta=\theta}(z) dP_\Theta(\theta) \quad (304)$$

$$= \frac{1}{n} \sum_{t=1}^n \int \int \ell(x, y, \theta) dP_{Z_t|\Theta=\theta}(x, y) dP_\Theta(\theta) \quad (305)$$

$$= \int \int \ell(x, y, \theta) dP_{Z|\Theta=\theta}(x, y) dP_\Theta(\theta), \quad (306)$$

where the equality (300) follows from Assumption (b) and [61, Theorem 2.2.3]; the equality in (301) follows by exchanging the order of the integrals [50, Theorem 2.6.6]; the equality (302) follows from Assumption (c) and [61,

Theorem 2.2.3]; the equality in (303) follows from Lemma 46 and Lemma 47 (in Appendix A), which hold under Assumption (b) and Assumption (c) and imply that for all $(z, \theta) \in (\mathcal{X} \times \mathcal{Y})^n \times \mathcal{M}$,

$$\frac{dP_{\Theta|Z=z}(\theta)}{dP_\Theta}(\theta) \frac{dP_Z}{dP_{Z|\Theta=\theta}}(z) = 1; \quad (307)$$

the equality in (304) follows from (7); the equality in (305) follows from [50, Theorem 1.6.3]; and finally, the equality in (306) follows from Lemma 5, which holds under Assumption (a).

The proof ends by using (298) and (306) in (292), which yields

$$\begin{aligned} \overline{\mathbb{G}}(P_{\Theta|Z}, P_Z) &= \int \int \ell(x, y, \theta) dP_Z(x, y) dP_\Theta(\theta) \\ & \quad - \int \int \ell(x, y, \theta) dP_{Z|\Theta=\theta}(x, y) dP_\Theta(\theta) \quad (308) \\ &= \int \mathbb{G}(\theta, P_Z, P_{Z|\Theta=\theta}) dP_\Theta(\theta), \end{aligned} \quad (309)$$

where the equality in (309) follows from (21). This completes the proof.