Information-Theoretic Generalization Bounds for Transductive Learning and its Applications

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Abstract

We develop data-dependent and algorithm-dependent generalization bounds for transductive learning algorithms based on information theory. We first show that the generalization error for a transductive learning algorithm can be controlled by the mutual information between training labels and the hypothesis. By introducing the concept of transductive supersamples, we go beyond inductiv learning setting further derive upper bounds in terms of various information measure. From this results, we derive PAC-Baysian bounds with faster rate and build connection between generalization and the sharpness of loss landscape under transductive learning setting. Finally, we present the upper bounds for adaptive optimization algorithms and demonstrate the applications of our results on semi-supervised and transductive graph learning scenarios.

1 Introduction

In the standard supervised learning paradigm [107], we receive a set of instances sampling independently from unknown distribution that are composed of features and targets. Our task is to build a learner (or model) by specific optimization algorithm that maps features to corresponding targets based on limited instances. A modern and popular practice of this paradigm is training a deep neural network for image classification via stochastic gradient descent [59]. Generalization, referring to the prediction performance of learner on unseen examples, is one of the fundamental questions in machine learning theory. The past decades have witnessed efforts devoted to characterizing and understanding the generalization of machine learning models. In the category of classical learning theory, generalization is connected to the complexity of hypothesis space [58, 8, 7], the stability of algorithm [13, 92] or the divergence between two probability measure on hypothesis space [95, 70]. Recently, mutual information and its variants are shown to serve as an ideal generalization metric, since they reflect both the impact of dataset and optimization on generalization. Research of this viewpoint originates from work [85, 86, 117], and is further developed by subsequent studies [73, 15, 45, 99, 46, 43, 89, 114]. Despite the diverse forms of these results, they possess a common key insight: the less information on training data (or its selection) a hypothesis (or the variables it induced) reveals, the better generalization it will have.

The aforementioned supervised learning setting are far not enough to cover all machine learning scenarios. Data collected from real-world scenarios could come from various domains, and some examples could lack of targets due to the expensive cost of annotations. This raises the need of exploring new theory to measure the generalization, where the key challenge is relaxing the identical and independent assumptions of instances. We move towards this direction by analyzing a classical but important regime termed as transductive learning [106]. In this learning paradigm, we are provided with a fixed set of instances containing both labeled example and unlabeled examples, and our task is to build a learner that make prediction for those unlabeled ones. Note that under this setting, the examples to be predicted are available to learner. As a comparison, the learning paradigm of supervised learning is inductive, since the examples to be predicted are not available

to learner during training. Popular practices of transductive learning are semi-supervised learning [91, 11, 52, 116] and graph learning [39, 87, 36, 57].

Existing results for transductive generalization bounds fall into three categories: complexity-based bounds derived by VC dimension [22] or transductive Rademacher complexity [30, 105], stability-based bounds [29, 23] and PAC-Bayesian bounds [26, 10]. These results are sufficient to provide learning guarantee for classical learner or algorithms such as transductive support vector machine and unlabeled-labeled representation. However, they are far from the optimal approaches to understanding the generalization behavior of deep transducitve model such as Graph Neural Networks (GNNs). The reasons are three folds. First, [32] shows that VC dimension results in trivial generalization error bounds, and transductive Rademacher complexity is algorithm-independent and fail to characterize the impact of optimization algorithms on generalization [101]. Second, stability-based bounds depend on Lipschitz and smoothness constant [21], which is difficulty to compute for deep models [74]. Third, existing transductive PAC-Bayesian bounds are of slow order and not sufficient to provide non-vacuous bounds. Furthermore, it is unclear to what extent they reflect the impact of optimization algorithms. In a nutshell, effort to establish data-dependent and algorithm-dependent generalization bounds for transductive learning is limited.

In this paper, we comprehensively study the generalization theory of transductive learning in the context of information theory. First, we derive upper bounds of transductive generalization gap in expectation and high probability. These results demonstrate that the dependence of output hypothesis on the randomness of training labels serve as a measure to quantify the generalization performance of tranductive learner. Second, we introduce the concept of transductive supersamples and establish upper bounds include the conditional mutual information between the indicator random variables and output hypothesis. These bounds are non-vacuous and convenient in computation. Third, by observing the connection between information theory and PAC-Bayesian theory, we give novel transductive PAC-Bayesian bounds that has weaker assumption and sharper bounds. With this result, we further show that the sharpness of loss landscape affects generalization still holds in transductive learning setting, as supported by the empirical evidence in recent study [17]. Forth, we provide the upper bounds for adaptive optimization algorithms composed of trajectory adaptive gradient norm and the sensitivity of the final parameter to noise under transductive setting. Fifth, we illustrates the applications of the established results on semi-supervised learning and graph learning scenarios. Our main contributions are summarized as follows:

- For the first time, we systematically establish information-theoretic generalization bounds for transductive learning and reveal their connection with PAC-Bayesian bounds, which provide new perspective to understanding the generalization transductive learning.
- We propose the concept of transductive supersamples and use it to bridge the gap between supersample setting in inductive learning and transductive learning setting. This also help us obtain the first non-vacuous bound for deep transductive learner.

2 Related Work

Information-theoretic Generalization Theory. [85, 86, 117] are the pioneer work that associates expected generalization error with the mutual information between training examples and algorithm output. The subsequent studies mainly fall into four categories: (i) deriving sharper upper bounds by introducing new information measure [46, 49, 114], problem setting [99, 81, 44] or proof techniques [6, 15, 41, 34, 125, 20], (ii) establishing bounds described by various divergences [64, 109, 31, 4, 3] (iii) applying existing results to establish upper bounds for optimization algorithms such as SGD [74, 113] or SDLD [78, 73, 110], and (iv) extending the theoretical results to diverse scenarios such as meta-learning [54, 83, 18, 55], transfer learning [115, 53, 67, 14], semi-supervised learning [2, 47], self-supervised learning [123] and domain adaption [114]. However, the training and test examples are independent in existing studies, which makes them not applicable on transductive learning. Another related topic is information bottleneck theory [102] and its applications to explaining the representation [103, 82] and generalization [98, 42, 112, 56] of deep neural networks, which are parallel to our work. Interested readers are referred to a recent monograph [50] for more illustrations.

PAC-Bayesian Generalization Theory. The classical results in PAC-Bayesian generalization theory include McAllester's bound [70], Seeger's bound [88], Catoni's bound [16] and Maurer's

bound [68]. Based on this, there have been numerous studies that applying or extending these results to the analysis of deep neural networks generalization, including computing non-vacuous bounds for deep neural networks [28, 126, 79, 65] and establishing upper bounds for optimization algorithms [63, 75, 84, 5, 72, 121, 61, 66]. We refer interested readers to a comprehensive survey [1] for more detail on this topic. All the above results require that training examples are independent to test examples and could not be applied on transductive learning setting.

Transductive Learning Generalization Theory. The concept of transductive learning and the earliest bounds are presented to [106]. The authors in [29] study the stability of transductive learning algorithms. They further propose another tool named transductive Rademacher Complexity [30] as a complexity of hypothesis space under transductive setting. Permutational Rademacher Complexity is latter presented in [105], which is shown to be more suitable for transductive learning setting than transductive Rademacher Complexity. By considering the variance of functions, the authors in [104] establish new concentration inequalities and sharper bounds. [26] is the first work to analyze the generalization of transductive learning in the context of PAC-Bayesian, and their results are improved latter in [10]. Furthermore, the above results have been applied on the theoretical analysis in graph learning [96, 97, 24, 76, 32, 21, 101], semi-supervised learning [69, 38, 118], matrix completion [37, 94], distributed optimization [93] and collaborative filtering [119, 25], among other areas. Our results also apply to these fields, particularly when the learner is deep neural network.

3 Preliminaries

3.1 Notations

We stipulate that random variables and their realization are denoted by uppercase and lowercase letters, respectively. For given random variable X, we denote its distribution measure by P_X. Similarly, the conditional distribution measure of X given Y is given by $P_{X|Y}$. We use $\mathrm{D}_{\mathrm{KL}}(P||Q)$ to denote the Kullback–Leibler (KL) divergence between two probability measure P and Q, where we have assumed that they are on the same measure space and the Radon-Nikodym derivative of P with respect to Q is well defined. With this notation, the mutual information between X and Y is defined as $I(X;Y) \triangleq \mathrm{D}_{\mathrm{KL}}(P_{X,Y}||P_X P_Y)$. Furthermore, the disintegrated mutual information is denoted by $I^z(X;Y) \triangleq \mathrm{D}_{\mathrm{KL}}(P_{X,Y|Z=z}||P_{X|Z=z}P_{Y|Z=z})$, whose expectation taking over $Z \sim P_Z$ is the conditional mutual information $I(X;Y|Z) = \mathbb{E}_{P_Z}[I^Z(X;Y)]$.

3.2 Transductive Learning

Let $D = \{\mathbf{z}_1, \ldots, \mathbf{z}_n\}$ be a given set with finite cardinality, where $\mathbf{z} = (\mathbf{x}, y)$ is an instance composed of attribute $\boldsymbol{x} \in \mathcal{X}$ and target $y \in \mathcal{Y}$ from $\mathcal{Z} \triangleq \mathcal{X} \times \mathcal{Y}$. We use $\mathrm{Perm}(D)$ to denote the set containing all bijections $\pi : D \to D$. Here each bijection $\pi \in \mathrm{Perm}(D)$ could be regarded as a permutation on D. Note that sampling without replacement from D is equivalent to firstly sampling a permutation from $\mathrm{Perm}(D)$ with equal probability and then applying it on D. Denote by Π a random variable follows uniform distribution over $\mathrm{Perm}(D)$, namely $\mathbb{P}\{\Pi = \pi\} = \frac{1}{n!}$ holds for any $\pi \in \mathrm{Perm}(D)$. With this notation, we use $Z \triangleq (Z_1, \ldots, Z_n)$ to denote the random permutation vector induced by Π, where $Z_j = \Pi(\mathbf{z}_j)$ represents the j-th element of the sequence after permutation. Once the permutation Z is determined, the training set is defined as $\mathrm{D}_{\mathrm{train}} \triangleq \{Z_1, \ldots, Z_m, X_{m+1}, \ldots, X_{m+u}\}$, where m and u are the number of training and test instances, respectively. Let $\mathcal{W}$ be the space of parameter, the transductive learning algorithm takes $\mathrm{D}_{\mathrm{train}}$ as input and outputs a random element $W \in \mathcal{W}$ as the hypothesis, which is characterized by a Markov kernel $P_{W|Z}$. Let $\ell : \mathcal{W} \times \mathcal{Z} \to \mathbb{R}_{\geq 0}$ be the objective function, the transductive training and test error of a hypothesis W are defined as $R_m(W,Z) \triangleq \frac{1}{m}\sum_{i=1}^{m} \ell(W, Z_i)$ and $R_u(W,Z) = \frac{1}{u}\sum_{i=m+1}^{m+u} \ell(W, Z_i)$, respectively. The *transductive generalization error* is then defined as $\mathcal{E}(W,Z) \triangleq R_u(W,Z) - R_m(W,Z)$. Furthermore, we use $\mathbb{E}_{W,Z}[\mathcal{E}(W,Z)]$ to denote the expectation of $\mathcal{E}(W,Z)$ taking over $P_{W,Z} = P_Z \otimes P_{W|Z}$, which represents the the average performance difference of the hypothesis W between testing and training instances over all permutation Z. Under certain circumstances, the objective $\ell(W,Z)$ is represented as $l(f_W(X), Y)$, where $f_\cdot(\cdot) : \mathcal{X} \times \mathcal{W} \to \widehat{\mathcal{Y}}$ is the learner parameterized by W and $l : \widehat{\mathcal{Y}} \times \mathcal{Y} \to \mathbb{R}_{\geq 0}$ is the criterion.

4 Information-Theoretic Generalization Bounds for Transductive Learning

4.1 Establishing Upper Bounds by Mutual Information

Different from supervised learning, the randomness of training and testing examples in transductive learning come from the partition determined by permutation rather than from sampling. This also brings another challenge, namely the dependence of training and testing examples, since the testing examples are uniquely determined once training examples are chosen. The most widely adopt technique to tackle dependence is the martingales method, which enables us to derive similar "sub-Gaussian" property for the transductive generalization error. Together with the Donsker-Varadhan's variational formula, we establish the following transductive generalization bounds.

Theorem 1. *Suppose $\ell(\mathbf{w}, \mathbf{z}) \leq B$ holds for any $\mathbf{w} \in \mathcal{W}$ and $\mathbf{z} \in D$, then*

$$|\mathbb{E}_{W,Z}\left[R_u(W,Z) - R_m(W,Z)\right]| \leq \sqrt{\frac{C_{m,u}}{2}\left(\frac{1}{m}+\frac{1}{u}\right) I(Z;W)}, \tag{1}$$

$$\mathbb{E}_{W,Z}\left[(R_u(W,Z) - R_m(W,Z))^2\right] \leq C_{m,u}\left(\frac{1}{m}+\frac{1}{u}\right)(I(Z;W) + \log 3). \tag{2}$$

where $C_{m,u} \triangleq \frac{2B^2(m+u)\max(m,u)}{(m+u-1/2)(2\max(m,u)-1)}$.

Theorem 1 shows that the expectation of transductive generalization error is upper bounded by the mutual information between permutation Z and hypothesis W. This result implies that the less dependence the output hypothesis has on the selection of training data, the better generalization a transductive learning algorithms will have. One can image that if the algorithm only "memorize" the partition of training and testing examples (or heavily depends on the training samples it sees), we could not expect that it will have strong generalization ability. As a comparison, similar results (Theorem 1 in [117]) under supervised learning setting say that the generalization error is upper bounded by the mutual information between training set S and hypothesis W, which could be regarded as a special case of our result that u is infinite. In this event, the transductive training and test error corresponding to the supervised training and test error, respectively. Also, m is the number of examples in S, and the term $\frac{1}{u}$ vanish. Note that since the test error is computed over infinite examples, there is no dependence between it and the training error. Furthermore, the assumption of Theorem 1 is slightly stronger than that in supervised learning setting, where they only requires the loss to be sub-Gaussian while we require the loss to be bounded. However, we believe that our result could be extend to the unbounded loss setting under proper assumptions.

The result presented in Theorem 1 is a expectation bound over all possible selection of training data. In real-world application particularly deep learning scenario, only a few partitions (determined by random seed) are adopted to verify the quality of a transductive learning algorithm, and the empirical results show that whose performance could generally be guaranteed. This urges us to establish the high probability bound in order to better describe the generalization behavior of deep transductive learners. Achieve this relies on the monitor technique proposed in [9]. Another derivant is the expectation bound on the absolute value of transductive generalization error, which serves as a supplement of Theorem 1. The aforementioned results are summarized in Theorem 2.

Theorem 2. *Suppose $\ell(\mathbf{w}, \mathbf{z}) \in [0, B]$ holds for any $\mathbf{w} \in \mathcal{W}$ and $\mathbf{z} \in D$, with probability at least $1-\delta$ over the randomness of Z, W:*

$$|R_u(W,Z) - R_m(W,Z)| \leq 2\sqrt{\frac{C_{m,u}}{2}\left(\frac{1}{m}+\frac{1}{u}\right)\left(\log\left(\frac{1}{\delta}\right) + \frac{I(Z;W)}{\delta}\right)}, \tag{3}$$

where $C_{m,u}$ follows the definition in Theorem 1. Furthermore, we have

$$\mathbb{E}\,|R_u(W,Z) - R_m(W,Z)| \leq \sqrt{\frac{C_{m,u}}{2}\left(\frac{1}{m}+\frac{1}{u}\right)(I(Z;W) + \log 2)}. \tag{4}$$

Since $C_{m,u} \approx B^2$ when $m+u$ is large, the high probability bound presented in Eq. 3 is of order $(1/m + 1/u)^{\frac{1}{2}}$. Despite a degenerated constant factor from $\log(1/\delta)$ to $1/\delta$, our bound is sharper

than that in existing studies [76, 32]. Although the mutual information term $I(Z;W)$ could not be easily computed, we will show in Sec. that it has a unique advantage when the learner is optimized by stochastic algorithms such as stochastic gradient descent and its variants. Besides, result similar to Eq. (4) can be derived from Eq. (2), despite the constant factor is slightly larger.

4.2 Establishing Upper Bounds by Conditional Information

So far, all the bounds we have established contains the mutual information term $I(Z;W)$, either in expectation or high probability. One unsatisfied property of mutual information is that it does not have a finite upper bound, which may lead to vacuous bounds under some circumstances. Fortunately, this issue could be addressed by adopting "supersamples" setting proposed in [99] under supervised learning setting. The key insight is that introducing another random variable to control the randomness of sampling training and test examples, which is independent of the instances. However, directly applying this technique on transductive learning setting is not feasible. The reason is that the training and test examples given returned by this setting is independent, which is yet dependent in transductive learning setting. To bridge this gap, we propose the following transductive supersamples under a specific condition that the number of training examples is equal to that of test examples.

Definition 1 (Transductive Supersamples). *Let $D = \{\mathbf{z}_i\}_{i=1}^n$ be a given set where n is a finite even number. Denote by $m = \frac{1}{2}n$, the transductive supersamples is a sequence $\widetilde{Z}^m \triangleq (\widetilde{Z}_1, \ldots, \widetilde{Z}_m)$ generated by sampling without replacement from D, where $\widetilde{Z}_i \triangleq \left\{\widetilde{Z}_{i,0}, \widetilde{Z}_{i,1}\right\}$ for $i \in [m]$ is an unordered set with cardinality 2.*

Definition 1 shows that the transductive supersamples is obtained by continuously sampling an unorderd instance pairs from a fixed set until there is no remained instances. Please refer to Appendix E for a illustrated example of this definition. As a comparison, transductive samples Z^n is obtained by each time sampling an instance from D. A deeper relationship between Z^m and $\widetilde{Z}^m$ is given by the following lemma.

Proposition 1. *Denote by $\widetilde{\mathcal{Z}}$ the set containing all $\widetilde{Z}^m$. Let $S = (S_1, \ldots, S_m) \sim \mathrm{Unif}(\{0,1\})^m$ be the sequence of random variables that is independent of $\widetilde{Z}^m$. Sampling without replacement from D is equivalent to firstly sampling $\widetilde{Z}$ from $\widetilde{\mathcal{Z}}$ and applying S to permute $\widetilde{Z}$.*

Proposition 1 implies that there is another way to obtain the random permutation vector Z^n with the help of transductive supersamples. Let $\widetilde{Z}^m$ and S be the random variables described in Proposition 1, Z can be expressed by $Z^n = (\widetilde{Z}_{1,S_1}, \ldots, \widetilde{Z}_{m,S_m}, \widetilde{Z}_{1,1-S_1}, \ldots, \widetilde{Z}_{m,1-S_m})$. Let $\mathcal{E}(W, \widetilde{Z}, S)$ be the transductive generalization error under supersampling setting defined by

$$\mathcal{E}(W, \widetilde{Z}, S) \triangleq \frac{1}{m}\sum_{i=1}^{m}(\ell(W, \widetilde{Z}_{i,S_i}) - \ell(W, \widetilde{Z}_{i,1-S_i})), \tag{5}$$

we have $\mathbb{E}[\mathcal{E}(W, \widetilde{Z}, S)] = \mathbb{E}[\mathcal{E}(W, Z)]$. This enables us to characterize the generalization bounds using conditional mutual information, as presented in Theorem 3.

Theorem 3. *Suppose that $\ell(\mathbf{w}, \mathbf{z}) \in [0, B]$ holds for any $\mathbf{w} \in \mathcal{W}$ and $\mathbf{z} \in D$, then*

$$|\mathbb{E}_{Z,W}\left[R_u(W,Z) - R_m(W,Z)\right]| \leq \mathbb{E}_{\widetilde{Z}}\sqrt{\frac{2B^2}{m} I^{\widetilde{Z}}(S;W)} \tag{6}$$

$$\mathbb{E}_{S,W}\left[(R_u(W,Z) - R_m(W,Z))^2\right] \leq \frac{4B^2}{m}(I(S;W|\widetilde{Z}) + \log 3). \tag{7}$$

By [99], we have $I(S;W|\widetilde{Z}) \leq H(S;Z) \leq m\log 2$ holds, suggesting that the conditional mutual information has a finite upper bound and thus provides a non-vacuous generalization bound. Eq. (6) is consistent with the results in supervised learning setting [99] in form, and the only difference is that $\widetilde{Z}$ should be interpreted as the transductive supersamples. Also, we can recover the result in supervised learning (Theorem 1.2 in [99]) whereas the full sample set D has a infinite cardinality. In this event, D is exactly the space containing all instances, implying that entries in the sequence $\widetilde{Z}^m$ are independent to each other.

Although the mutual information term $I(S;W|\widetilde{Z})$ in Theorem 3 is bounded, computing its numerical value is still difficult, due to W is always a high-dimensional random variable. Thanks to the transductice supersampling setting, various information-theoretical measures [46, 49, 114] adopted in supervised learning setting can be extended to transductive learning setting, as shown in the following Corollary.

Corollary 1. *Suppose the criterion l satisfies $l(\hat{y},y)\in[0,B]$ holds for any $\hat{y}\in\widehat{\mathcal{Y}},y\in\mathcal{Y}$. Let $f_w(\mathbf{x})\in\mathbb{R}^d$ be the prediction given by the learner. Denote by $F\in\mathbb{R}^{m\times 2d}$ the prediction matrix where the i-th row is given by $F_{i,:}\triangleq(f_W(\widetilde{X}_{i,0}),f_W(\widetilde{X}_{i,1}))$, where $\widetilde{X}$ is the feature of $\widetilde{Z}=(\widetilde{X},\widetilde{Y})$. We have*

$$|\mathbb{E}_{Z,W}\left[R_u(W,Z)-R_m(W,Z)\right]|\leq\frac{B}{m}\sum_{i=1}^{m}\mathbb{E}_{\widetilde{Z}}\sqrt{2I(F_i;S_i|\widetilde{Z})}. \tag{8}$$

Denote by $L\in\{0,1\}^{m\times 2}$ the loss value matrix, where the i-th row is $L_{i,:}\triangleq(\ell(W,\widetilde{z}_{i,0}),\ell(W,\widetilde{z}_{i,1}))$. Let $\Delta_i\triangleq\ell(W,\widetilde{z}_{i,1})-\ell(W,\widetilde{z}_{i,0})$ be the difference of loss value. We have

$$|\mathbb{E}_{S,W}\left[R_u(W,Z)-R_m(W,Z)\right]|\leq\frac{B}{m}\sum_{i=1}^{m}\mathbb{E}_{\widetilde{Z}}\sqrt{2I^{\widetilde{Z}}(L_i;S_i)}, \tag{9}$$

$$|\mathbb{E}_{S,W}\left[R_u(W,Z)-R_m(W,Z)\right]|\leq\frac{B}{m}\sum_{i=1}^{m}\mathbb{E}_{\widetilde{Z}}\sqrt{2I^{\widetilde{Z}}(\Delta_i;S_i)}. \tag{10}$$

Compared with previous studies, we termed the bounds in Eqs. (8,9,10) as transductive f-CMI, transductive e-CMI and transductive Id-CMI bounds, respectively. In applications, the prediction of learner is a low-dimension vector and thus reduce the difficulty of computing the conditional mutual information $I(W;S|\widetilde{Z})$. Note that L_i in Eq. (9) and Δ_i in Eq. (10) are two-dimensional and one-dimensional random variable, yielding more convenient computation and sharper bounds. Here we point out that each result has its advantage. The vanilla bound in Eq. (6) is more informative to understanding generalization, and the expense is is difficulty of calculating numerical value. In contrast, the other bounds in Corollary 1 has computation convenience, yet they are inferior in reflecting factors that affect generalization. Despite the exist of this trade-off, these results are sufficient for us to understand the generalization behavior of transductive learner or establish non-vacuous bounds for them.

We close this part by briefly discuss how to extend the aforementioned results to more ordinary cases. According to Definition 1, Theorem 3 and Corollary 1 only apply to the case that $m=u$. Here we point out that they can be extended to cases that $m=ku$ or $u=km$ where $k\in\mathbb{N}_+$. Considering the symmetric, it is sufficient to discuss the case that $u=km$. To this end, the transductive supersamples are extended to the following k-transductive supersamples.

Definition 2 (k-Transductive Supersamples). *Let $D=\{\mathbf{z}_i\}_{i=1}^{n}$ be a given set where n is a finite even number. Let $k\in\{1,\ldots,n-1\}$ be a given integer. Denote by $m=\frac{n}{k+1}\in\mathbb{N}_+$, the k-transductive supersamples is a sequence $\widetilde{Z}^m\triangleq(\widetilde{Z}_1,\ldots,\widetilde{Z}_m)$ generated by sampling without replacement from D, where $\widetilde{Z}_i\triangleq\{\widetilde{Z}_{i,0},\ldots,\widetilde{Z}_{i,k}\}$ is an unordered set with cardinality $k+1$.*

Note that Definition 1 is a special case of Definition 2 where $k=1$. Similarly we need to extend the definition of the indicator variable S. Let $S=(S_1,\ldots,S_m)\sim\mathrm{Unif}(\{0,\ldots,k\})^m$ be the sequence of random variables that is independent of $\widetilde{Z}^m$. Let $U=(U_1,\ldots,U_m)\sim\mathrm{Unif}(\{0,\ldots,(k-1)!\})^m$ be the sequence of random variables that is independent of $\widetilde{Z}^m$ and S. For a fixed set $\mathcal{S}$, we use $\Pi(\mathcal{S},U)$ to represent the permutation of $\mathcal{S}$ induced by random variable U. For example, $\Pi(\widetilde{Z}_i\setminus\widetilde{Z}_{i,0},U_1)$ denote the result of drawing a permutation of $\widetilde{Z}_i\setminus\widetilde{Z}_{i,0}$ according to U_1, which is essentially equivalent to sampling without replacement from $\widetilde{Z}_i\setminus\widetilde{Z}_{i,0}$. With this definition, the permutation vector Z can be expressed by $Z^n=(\widetilde{Z}_{1,S_1},\ldots,\widetilde{Z}_{m,S_m},\Pi_{U_1}(\widetilde{Z}_1\setminus\widetilde{Z}_{1,S_1}),\ldots,\Pi_{U_m}(\widetilde{Z}_m\setminus\widetilde{Z}_{m,S_m}))$. By this way, all results in Theorem 3 and Corollary 1 can be extended to the case that $u=km$, and we place the details in Appendix E. One main differences between the case that $k=1$ and $k>1$ is the increased cost of estimating the mutual information, since each entry of S has more possible values to take. In other words, with the increase of k, we need to accordingly increase the samples of S to reduce the estimated error of the mutual information.

4.3 Connection with Transductive PAC-Bayesian Bounds

PAC-Bayesian methods and Information-theoretic methods are closely related, since both of them are based on Donsker-Varadhan's variational formulation. Borrowing the proof of Theorem 1, we obtain the following new transductive PAC-Bayesian bounds.

Theorem 4. *Suppose that $\ell(w, \mathbf{z}) \leq B$ holds for any $w \in \mathcal{W}$ and $\mathbf{z} \in D$. Let P be a prior distribution P on $\mathcal{W}$. With probability at least $1-\delta$ over the randomness of Z, for any distribution Q on $\mathcal{W}$ we have*

$$|\mathbb{E}_{W\sim Q}\left[R_u(W,Z) - R_m(W,Z)\right]| \leq \sqrt{\frac{C_{m,u}}{2}\left(\frac{1}{m}+\frac{1}{u}\right)\left(\mathrm{D}_{\mathrm{KL}}(Q||P) + \log\left(\frac{1}{\delta}\right)\right)}, \tag{11}$$

where $C_{m,u}$ follows the definition in Theorem 1.

Compared with previous transductive PAC-Bayesian bound (Corollary 7(b) in [10]), the result in Theorem 4 are as follows. For one hand, the assumptions of our bound is weaker. Previous result only apply to zero-one loss, and the value of m and n are required to satisfy $m \geq 40$ and $20 \leq m \leq n-20$. In contrast, our result apply to any bounded loss and there are no constraints on the value of m and n. For the other hand, our result is strictly sharper than previous result by removing the term $\log\left(\log(m)\sqrt{\frac{mu}{m+u}}\right)$. Furthermore, incorporating the technique in [75], the results in [62] could be directly extend to transductive learning setting and thus providing generalization guarantee for many GNNs models on node classification and link prediction task.

One of the most important insights provided by PAC-Bayesian bounds in that the generalization performance is closely related with the sharpness of the loss landscape, and a flat minimum is beneficial for generalization [75]. With the help of Theorem 4, this result can be extended to transductive learning setting when the criterion is 0-1 loss.

Corollary 2. *Suppose that $R_u(\mathbf{w}, Z) \leq \mathbb{E}_{\boldsymbol{\epsilon}\sim\mathcal{N}(\mathbf{0},\sigma^2\mathbf{I})}[R_u(\mathbf{w}+\boldsymbol{\epsilon}, Z)]$ holds for any Z, where $\mathbf{w} \in \mathbb{R}^d$ is the parameter returned by given transductive learning algorithm and $\boldsymbol{\epsilon} \in \mathbb{R}^d$ is a random noise. With probability at least $1-\delta$ over the randomness of Z,*

$$\begin{aligned} &R_u(\mathbf{w}, Z) \\ &\leq \max_{\|\boldsymbol{\epsilon}\|_2\leq\rho} R_m(\mathbf{w}+\boldsymbol{\epsilon}, Z) \\ &\quad + \sqrt{\frac{C_{m,u}(m+u)\left(1+\frac{d}{2}\log\left(1+\frac{\left(1+\widetilde{C}_{m,u}\right)^2\|\mathbf{w}\|_2^2}{\rho^2}\right)+\log\left(\frac{1}{6\delta}\right)+2\log\left(\frac{4\pi mu}{m+u}\right)\right)}{mu}}, \end{aligned} \tag{12}$$

where $\widetilde{C}_{m,u} \triangleq \sqrt{\log(4mu/(m+u))/d}$ and $C_{m,u}$ follows the definition in Theorem 1.

The term $\max_{\|\boldsymbol{\epsilon}\|_2\leq\rho} R_m(\mathbf{w}+\boldsymbol{\epsilon}, Z)$ characterizes the change of loss landscape within a ball with $\mathbf{w}$ as the center and ρ as the radius. Formally, we call $\mathbf{w}$ as sharp minima if the loss values around it differ significantly from itself, namely $R_m(\mathbf{w}+\boldsymbol{\epsilon}, Z) > R_m(\mathbf{w}, Z)$. Therefore, Corollary 2 suggests that a flat optima could have better transductive generalization performance. This theoretical result has been verify by recent work [17], which applies sharpness-aware minimization [33] on recommendation task to achieve better generalization performance for GNNs. We believe that this result could shed light in understanding the correlation between sharpness and generalization in transductive learning.

4.4 Upper Bounds for Adaptive Optimization Algorithms

As we have mentioned, one advantages of our theoretical results against previous one is that the effect of optimization algorithm on generalization can be fully considered. In this work we focus on AdaGrad, which is one of the most widely adopted optimization algorithms in practice. Different from SGD, the learning rate is adaptively adjusted during training. Denote by $\{W_t\}_{t\in[T]}$ the weights along the training trajectory of AdaGrad. Following [113], we consider the setting that mini-batches examples are fixed. Denote by $(B_1, \ldots, B_T)$ the sequence of mini-batches where B_i is the of examples used in the t-th epoch. For concise we assume that the learner only minimizes the loss

on labeled examples, and the number of each mini-batch examples are equal to b. Then the average gradient on the B_t is defined as

$$g(w, B_t(Z)) \triangleq \frac{1}{b} \sum_{\mathbf{z} \in B_t} \nabla_w \ell(w, \mathbf{z}), \tag{13}$$

where $B_t(Z) \subseteq \{\mathbf{z} | \mathbf{z} \in Z^m\}$. For $t \in [T]$, the update rule of AdaGrad can be formulated as

$$v_t = \sum_{k=1}^{t-1} g(W_k, B_k(Z)) \odot g(W_k, B_k(Z)), W_t = W_{t-1} - \frac{\eta}{\sqrt{v_t} + \epsilon} \odot g(W_{t-1}, B_t(Z)), \tag{14}$$

where W_0 is the initial parameter and $\odot$ is the Hadamard product. η and ϵ are two hyper-parameters. Note that v_t is a random variable determined by $W^{[t-1]} \triangleq (W_0, \ldots, W_{t-1})$. For the concise of notations we use $\Psi(W^{[t-1]}, Z) \triangleq \left(\eta/(\sqrt{v_t} + \epsilon)\right) \odot g(W_{t-1}, B_t(Z))$ to denote the "adaptive gradient", which is computed by normalizing the current gradient with accumulate squared gradient. Inspired by [74, 113], we introduce the following auxiliary weight process $\{\widetilde{W}_t\}_{t \in [T]}$ for analysis:

$$\widetilde{W}_0 = W_0, \widetilde{W}_t = \widetilde{W}_{t-1} - \Psi(W^{[t-1]}, Z) + N_t, \tag{15}$$

where $N_t \triangleq \sigma_t N$. Here $\{\sigma_t\}_{t \in [T]}$ are predefined hyperparameters and N is a Gaussian random variable that is independent to $W^{[T]}$ and Z. For concise, we define $U_t \triangleq \sum_{k=1}^{t} N_k$. The upper bound for a transductive learner trained by AdaGrad is presented in the following theorem.

Theorem 5. *Suppose that (i) $\ell(w, \mathbf{z}) \leq B$ holds for any $w \in \mathcal{W}$ and $\mathbf{z} \in D$ and (ii) $\mathbb{E}\left[R_u(w_T + U_T, Z) - R_u(w_T, Z)\right] \geq 0$ holds for any realization of $W_T = w_T$. Then we have*

$$\begin{aligned}
&\mathbb{E}_{Z, W_T}\left[R_u(W_T, Z) - R_m(W_T, Z)\right] \\
\leq &\sqrt{\frac{C_{m,u}}{2}\left(\frac{1}{m} + \frac{1}{u}\right) \sum_{t=1}^{T} \frac{d}{2} \log\left(\frac{1}{d\sigma_t^2} \mathbb{E}\left[\left\|\Psi(W^{[t-1]}, Z) - \mathbb{E}_{W^{[t-1]}, Z}\left[\Psi(W^{[t-1]}, Z)\right]\right\|_2^2\right] + 1\right)} \\
&+ \mathbb{E}_{Z, W_T, U_T}\left[R_m(W_T + U_T, Z) - R_m(W_T, Z)\right].
\end{aligned} \tag{16}$$

Assumption (ii) in Theorem 5 is also used in Corollary 2 to establish the PAC-Bayesian bound. This assumption requires that adding random noise to the final parameter does not decrease the risk on unlabeled examples in expectation. The first term in Eq. (16) records the variance of "adaptive gradient" along the training trajectory, and the second term measures the expected change of training risk after adding random noise. Compared with stability based [21] or complexity based [101] methods, our results do not contain any Lipschitz or smoothness constants and thus more easier to computed. Besides, the smoothness or Hölder smoothness assumption limit the application scope of previous results, *e.g.*, they could not be applied to neural networks with ReLU as activation function. As a comparison, our result does not rely on these assumptions and has a wider applicability. Also, since the Lipschitz constant is the upper bound of the norm of gradient, our results can more finely depict the impact of optimization trajectories on generalization. Furthermore, the second term characterizes the flatness of the final parameter, which conveys the same insight as Theorem 4, namely a flat optima is beneficial to achieve smaller generalization gap. If u is infinity and v_t is set to all-ones vector, the result for SGD under supervised learning setting [74, 113] are recovered from our result. Considering the popularity of Adam in real-world applications, we also derive the corresponding results. The reflected insights are similar yet the formulations are more tedious, and we place the details in Appendix I.

5 Applications

In this section, we demonstrate the application of theoretical results through two specific examples: semi-supervised learning and graph learning.

5.1 Semi-supervised Learning

Due to the expensive cost of collecting high-quality labeled data, semi-supervised learning aims to train a learner with a few labeled examples and a large amount of unlabeled data. The analysis for the

generalization of semi-supervised learner has been widely explored [71], and the theoretical results differ by the problem setting and assumptions. Here we focus on the transductive setting, which is also termed as setting 2 of transudctive learning [106]. Formally, the labeled and unlabeled data is represented as $D_m \triangleq \{(X_i, Y_i)\}_{i\in[m]}$ and $D_u \triangleq \{(X_i, Y_i)\}_{i\in[u]}$, which are samples independently from certain distribution. The semi-supervised learner takes $D_m \cup D_u^X$ as input and outputs the hypothesis characterized by $W \in P_{W|D_m\cup D_u^X}$, where $D_u^X \triangleq \{X_i\}_{i\in[u]}$. Different from the setting we present in Subsection 3.2, here each example (X, Y) should be regarded as random variable rather than constant pair. Furthermore, the training and test risk are defined as $R(W, D_m) \triangleq \frac{1}{m}\sum_{i=1}^{m} \ell(W, (X_i, Y_i))$ and $R(W, D_u) \triangleq \frac{1}{u}\sum_{i=m+1}^{m+u} \ell(W, (X_i, Y_i))$, respectively. Leveraging the theoretical results established in Section 4, the generalization of semi-supervised learner is described as follows.

Proposition 2. *Suppose $\ell(\mathbf{w}, \mathbf{z}) \in [0, B]$ holds for any $\mathbf{w} \in \mathcal{W}$ and $\mathbf{z} \in D$, then we have*

$$\left|\mathbb{E}_{D_m, D_u^X, W}\left[R(W, D_u) - R(W, D_m)\right]\right| \leq \mathbb{E}_{D_{m+u}}\sqrt{\frac{C_{m,u}}{2}\left(\frac{1}{m} + \frac{1}{u}\right) I(Z; W|D_{m+u})}, \tag{17}$$

where $C_{m,u}$ follows the definition in Theorem 1. Denote by $R_\mu(W) \triangleq \mathbb{E}_{(X,Y)\sim\mu}\ell(W, (X, Y))$ the population risk of the semi-supervised learner, under the same assumption we have

$$\mathbb{E}_{D_m, D_u^X, W} R_\mu(W) \leq R(W, D_m) + \sqrt{\frac{2B^2 I(D_{m+u}, Z; W)}{m+u}} + \mathbb{E}_{D_{m+u}}\sqrt{\frac{C_{m,u} I(Z; W|D_{m+u})}{2m(m/u+1)}}. \tag{18}$$

Compared with Theorem 1, the upper bound in Eq. (17) includes the conditional mutual information $I(Z, W|D_{m+u})$ rather than mutual information $I(Z, W)$. The reason is that each element in D_{m+u} is random variables rather than constants, and the randomness of D_{m+u} should also be taken into consideration. Eq. (18) reveals that if the unlabeled data follows the same distribution as that of labeled data, the population risk decreases with the number of u, namely increasing the number of unlabeled data is beneficial for generalization. However, label/data noise and distribution shift could occur in unlabeled data collected from real-world scenario. Thus, developing robust semi-supervised learners is more urgent.

5.2 Transductive Graph Learning

Composed of several objects and their relationship, graph-structured data plays an important role in real-world applications, *e.g.*, recommendation system [111, 48, 51] drug discovery [100, 12] and traffic prediction. Recent years have witnessed the success of GNNs in various learning and inference tasks on graph-structured data. The graph learning tasks can be divided into transductive task and inductive task, and we only discuss the first one. Transductive graph learning tasks include graph-level task and node/edge-level task. The goal for node-level task is to predict the label of nodes. As for edge-level task, the learner is required to predict whether there is a link between two nodes. Both of them fall into the category of transductive learning. Taking node classification as an example, partial nodes features together with labels randomly selected from the graph are used for training, and the GNN model need to predict the labels of remaining nodes. During this process, all node features are visible. Let D be the set containing all nodes and all edges respectively, our results can be applied on analyzing the generalization gap of GNNs on node classification task and link prediction task. Notably, the upper bound in Theorem 5 includes the norms along trajectory, which has close relation to both the architecture of GNN model and property of graph-structured information. Following the technique in [21, 101], we believe that it is possible to derive fine-grained upper bounds for specific GNN models and obtain more insights on its generalization behavior.

6 Experiments

In this section, we conduct experiments on semi-supervised learning and transductive graph learning scenarios to validate our theoretical findings.

6.1 Semi-supervised Learning

Datasets and Learning Algorithms. We choose semi-supervised image classification on MNIST and CIFAR-10 as the learning tasks. The semi-supervised learning loss for unlabeled images is defined as the mean square error between the prediction of the augmented images and the vanilla images by the model, which is also termed as consistency regularization in semi-supervised learning. Following [46, 40], we adopt a four-layer CNN and Wide ResNet-28-10 [124] as the model for MNIST and CIFAR-10, respectively. Please refer to Appendix for the detail of network architecture. For both these two experiments, we train the model on xx mini batches using Adam optimizer with learning rate 0.001, and the number per mini batch is fixed to xx. The loss is set to zero-one loss. Following [46], we make the training process be deterministic by fixing the sequence of mini batch and the initialization of parameters via random seed.

Estimating the Expected Transductive Generalization Gaps and the Derived Bounds. Notice that compute the accurate value of the expected transductive generalization gap (and also the derived upper bounds) is not applicable since we need to run the algorithm on $(m+u)!$ partitions in total. Therefore we use Monte Carlo simulation to estimate these expectations based on finite samples. The sampling process are as follows: (i) randomly draw t_1 full samples set s_{m+u} by each time sampling $m+u$ images from the raw images set, (ii) randomly draw t_2 transductive supersamples $\widetilde{z}^m$ based on Definition 2, (iii) randomly draw t_3 train/test split variables s and obtain the training and test samples set according to Subsection 4.2. Notice that here we do not consider the randomness of U for the case $k \geq 2$. The reason is that U control the permutation of test samples, and the learning algorithm we consider is independent of this permutation. Now we discuss the estimation of transductive generalization gap and the upper bounds established in Corollary 1. Taking Eq. () as an example, for each $(s_{m+u}, \widetilde{z})$ we use the mean value over t_3 samples of S to estimate the conditional term expectation term $\frac{1}{m}\sum_{i=1}^{m}\mathbb{E}_{F_i,U_i|\widetilde{z},s_{m+u}}g(F_i,S_i,\widetilde{y}_i)$. After that we use t_1t_2 samples of S_{m+u} and $\widetilde{Z}$ to estimate the expected generalization gap, whose mean and standard deviation are shown in Figure. Similarly, we use a plug-in estimator [77] to estimate the disentangled mutual information $I^{s_{m+u},\widetilde{z}}(F_i;S_i)$ over the t_3 samples of S. Then the upper bound in Eq. () is estimated by the t_1t_2 samples of S_{m+u} and $\widetilde{Z}$, whose mean and standard deviation are shown in Figure.

6.2 Transductive Graph Learning

Datasets and Learning Algorithms. We choose semi-supervised node classification on synthetic and real world datasets as the learning tasks. Specifically, we select cSBMs [27] to be the synthetic data, and Cora, CiteSeer, PubMed [90, 122] to be the real world dataset. For each of these dataset, we adopt GCN [57], GAT [108], JKNet [120], APPNP [35] and GPR-GNN [19] as the learner, which are popular baselines in graph learning literature. Please refer to Appendix for the detail of network architecture. Following , we train the model on all labeled nodes for 200 epochs with Adam optimizer with learning rate

Estimating the Expected Transductive Generalization Gaps and the Derived Bounds. The estimation process is generally follows that of semi-supervised learning, expect that we do not need to consider the sample of S_{m+u}. Concretely, the sampling process is only composed of (ii) and (iii). Accordingly, we use t_2 samples of $\widetilde{Z}$ to estimate the expected bounds and the conditional mutual information.

7 Conclusion

In this work, we study the generalization of transductive learning under the viewpoint of information theory, and establish upper bounds for general transductive algorithms and iterative algorithms in terms of different information measure. Furthermore, we demonstrate their applications in semi-supervised learning and transductive graph learning. Promising future directions include apply our results to other scenarios and develop the lower bounds that matched the upper bounds.

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A Notations and Lemma

We introduce additional notations used throughout the paper. We use $[m]$ to denote the set $\{1, 2, \ldots, n\}$. The combination number is denoted as $C_m^n = \frac{m!}{n!(m-n)!}$, where ! represents factorial. Furthermore, we use $\mathbb{N}$ to denote the set of all non-negative integers, and $\mathbb{N}_+$ to denote the set of all positive integers. Also, $\mathbb{R}$ is the set of real number and $\mathbb{R}_{\geq 0}$ is the set of non-negative real numbers. The gamma function is denoted as $\Gamma(\cdot)$. We finish this section by introducing the following lemma, which is also termed as the Donsker-Varadhan dual characterization of KL divergence or Gibbs variational principle in the literature. This lemma is the foundation of most information-theoretic and PAC-Bayesian theoretical results.

Lemma 1 (Theorem 4.6 in [80]). *Let P, and Q be two probability measure on $\mathcal{X}$ and $\mathcal{F} \triangleq \{f : \mathcal{X} \to \mathbb{R}\}$ the family of bounded measurable function. Then we have*

$$\mathrm{D}_{\mathrm{KL}}(P||Q) = \sup_{f \in \mathcal{F}} \mathbb{E}_P\left[f(X)\right] - \log \mathbb{E}_Q\left[\exp\left\{f(X)\right\}\right]. \tag{19}$$

B Proof of Theorem 1

We firstly show that $\mathcal{E}(w, Z)$ satisfies sub-gaussian property for a fixed realization w of W. Inspired by [23, 30], we construct the following martingale difference sequences:

$$V_i \triangleq \mathbb{E}[\mathcal{E}(w, Z)|Z_1, \ldots, Z_i] - \mathbb{E}[\mathcal{E}(w, Z)|Z_1, \ldots, Z_{i-1}], i \in [n]. \tag{20}$$

With this definition, one can verify that $\mathcal{E}(w, Z) - \mathbb{E}[\mathcal{E}(w, Z)] = \sum_{i=1}^n V_i$. Note that V_i is a function of $Z_1, \ldots, Z_i$. Define

$$\begin{aligned}
L_i &\triangleq \inf_z \mathbb{E}[\mathcal{E}(w, Z)|Z_1, \ldots, Z_{i-1}, Z_i = z] - \mathbb{E}[\mathcal{E}(w, Z)|Z_1, \ldots, Z_{i-1}], \\
U_i &\triangleq \sup_z \mathbb{E}[\mathcal{E}(w, Z)|Z_1, \ldots, Z_{i-1}, Z_i = z] - \mathbb{E}[\mathcal{E}(w, Z)|Z_1, \ldots, Z_{i-1}],
\end{aligned}$$

we have $L_i \leq V_i \leq U_i$. Then we show that $U_i - L_i$ is a bounded random variable when $Z_1, \ldots, Z_{i-1}$ are given:

$$\begin{aligned}
&U_i - L_i \\
=&\sup_z \mathbb{E}[\mathcal{E}(w, Z)|Z_1, \ldots, Z_{i-1}, Z_i = z] - \inf_z \mathbb{E}[\mathcal{E}(w, Z)|Z_1, \ldots, Z_{i-1}, Z_i = z] \\
=&\sup_{z, \tilde{z}} \left\{\mathbb{E}[\mathcal{E}(w, Z)|Z_1, \ldots, Z_{i-1}, Z_i = z] - \mathbb{E}[\mathcal{E}(w, Z)|Z_1, \ldots, Z_{i-1}, Z_i = \tilde{z}]\right\} \\
=&\frac{u!(m-i)!C_{n-i-1}^{m-i}}{(n-i)!} \cdot \frac{(m+u)B}{mu} \\
=&\frac{(m+u)B}{m(m+u-i)} \triangleq c_i.
\end{aligned} \tag{21}$$

Since $\mathbb{E}[V_i|Z_1, \ldots, Z_{i-1}] = 0$, by Hoeffding's lemma, $\mathbb{E}\left[e^{\lambda V_i}|Z_1, \ldots, Z_{i-1}\right] \leq e^{\frac{\lambda^2 c_i^2}{8}}$ holds for any $\lambda \in \mathbb{R}$. Note that

$$\begin{aligned}
\mathbb{E}\left[\exp\left\{\lambda \sum_{i=1}^n V_i\right\}\right] =& \mathbb{E}\left[\mathbb{E}\left[\exp\left\{\lambda \sum_{i=1}^{n-1} V_i\right\} \exp\left\{V_n\right\}\right] \middle| Z_1, \ldots, Z_{n-1}\right] \\
=& \mathbb{E}\left[\exp\left\{\lambda \sum_{i=1}^{n-1} V_i\right\} \mathbb{E}\left[\exp\left\{V_n\right\}\right] \middle| Z_1, \ldots, Z_{n-1}\right] \\
\leq& \exp\left\{\frac{\lambda^2 c_n^2}{8}\right\} \mathbb{E}\left[\exp\left\{\lambda \sum_{i=1}^{n-1} V_i\right\}\right].
\end{aligned} \tag{22}$$

By recursively repeating the above process, we obtain

$$\begin{aligned}
&\mathbb{E}\left[\exp\left\{\lambda \sum_{i=1}^n V_i\right\}\right] \\
\leq& \exp\left\{\frac{\lambda^2}{8} \sum_{i=1}^n c_i^2\right\} = \exp\left\{\frac{\lambda^2 (m+u)^2 B^2}{8m^2} \sum_{i=1}^n \frac{1}{(m+u-i)^2}\right\} \\
\leq& \exp\left\{\frac{\lambda^2 B^2 (m+u)^2}{8m(u-1/2)(m+u-1/2)}\right\}.
\end{aligned} \tag{23}$$

Due to the symmetric of training and test partition, the final bound is obtained by taking the largest one among them:

$$\mathbb{E}\left[\exp\left\{\lambda\sum_{i=1}^{n}V_i\right\}\right]\leq\exp\left\{\frac{\lambda^2B^2(m+u)^2}{8mu(m+u-1/2)}\cdot\frac{2\max(m,u)}{2\max(m,u)-1}\right\} \tag{24}$$

Combining Eq. (24) and the facts that $\mathcal{E}(w,Z)-\mathbb{E}[\mathcal{E}(w,Z)]=\sum_{i=1}^{n}V_i$ and $\mathbb{E}[\mathcal{E}(w,Z)]=0$, we obtain

$$\begin{aligned}&\mathbb{E}_Z\left[\exp\left\{\lambda(R_u(w,Z)-R_m(w,Z))\right\}\right]\\ \leq&\exp\left\{\frac{\lambda^2B^2(m+u)^2}{8mu(m+u-1/2)}\cdot\frac{2\max(m,u)}{2\max(m,u)-1}\right\}\\ =&\exp\left\{\frac{\lambda^2(m+u)C_{m,u}}{8mu}\right\}\end{aligned} \tag{25}$$

where $C_{m,u}\triangleq\frac{2B^2(m+u)\max(m,u)}{(m+u-1/2)(2\max(m,u)-1)}$. Denote by Z' the independent copy of Z, which is independent from W and has the same distribution as Z. Then we have

$$\begin{aligned}&\log\mathbb{E}_{W,Z'}\left[\exp\left\{\lambda(R_u(W,Z')-R_m(W,Z'))\right\}\right]\\ =&\log\left(\int_w\mathbb{E}_{Z'}\left[\exp\left\{\lambda(R_u(w,Z')-R_m(w,Z'))\right\}\right]\mathrm{d}P_W(w)\right)\\ \leq&\log\left(\int_w\exp\left\{\frac{\lambda^2(m+u)C_{m,u}}{8mu}\right\}\mathrm{d}P_W(w)\right)\\ =&\frac{\lambda^2C_{m,u}}{8}\left(\frac{1}{m}+\frac{1}{u}\right).\end{aligned} \tag{26}$$

By Donsker-Varadhan's variational formula, for any $\lambda\in\mathbb{R}$:

$$\begin{aligned}&\mathrm{D}_{\mathrm{KL}}(P_{Z,W}||P_{Z',W})\\ \geq&\mathbb{E}_{Z,W}\left[\lambda(R_u(W,Z)-R_m(W,Z))\right]-\log\mathbb{E}_{Z',W}\left[\exp\left\{\lambda(R_u(W,Z')-R_m(W,Z'))\right\}\right]\\ \geq&\mathbb{E}_{Z,W}\left[\lambda(R_u(W,Z)-R_m(W,Z))\right]-\frac{\lambda^2C_{m,u}}{8}\left(\frac{1}{m}+\frac{1}{u}\right),\end{aligned} \tag{27}$$

which implies that

$$\left|\mathbb{E}_{Z,W}\left[R_u(W,Z)-R_m(W,Z)\right]\right|\leq\sqrt{\frac{C_{m,u}}{2}\left(\frac{1}{m}+\frac{1}{u}\right)I(Z;W)}. \tag{28}$$

This finishes the proof for the first part. For the second part, note that Eq. (25) can be rewritten as $\mathbb{E}_Z[\exp\{\lambda\mathcal{E}(w,Z)\}]\leq\exp\{\lambda^2\sigma_{m,u}\}$, where $\sigma_{m,u}\triangleq C_{m,u}(1/m+1/u)/8$. Similarly we have $\mathbb{E}_Z[\exp\{-\lambda\mathcal{E}(w,Z)\}]\leq\exp\{\lambda^2\sigma_{m,u}\}$. Then we have

$$\mathbb{P}\left\{|\mathcal{E}(w,Z)|\geq t\right\}\leq\mathbb{P}\left\{\mathcal{E}(w,Z)\geq t\right\}+\mathbb{P}\left\{\mathcal{E}(w,Z)\leq-t\right\}\leq2\exp\left\{-\frac{t^2}{4\sigma_{m,u}}\right\}. \tag{29}$$

where the first and the second inequality are due to the Boole's inequality and the Chernoff technique, respectively. For any $k\in\mathbb{N}_+$, we have

$$\begin{aligned}\mathbb{E}\left[|\mathcal{E}(w,Z)|^k\right]=&\int_0^\infty\mathbb{P}\{|\mathcal{E}(w,Z)|^k\geq u\}\,\mathrm{d}u\\ =&k\int_0^\infty\mathbb{P}\{|\mathcal{E}(w,Z)|\geq t\}\,t^{k-1}\,\mathrm{d}t\\ \leq&2k\int_0^\infty\exp\left\{-\frac{t^2}{4\sigma_{m,u}}\right\}t^{k-1}\,\mathrm{d}t=(4\sigma_{m,u})^{\frac{k}{2}}k\Gamma(k/2),\end{aligned} \tag{30}$$

which implies that

$$\mathbb{E}\left[\exp\{\lambda\mathcal{E}^2(w,Z)\}\right]=1+\sum_{k=1}^{\infty}\frac{\lambda^k}{k!}\mathbb{E}\left[|\mathcal{E}(w,Z)|^{2k}\right]\leq1+2\sum_{k=1}^{\infty}(4\lambda\sigma_{m,u})^k. \tag{31}$$

By Donsker-Varadhan's variational formula, for any $\lambda\in\mathbb{R}$:

$$\begin{aligned}&\mathrm{D}_{\mathrm{KL}}(P_{Z,W}||P_{Z,W'})\\ \geq&\mathbb{E}_{Z,W}\left[\lambda(R_u(W,Z)-R_m(W,Z))^2\right]-\log\mathbb{E}_{Z,W'}\left[\exp\left\{\lambda(R_u(W',Z)-R_m(W',Z))^2\right\}\right]\\ \geq&\mathbb{E}_{Z,W}\left[\lambda(R_u(W,Z)-R_m(W,Z))^2\right]-\log\left(1+2\sum_{k=1}^{\infty}(4\lambda\sigma_{m,u})^k\right),\end{aligned} \tag{32}$$

Let $\lambda=1/8\sigma_{m,u}$ and plugging into $\sigma_{m,u}\triangleq C_{m,u}(1/m+1/u)/8$, we obtain

$$\mathbb{E}_{Z,W}\left[(R_u(W,Z)-R_m(W,Z))^2\right]\leq C_{m,u}\left(\frac{1}{m}+\frac{1}{u}\right)(I(Z;W)+\log3). \tag{33}$$

C Proof of Theorem 2

Denote by $Z^{(1)}, \ldots, Z^{(k)}$ the k independent copy of Z. By running a transductive algorithm $\mathcal{A}$ on each $Z^{(j)}$ respectively, we obtain the corresponding output $W^{(j)} = \mathcal{A}(Z^{(j)})$ for $j \in [k]$. By this way, $(Z^{(j)}, W^{(j)})$ can be regarded as independent copy of (Z, W) for $j \in [k]$. Now assume that there is a monitor that returns

$$(J^*, R^*) \triangleq \underset{j\in[k], r\in\{\pm 1\}}{\operatorname{argmax}} \; r\mathcal{E}(W^{(j)}, Z^{(j)}), \; W^* = W_{J^*}.$$

One can verify that

$$R^*\mathcal{E}(W^{(J^*)}, Z^{(J^*)}) = \max_{j\in[k]} |\mathcal{E}(Z^{(j)}, W^{(j)})|.$$

Now taking expectation on both side, we have

$$\mathbb{E}_{Z^{(1)},\ldots,Z^{(k)},J^*,R^*,W^*}\left[R^*\mathcal{E}(W^{(J^*)}, Z^{(J^*)})\right] = \mathbb{E}_{Z^{(1)},\ldots,Z^{(k)},W_1,\ldots,W_k}\left[\max_{j\in[k]} |\mathcal{E}(Z^{(j)}, W^{(j)})|\right].$$

Using the same procedure used in the proof of Theorem 1, we have

$$\log \mathbb{E}_{J^*,R^*,W^*}\mathbb{E}_{Z^{(1)},\ldots,Z^{(k)}}\left[\exp\left\{\lambda R^*\mathcal{E}(W^{(J^*)}, Z^{(J^*)})\right\}\right] \le \frac{\lambda^2 C_{m,u}}{8}\left(\frac{1}{m}+\frac{1}{u}\right).$$

By Donsker-Varadhan's variational formula, the following inequality holds for any $\lambda \in \mathbb{R}$:

$$\begin{aligned}
&D(P_{Z^{(1)},\ldots,Z^{(k)},J^*,R^*,W^*} || P_{Z^{(1)},\ldots,Z^{(k)}} \otimes P_{J^*,R^*,W^*}) \\
\ge&\mathbb{E}_{Z^{(1)},\ldots,Z^{(k)},J^*,R^*,W^*}\left[\lambda R^*\mathcal{E}(W^{(J^*)}, Z^{(J^*)})\right] \\
&- \log \mathbb{E}_{J^*,R^*,W^*}\mathbb{E}_{Z^{(1)},\ldots,Z^{(k)}}\left[\exp\left\{\lambda R^*\mathcal{E}(W^{(J^*)}, Z^{(J^*)})\right\}\right] \\
\ge&\lambda\mathbb{E}_{Z^{(1)},\ldots,Z^{(k)},J^*,R^*,W^*}\left[R^*\mathcal{E}(W^{(J^*)}, Z^{(J^*)})\right] - \frac{\lambda^2 C_{m,u}}{8}\left(\frac{1}{m}+\frac{1}{u}\right).
\end{aligned}$$

which implies

$$\begin{aligned}
&\mathbb{E}_{Z^{(1)},\ldots,Z^{(k)},J^*,R^*,W^*}\left[R^*\mathcal{E}(W^{(J^*)}, Z^{(J^*)})\right] \\
\le&\sqrt{\frac{C_{m,u}}{2}\left(\frac{1}{m}+\frac{1}{u}\right) I(Z^{(1)},\ldots,Z^{(k)}; J^*, R^*, W^*)}.
\end{aligned} \tag{34}$$

Next we provide a upper bound for the mutual information. Note that

$$\begin{aligned}
&I(Z^{(1)},\ldots,Z^{(k)}; J^*, R^*, W^*) \\
\le&I(S(\pi_1),\ldots,S(\pi_k); J^*, R^*, W^*, W_1,\ldots,W_k) \\
=&I(Z^{(1)},\ldots,Z^{(k)}; W_1,\ldots,W_k) + I(S(\pi_1),\ldots,S(\pi_k); J^*, R^*, W^* | W_1,\ldots,W_k) \\
=&\sum_{j=1}^{k} I(S(\pi_j); W_j) + I(Z^{(1)},\ldots,Z^{(k)}; J^*, R^*, W^* | W_1,\ldots,W_k) \\
\le&kI(Z; W) + \log(2k).
\end{aligned} \tag{35}$$

where we have use that $(S(\pi_j), W_j), j \in [k]$ are independent. Plugging Eq. (35) into Eq. (34) yields

$$\mathbb{E}_{Z^{(1)},\ldots,Z^{(k)},W^{(1)},\ldots,W^{(k)}}\left[\max_{j\in[k]} |\mathcal{E}(Z^{(j)}, W^{(j)})|\right] \le \sqrt{\frac{C_{m,u}}{2}\left(\frac{1}{m}+\frac{1}{u}\right)(\log(2k) + kI(Z,W))}.$$

Since $(Z^{(j)}, W^{(j)})$ are independent copy of (Z, W), for any $\alpha > 0$ we have

$$\mathbb{P}_{Z^{(1)},W^{(1)},\ldots,Z^{(k)},W^{(k)}}\left\{\max_{j\in[k]} |\mathcal{E}(Z^{(j)}, W^{(j)})| < \alpha\right\} = \left(\mathbb{P}_{Z,W}\left\{|\mathcal{E}(Z,W)| < \alpha\right\}\right)^k.$$

By Markov's inequality:

$$\begin{aligned}
&\mathbb{P}_{Z^{(1)},W^{(1)},\ldots,Z^{(k)},W^{(k)}}\left\{\max_{j\in[k]} |\mathcal{E}(Z^{(j)}, W^{(j)})| \ge \alpha\right\} \\
\le&\frac{1}{\alpha}\mathbb{E}_{Z^{(1)},\ldots,Z^{(k)},W^{(1)},\ldots,W^{(k)}}\left[\max_{j\in[k]} |\mathcal{E}(Z^{(j)}, W^{(j)})|\right] \\
\le&\frac{1}{\alpha}\sqrt{\frac{C_{m,u}}{2}\left(\frac{1}{m}+\frac{1}{u}\right)(\log(2k) + kI(Z,W))}.
\end{aligned}$$

Therefore,

$$\begin{aligned}
&\mathbb{P}_{Z,W}\left\{|\mathcal{E}(Z,W)|\geq\alpha\right\}\\
=&1-\mathbb{P}_{Z,W}\left\{|\mathcal{E}(Z,W)|<\alpha\right\}\\
=&1-\left(\mathbb{P}_{Z^{(1)},W^{(1)},\ldots,Z^{(k)},W^{(k)}}\left\{\max_{j\in[k]}|\mathcal{E}(Z^{(j)},W^{(j)})|<\alpha\right\}\right)^{\frac{1}{k}}\\
=&1-\left(1-\mathbb{P}_{Z^{(1)},W^{(1)},\ldots,Z^{(k)},W^{(k)}}\left\{\max_{j\in[k]}|\mathcal{E}(Z^{(j)},W^{(j)})|<\alpha\right\}\right)^{\frac{1}{k}}\\
\leq&1-\left(1-\frac{1}{\alpha}\sqrt{\frac{C_{m,u}}{2}\left(\frac{1}{m}+\frac{1}{u}\right)\left(\log(2k)+kI(Z,W)\right)}\right)^{\frac{1}{k}}.
\end{aligned}$$

Let $\alpha=2\sqrt{\frac{C_{m,u}}{2}\left(\frac{1}{m}+\frac{1}{u}\right)\left(\log(2k)+kI(Z,W)\right)}$ and $k=\lfloor\frac{1}{\delta}\rfloor$, we have obtained the result. Let $k=1$, we obtain

$$\mathbb{E}_{Z,W}\left[|\mathcal{E}(Z,W)|\right]\leq\sqrt{\frac{C_{m,u}}{2}\left(\frac{1}{m}+\frac{1}{u}\right)\left(\log 2+I(Z,W)\right)}.$$

D Proof of Proposition 1

Denote by $\mathcal{S}$ the set containing all value of S. For any $\widetilde{z}\in\widetilde{\mathcal{Z}}$ and $s\in\mathcal{S}$, we use

$$\bar{z}(\widetilde{z},s)\triangleq(\widetilde{z}_{1,s_1},\ldots,\widetilde{z}_{m,s_m},\widetilde{z}_{1,1-s_1},\ldots,\widetilde{z}_{m,1-s_m}) \tag{36}$$

to denote the random permutation vector induced by $\widetilde{z}$ and s. Let $\bar{Z}:\{\bar{z}(\widetilde{z},s)|\widetilde{z}\in\widetilde{\mathcal{Z}},s\in\mathcal{S}\}$, it is sufficient to proof that $\bar{Z}=\mathfrak{Z}$, where $\mathfrak{Z}$ is the set includes all possible values of Z^n defined in Subsection 3.2. Note that each element $\widetilde{z}$ in $\widetilde{\mathcal{Z}}$ differs by each other, since $\widetilde{z}$ is a partitions of $m+u$ elements into m subsets, where each subset contains 2 elements. Thus, the cardinality of $\widetilde{\mathcal{Z}}$ is $\frac{(2m)!}{2^m}$. Furthermore, for fixed $\widetilde{z}$ and $s_1,s_2\in\mathcal{S}$, it is clear that $s_1\neq s_2$ implies $\bar{z}(\widetilde{z},s_1)\neq\bar{z}(\widetilde{z},s_2)$, due to the fact that $\bar{z}(\widetilde{z},s_1)=\bar{z}(\widetilde{z},s_2)$ if and only if $\bar{z}(\widetilde{z},s_1)_j=\bar{z}(\widetilde{z},s_2)_j$ for $j\in[2m]$. Here $\bar{z}(\widetilde{z},s)_j$ represents the j-th entry in the sequence. Now we claim that for any two element $\bar{z}_1(\widetilde{z}_1,s_1),\bar{z}_2(\widetilde{z}_2,s_2)\in\bar{Z}$, if $\bar{z}_1(\widetilde{z}_1,s_1)=\bar{z}_2(\widetilde{z}_2,s_2)$, then $\widetilde{z}_1=\widetilde{z}_2$ holds. To see this, we show that $\widetilde{z}$ can be uniquely determined when seeing $\bar{z}(\widetilde{z},s)$. Recall that $\widetilde{z}$ is a sequence containing m element, and each element $\widetilde{z}_j$ is a set. By Eq. (36), we conclude that $\widetilde{z}_{1,s_1}$ comes from $\widetilde{z}_1$, $\widetilde{z}_{2,s_2}$ comes from $\widetilde{z}_2$, and so on. Similarly, $\widetilde{z}_{1,1-s_1}$ comes from $\widetilde{z}_1$, $\widetilde{z}_{2,1-s_2}$ comes from $\widetilde{z}_2$, and so on. By this way, we have recovered $\widetilde{z}$ from $\bar{z}(\widetilde{z},s)$ and it is unique. Together with the fact $\bar{z}(\widetilde{z},s_1)=\bar{z}(\widetilde{z},s_2)\Longrightarrow s_1=s_2$ that we have just shown, we conclude that $\bar{z}_1(\widetilde{z}_1,s_1)=\bar{z}_2(\widetilde{z}_2,s_2)\Longrightarrow\widetilde{z}_1=\widetilde{z}_2,s_1=s_2$, which suggest that $(\widetilde{z},s)\to\bar{z}(\widetilde{z}_1,s_1)$ is a one-to-one mapping. Since $|\mathcal{S}|=2^m$, we have $|\bar{Z}|=|\widetilde{\mathcal{Z}}||\mathcal{S}|=(2m)!$. Note that $\bar{Z}\subseteq\mathfrak{Z}$ and $|\bar{Z}|=|\mathfrak{Z}|$, we conclude that $\bar{Z}=\mathfrak{Z}$.

E Proof of Theorem 3

We firstly present a warm-up example for illustrating the proposed transductive supersamples. Suppose $m=2$, all entries in $\widetilde{Z}$ are as follows:

- $(\{\mathbf{z}_1,\mathbf{z}_2\},\{\mathbf{z}_3,\mathbf{z}_4\})$
- $(\{\mathbf{z}_1,\mathbf{z}_3\},\{\mathbf{z}_2,\mathbf{z}_4\})$
- $(\{\mathbf{z}_1,\mathbf{z}_4\},\{\mathbf{z}_2,\mathbf{z}_3\})$
- $(\{\mathbf{z}_2,\mathbf{z}_3\},\{\mathbf{z}_1,\mathbf{z}_4\})$
- $(\{\mathbf{z}_2,\mathbf{z}_4\},\{\mathbf{z}_1,\mathbf{z}_3\})$
- $(\{\mathbf{z}_3,\mathbf{z}_4\},\{\mathbf{z}_1,\mathbf{z}_2\})$

Here we use set $\{\cdot\}$ and tuple $(\cdot)$ to indicate whether we consider the order or not. Now we give the formal proof. Denote by w and $\widetilde{z}$ the fixed realizations of W and $\widetilde{Z}$. For any $\lambda\in\mathbb{R}$, by Hoeffding's Lemma:

$$\begin{aligned}
&\mathbb{E}_S\left[\exp\left\{\lambda\mathcal{E}(w,\widetilde{z},S)\right\}\right]\\
=&\mathbb{E}_S\left[\exp\left\{\frac{\lambda}{m}\sum_{i=1}^{m}\ell(w,\widetilde{z}_{i,S_i})-\ell(w,\widetilde{z}_{i,1-S_i})\right\}\right]\leq\exp\left\{\frac{\lambda^2B^2}{2m}\right\}.
\end{aligned}\tag{37}$$

Let S' be the independent copy of S, we have

$$\begin{aligned}&\log \mathbb{E}_{S',W|\widetilde{Z}=\widetilde{z}}\left[\exp\left\{\lambda\mathcal{E}(W,\widetilde{z},S')\right\}\right]\\=&\log\left(\int_w \mathbb{E}_{S'}\left[\exp\left\{\lambda\mathcal{E}(w,\widetilde{z},S')\right\}\right]\mathrm{d}P_{W|\widetilde{Z}=\widetilde{z}}(w)\right)\leq\frac{\lambda^2B^2}{2m}.\end{aligned}\tag{38}$$

where we have used the fact that $P_{S',W|\widetilde{Z}=\widetilde{z}}=P_{W|\widetilde{Z}=\widetilde{z}}P_{S'}$, due to S' is independent from both $\widetilde{Z}$ and W. By Donsker-Varadhan's variational formula, for any $\lambda\in\mathbb{R}$:

$$\begin{aligned}&I(S;W|\widetilde{Z}=\widetilde{z})=\mathrm{D}_{\mathrm{KL}}(P_{S,W|\widetilde{Z}=\widetilde{z}}||P_{S',W|\widetilde{Z}=\widetilde{z}})\\\geq&\mathbb{E}_{S,W|\widetilde{Z}=\widetilde{z}}\left[\lambda\mathcal{E}(W,\widetilde{z},S)\right]-\log\mathbb{E}_{S',W|\widetilde{Z}=\widetilde{z}}\left[\exp\left\{\lambda\mathcal{E}(W,z,S')\right\}\right]\\\geq&\lambda\mathbb{E}_{S,W|\widetilde{Z}=\widetilde{z}}\left[\mathcal{E}(W,\widetilde{z},S)\right]-\frac{\lambda^2B^2}{2m},\end{aligned}\tag{39}$$

which implies that

$$\left|\mathbb{E}_{S,W|\widetilde{Z}=\widetilde{z}}\left[\mathcal{E}(W,\widetilde{z},S)\right]\right|\leq\sqrt{\frac{2B^2}{m}I(S;W|\widetilde{Z}=\widetilde{z})}.$$

Taking expectation over $\widetilde{Z}$ on both side, we have obtain

$$\begin{aligned}&\left|\mathbb{E}_{Z,W}\left[R_u(W,Z)-R_m(W,Z)\right]\right|=\left|\mathbb{E}_{\widetilde{Z},S,W}\left[\mathcal{E}(W,\widetilde{Z},S)\right]\right|\\\leq&\mathbb{E}_{\widetilde{Z}}\left|\mathbb{E}_{S,W|\widetilde{Z}}\left[\mathcal{E}(W,\widetilde{Z},S)\right]\right|\leq\mathbb{E}_{\widetilde{Z}}\sqrt{\frac{2B^2}{m}I(S;W|\widetilde{Z})}.\end{aligned}\tag{40}$$

For the second part, note that Eq. (37) can be rewritten as $\mathbb{E}_S\left[\exp\left\{\lambda\mathcal{E}(w,\widetilde{z},S)\right\}\right]\leq\exp\{\lambda^2B^2/2m\}$. Similarly we have $\mathbb{E}_S\left[\exp\left\{-\lambda\mathcal{E}(w,\widetilde{z},S)\right\}\right]\leq\exp\{\lambda^2B^2/2m\}$. By the same technique in Section B, we have

$$\mathbb{E}_{S,W|\widetilde{Z}=\widetilde{z}}\left[\mathcal{E}^2(W,\widetilde{z},S)\right]\leq\frac{4B^2}{m}(I(S;W|\widetilde{Z}=\widetilde{z})+\log 3).\tag{41}$$

Taking expectation on both side, we have obtain

$$\mathbb{E}_{S,W}\left[(R_u(W,Z)-R_m(W,Z))^2\right]=\mathbb{E}_{\widetilde{Z},S,W}\left[\mathcal{E}^2(W,\widetilde{Z},S)\right]\leq\frac{4B^2}{m}(I(S;W|\widetilde{Z})+\log 3).\tag{42}$$

We close this proof by presenting the results for more ordinary cases where $u=km$ with $k\in\mathbb{N}_+$. By Definition 2, the transductive generalization under this setting is defined by

$$\mathcal{E}(W,\widetilde{Z},S)\triangleq\frac{1}{m}\sum_{i=1}^{m}\ell(W,\widetilde{Z}_{i,S_i})-\frac{1}{km}\sum_{i=1}^{m}\sum_{j=0}^{k}\ell(W,\widetilde{Z}_{i,\bar{S}_{i,j}}).\tag{43}$$

One can verify that $\mathbb{E}_{S,W}\left[R_u(W,Z)-R_m(W,Z)\right]=\mathbb{E}_{\widetilde{Z},S,W}\left[\mathcal{E}(W,\widetilde{Z},S)\right]$ holds. Following the same procedure we have

$$\begin{aligned}&\left|\mathbb{E}_{S,W}\left[R_u(W,Z)-R_m(W,Z)\right]\right|\leq\mathbb{E}_{\widetilde{Z}}\sqrt{\frac{2(k+1)B^2}{n}I(S;W|\widetilde{Z})}\\&\mathbb{E}_{S,W}\left[(R_u(W,Z)-R_m(W,Z))^2\right]\leq\frac{4(k+1)B^2}{n}(I(S;W|\widetilde{Z})+\log 3).\end{aligned}\tag{44}$$

F Proof of Corollary 1

Denote by $g(F_i,S_i,\widetilde{Y}_i)\triangleq l(F_{i,S_i},\widetilde{Y}_{i,S_i})-l(F_{i,1-S_i},\widetilde{Y}_{i,1-S_i})$ the function of $(F_i,S_i,\widetilde{Y}_i)$. Let f_i and $\widetilde{z}_i=(\widetilde{x}_i,\widetilde{y}_i)$ be the fixed realizations of F_i and $\widetilde{Z}_i$. For any $\lambda\in\mathbb{R}$ and $i\in[m]$, by Hoeffding's Lemma:

$$\mathbb{E}_{S_i}\left[\exp\left\{\lambda g(f_i,S_i,\widetilde{y}_i)\right\}\right]\leq\exp\left\{\frac{\lambda^2B^2}{2}\right\}.\tag{45}$$

Let S_i' be the independent copy of S_i, by Donsker-Varadhan's variational formula:

$$\begin{aligned}I(F_i;S_i|\widetilde{Z}=\widetilde{z})&\geq\lambda\mathbb{E}_{F_i,S_i|\widetilde{Z}=\widetilde{z}}\left[g(F,S_i,\widetilde{y}_i)\right]-\log\mathbb{E}_{F_i,S_i'|\widetilde{Z}=\widetilde{z}}\left[\exp\left\{\lambda g(F_i,S_i',\widetilde{y}_i)\right\}\right]\\&\geq\lambda\mathbb{E}_{F_i,S_i|\widetilde{Z}=\widetilde{z}}\left[g(F_i,S_i,\widetilde{y}_i)\right]-\frac{\lambda^2B^2}{2}.\end{aligned}\tag{46}$$

Then we have

$$\left|\mathbb{E}_{S,W|\widetilde{Z}=\widetilde{z}}\left[\ell(W,\widetilde{z}_{i,S_i})-\ell(W,\widetilde{z}_{i,1-S_i})\right]\right|=\left|\mathbb{E}_{F_i,S_i|\widetilde{Z}=\widetilde{z}}\left[g(F_i,S_i,\widetilde{y}_i)\right]\right|\leq B\sqrt{2I(F_i;S_i|\widetilde{Z}=\widetilde{z})},\tag{47}$$

which implies that

$$\begin{aligned}
&|\mathbb{E}_{Z,W}\left[R_u(W,Z)-R_m(W,Z)\right]| = \left|\mathbb{E}_{\widetilde{Z},S,W}\left[\mathcal{E}(W,\widetilde{Z},S)\right]\right| \\
\leq &\mathbb{E}_{\widetilde{Z}}\left|\frac{1}{m}\sum_{i=1}^{m}\mathbb{E}_{S,W|\widetilde{Z}}\left[\ell(W,\widetilde{Z}_{i,S_i})-\ell(W,\widetilde{Z}_{i,1-S_i})\right]\right| \\
\leq &\frac{1}{m}\sum_{i=1}^{m}\mathbb{E}_{\widetilde{Z}}\left|\mathbb{E}_{S,W|\widetilde{Z}}\left[\ell(W,\widetilde{Z}_{i,S_i})-\ell(W,\widetilde{Z}_{i,1-S_i})\right]\right| \\
= &\frac{1}{m}\sum_{i=1}^{m}\mathbb{E}_{\widetilde{Z}}\left|\mathbb{E}_{F_i,S_i|\widetilde{Z}}\left[g(F_i,S_i,\widetilde{Y}_i)\right]\right| \leq \frac{B}{m}\sum_{i=1}^{m}\mathbb{E}_{\widetilde{Z}}\sqrt{2I(\ell(F_i;S_i|\widetilde{Z})}.
\end{aligned} \tag{48}$$

Denote by $g(L_i,S_i)=L_{i,S_i}-L_{i,1-S_i}$, by the same technique we have

$$|\mathbb{E}_{S,W}\left[R_u(W,Z)-R_m(W,Z)\right]| \leq \frac{1}{m}\sum_{i=1}^{m}\mathbb{E}_{\widetilde{Z}}\sqrt{2I(L_i;S_i|\widetilde{Z})}. \tag{49}$$

Denote by $g(\Delta_i,S_i)\triangleq(-1)^{S_i}\Delta_i$, by the same technique we have

$$|\mathbb{E}_{S,W}\left[R_u(W,Z)-R_m(W,Z)\right]| \leq \frac{1}{m}\sum_{i=1}^{m}\mathbb{E}_{\widetilde{Z}}\sqrt{2I(\Delta_i;S_i|\widetilde{Z})}. \tag{50}$$

G Proof of Theorem 4

By Markov inequality, for any distribution P that independent to Z:

$$\mathbb{P}\left\{\mathbb{E}_{W\sim P}\left[e^{\lambda(R_u(W,Z)-R_m(W,Z))}\right] \geq \frac{1}{\delta}\mathbb{E}_Z\mathbb{E}_{W\sim P}\left[e^{\lambda(R_u(W,Z)-R_m(W,Z))}\right]\right\} \leq \delta. \tag{51}$$

By Donsker-Varadhan's variational formula and Eq. (25), for any distribution Q, with probability at least $1-\delta$ over the randomness of Z:

$$\begin{aligned}
&\lambda\mathbb{E}_{W\sim Q}\left[R_u(W,Z)-R_m(W,Z)\right] \\
\leq &\mathrm{D}_{\mathrm{KL}}(Q||P)+\log\left(\mathbb{E}_{W\sim P}\left[e^{\lambda(R_u(W,Z)-R_m(W,Z))}\right]\right) \\
\leq &\mathrm{D}_{\mathrm{KL}}(Q||P)+\log\left(\frac{1}{\delta}\right)+\log\mathbb{E}_Z\mathbb{E}_{W\sim P}\left[e^{\lambda(R_u(W,Z)-R_m(W,Z))}\right] \\
= &\mathrm{D}_{\mathrm{KL}}(Q||P)+\log\left(\frac{1}{\delta}\right)+\log\left(\int_w \mathbb{E}_{Z'}\left[\exp\left\{\lambda(R_u(w,Z')-R_m(w,Z'))\right\}\right]\mathrm{d}P(w)\right) \\
\leq &\mathrm{D}_{\mathrm{KL}}(Q||P)+\log\left(\frac{1}{\delta}\right)+\frac{\lambda^2 C_{m,u}}{8}\left(\frac{1}{m}+\frac{1}{u}\right),
\end{aligned} \tag{52}$$

which implies that: for any distribution Q, with probability at least $1-\delta$ over the randomness of Z,

$$|\mathbb{E}_{W\sim Q}\left[R_u(W,Z)-R_m(W,Z)\right]| \leq \sqrt{\frac{C_{m,u}}{2}\left(\frac{1}{m}+\frac{1}{u}\right)\left(\mathrm{D}_{\mathrm{KL}}(Q||P)+\log\left(\frac{1}{\delta}\right)\right)}. \tag{53}$$

Note that by setting $Q=P_{W|S}$ and $P=P_W$, we recover a degenerated version of Theorem 1 holds with probability $1-\delta$:

$$\begin{aligned}
&|\mathbb{E}_{W,Z}\left[R_u(W,Z)-R_m(W,Z)\right]| \leq \mathbb{E}_Z\left[|\mathbb{E}_{W\sim Q}\left[R_u(W,Z)-R_m(W,Z)\right]|\right] \\
\leq &\mathbb{E}_Z\left[\sqrt{\frac{C_{m,u}}{2}\left(\frac{1}{m}+\frac{1}{u}\right)\left(\mathrm{D}_{\mathrm{KL}}(P_{W|S}||P_W)+\log\left(\frac{1}{\delta}\right)\right)}\right] \\
\leq &\sqrt{\frac{C_{m,u}}{2}\left(\frac{1}{m}+\frac{1}{u}\right)\left(\mathbb{E}_Z\left[\mathrm{D}_{\mathrm{KL}}(P_{W|S}||P_W)\right]+\log\left(\frac{1}{\delta}\right)\right)} \\
= &\sqrt{\frac{C_{m,u}}{2}\left(\frac{1}{m}+\frac{1}{u}\right)\left(I(S;W)+\log\left(\frac{1}{\delta}\right)\right)}.
\end{aligned} \tag{54}$$

It is worth mentioning that we can also recover Theorem 1 from PAC-Bayesian perspective. Denote by $R_{m+u}(W,Z)\triangleq\frac{1}{m+u}\sum_{i=1}^{m+u}\ell(W,Z_i)=\frac{m}{m+u}R_m(W,Z)+\frac{u}{m+u}R_u(W,Z)$ the error on Z. Denote by

$\mathcal{D}(p,q) \triangleq p\log\frac{p}{q} + (1-p)\log\frac{1-p}{1-q}$ the KL divergence between two Bernoulli distributions with success probability p and q. Then the $\mathcal{D}$-function introduced in [10] is expressed by $\mathcal{D}^*_\beta(p,q) \triangleq \mathcal{D}(p,q) + \frac{1-\beta}{\beta}\mathcal{D}(\frac{q-\beta p}{1-\beta}, q)$. By Theorem 5 and Theorem 6 in [10], for fixed realization w of W:

$$\mathbb{E}_Z\left[\exp\left\{m\mathcal{D}^*_\beta(R_m(w,Z), R_{m+u}(w,Z))\right\}\right] \leq 3\log(m)\sqrt{\frac{mu}{m+u}}, \tag{55}$$

which implies that

$$\begin{aligned}
&\log\mathbb{E}_{W\otimes Z}\left[\exp\left\{m\mathcal{D}^*_\beta(R_m(W,Z), R_{m+u}(W,Z))\right\}\right] \\
=&\log\left(\int_w \mathbb{E}_Z\left[\exp\left\{m\mathcal{D}^*_\beta(R_m(w,Z), R_{m+u}(w,Z))\right\}\right] \mathrm{d}P_W(w)\right) \\
\leq&\log\left(3\log(m)\sqrt{\frac{mu}{m+u}}\right).
\end{aligned} \tag{56}$$

By Donsker-Varadhan's variational formula we have

$$\begin{aligned}
&\mathrm{D}_{\mathrm{KL}}(P_{Z,W}||P_{Z,W'}) \\
\geq&\mathbb{E}_{Z,W}\left[m\mathcal{D}^*_\beta(R_m(W,Z), R_{m+u}(W,Z))\right] - \log\mathbb{E}_{W\otimes Z}\left[e^{m\mathcal{D}^*_\beta(R_m(W,Z), R_{m+u}(W,Z))}\right] \\
\geq&m\mathbb{E}_{Z,W}\left[\mathcal{D}^*_\beta(R_m(W,Z), R_{m+u}(W,Z))\right] - \log\left(3\log(m)\sqrt{\frac{mu}{m+u}}\right).
\end{aligned} \tag{57}$$

By the Pinsker's inequality and plugging in $\beta = \frac{m}{m+u}$, the expectation term can be lower bounded by

$$\begin{aligned}
&\mathbb{E}_{Z,W}\left[\mathcal{D}^*_\beta(R_m(W,Z), R_{m+u}(W,Z))\right] \\
=&\mathbb{E}_{Z,W}\left[\mathcal{D}(R_m(W,Z), R_{m+u}(W,Z))\right] \\
&+\frac{u}{m}\mathbb{E}_{Z,W}\left[\mathcal{D}\left(\frac{m+u}{u}R_{m+u}(W,Z) - \frac{m}{u}R_m(W,Z), R_{m+u}(W,Z)\right)\right] \\
\geq&2\mathbb{E}_{Z,W}\left[(R_m(W,Z) - R_{m+u}(W,Z))^2\right] + 2\frac{m}{u}\mathbb{E}_{Z,W}\left[(R_m(W,Z) - R_{m+u}(W,Z))^2\right] \\
=&2\frac{m+u}{u}\mathbb{E}_{Z,W}\left[\left(R_m(W,Z) - \frac{m}{m+u}R_m(W,Z) + \frac{u}{m+u}R_u(W,Z)\right)^2\right] \\
=&\frac{2u}{m+u}\mathbb{E}_{Z,W}\left[(R_m(W,Z) - R_u(W,Z))^2\right] \\
\geq&\frac{2u}{m+u}\left(\mathbb{E}_{Z,W}[R_m(W,Z) - R_u(W,Z)]\right)^2.
\end{aligned} \tag{58}$$

Combining Eq. (57) and Eq. (58) we obtain a degenerated bound compared with that provided in Theorem 1 with extra factors $\log\left(3\log(m)\sqrt{\frac{mu}{m+u}}\right)$:

$$|\mathbb{E}_{Z,W}[R_m(W,Z) - R_u(W,Z)]| \leq \sqrt{\frac{1}{2}\left(\frac{1}{m}+\frac{1}{u}\right)\left[I(Z;W) + \log\left(3\log(m)\sqrt{\frac{mu}{m+u}}\right)\right]}.$$

H Proof of Corollary 2

The proof generally follows the proof of Theorem 2 in [33]. For given posterior distribution Q, we need to properly select the optimal prior distribution P^* such that the KL divergence term $\mathrm{D}_{\mathrm{KL}}(Q||P)$ can be minimized. However, this solution is not applicable. The reason is that P will depend on Q and Z, yet we require that P should be chosen before observing Z. Therefore, the most widely adopted method is to construct a predefined set of prior distribution $\mathcal{P} = \{P_j\}_{j\in\mathbb{N}}$, and then establishing a high probability guarantee for each $P \in \mathcal{P}$. After that, we can establish a high probability guarantee for the optimal prior P^* by using union bound inequality.

Formally, denote by $\mathbf{w} \in \mathbb{R}^d$ the parameter return by the learning algorithm and σ a predefined hyper-parameter, we define the posterior distribution as $Q \triangleq \mathcal{N}(\mathbf{w}+\boldsymbol{\epsilon}, \sigma^2\mathbf{I}_d)$. Let $c = \sigma_Q^2(1+e^{4n/d})$, the predefined set $\mathcal{P}$ is constructed as

$$\mathcal{P} \triangleq \left\{\mathcal{N}(\boldsymbol{\epsilon}, \sigma_j^2\mathbf{I}) | \sigma_j = ce^{(1-j)/d}\right\}.$$

Here c is a constant depends on m, n, d, σ, whose value will be discussed later. For any $P \triangleq \mathcal{N}(\boldsymbol{\epsilon}, \sigma_P^2\mathbf{I}) \in \mathcal{P}$, by calculating the KL divergence term, we have

$$\mathrm{D}_{\mathrm{KL}}(Q||P) = \frac{1}{2}\left[\frac{d\sigma^2 + \|\mathbf{w}\|_2^2}{\sigma_P^2} - d + d\log\left(\frac{\sigma_P^2}{\sigma^2}\right)\right],$$

which implies that

$$\operatorname*{argmin}_{\sigma_P} \mathrm{D}_{\mathrm{KL}}(Q||P) = \sqrt{\sigma^2 + \|\mathbf{w}\|_2^2/d}.$$

Therefore, we can define the optimal prior distribution as $P^* = \mathcal{N}(\boldsymbol{\epsilon}, \sigma_{j^*}^2 \mathbf{I})$ where

$$j^* = \left\lfloor 1 - d\log\left(\frac{\sigma^2 + \|\mathbf{w}\|_2^2/d}{c}\right)\right\rfloor,$$

which implies that

$$-d\log\left(\frac{\sigma^2 + \|\mathbf{w}\|_2^2/d}{c}\right) \le j^* \le 1 - d\log\left(\frac{\sigma^2 + \|\mathbf{w}\|_2^2/d}{c}\right), \tag{59}$$

and

$$\sigma^2 + \frac{\|\mathbf{w}\|_2^2}{d} \le \sigma_{j^*}^2 \le e^{1/d}\left(\sigma^2 + \frac{\|\mathbf{w}\|_2^2}{d}\right). \tag{60}$$

Here we have used a fact that $\sigma^2 + \|\mathbf{w}\|_2^2/d < c$, which will be shown later. Therefore, we have

$$\begin{aligned}
\mathrm{D}_{\mathrm{KL}}(Q||P^*) &= \frac{1}{2}\left[\frac{d\sigma_Q^2 + \|\mathbf{w}\|_2^2}{\sigma_{j^*}^2} - d + d\log\left(\frac{\sigma_{j^*}^2}{\sigma_Q^2}\right)\right] \\
&\le \frac{1}{2}\left[\frac{d(\sigma_Q^2 + \|\mathbf{w}\|_2^2/d)}{\sigma_Q^2 + \|\mathbf{w}\|_2^2/d} - d + d\log\left(\frac{e^{1/d}\left(\sigma_Q^2 + \|\mathbf{w}\|_2^2/d\right)}{\sigma^2}\right)\right] \\
&= \frac{1}{2}\left[d\log\left(\frac{e^{\frac{1}{d}}\left(\sigma^2 + \|\mathbf{w}\|_2^2/d\right)}{\sigma^2}\right)\right] = \frac{1}{2}\left[1 + d\log\left(1 + \frac{\|\mathbf{w}\|_2^2}{d\sigma^2}\right)\right].
\end{aligned} \tag{61}$$

Denote by A_j the event that

$$A_j \triangleq \left\{|\mathbb{E}_{W\sim Q}\left[R_u(W,Z) - R_m(W,Z)\right]| \ge \sqrt{\frac{C_{m,u}}{2}\left(\frac{1}{m} + \frac{1}{u}\right)\left(\mathrm{D}_{\mathrm{KL}}(Q||P_j) + \log\left(\frac{1}{\delta_j}\right)\right)}\right\}.$$

Let $\delta_j \triangleq \frac{6\delta}{\pi^2 j^2}$, by Theorem 4, for any distribution Q we have

$$\mathbb{P}\left\{A_{j^*}\right\} \le \mathbb{P}\left\{\cup_{j=1}^{\infty} A_j\right\} \le \sum_{j=1}^{\infty}\mathbb{P}\left\{A_j\right\} = \sum_{j=1}^{\infty}\delta_j = \sum_{j=1}^{\infty}\frac{6\delta}{\pi^2 j^2} = \delta. \tag{62}$$

Therefore, with probability at least $1-\delta$,

$$\begin{aligned}
&\mathbb{E}_{W\sim Q}\left[R_u(W,Z) - R_m(W,Z)\right] \\
=&\mathbb{E}_{\boldsymbol{\epsilon}\sim\mathcal{N}(\mathbf{0},\sigma^2\mathbf{I})}\left[R_u(\mathbf{w}+\boldsymbol{\epsilon},Z) - R_m(\mathbf{w}+\boldsymbol{\epsilon},Z)\right] \\
\le&\sqrt{\frac{C_{m,u}}{2}\left(\frac{1}{m} + \frac{1}{u}\right)\left(\mathrm{D}_{\mathrm{KL}}(Q||P_{j^*}) + \log\left(\frac{1}{\delta_j}\right)\right)} \\
\le&\sqrt{\frac{C_{m,u}}{2}\left(\frac{1}{m} + \frac{1}{u}\right)\left(\frac{1}{2}\left[1 + d\log\left(1 + \frac{\|\mathbf{w}\|_2^2}{d\sigma^2}\right)\right] + \log\left(\frac{1}{6\delta}\right) + 2\log\left(\pi j^*\right)\right)}.
\end{aligned} \tag{63}$$

Since $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \sigma^2\mathbf{I})$, Lemma 1 in [60] suggests that

$$\mathbb{P}\{\|\boldsymbol{\epsilon}\|_2^2 \ge d\sigma^2 + 2\sigma^2\sqrt{dt} + 2t\sigma^2\} \le e^{-t}. \tag{64}$$

Let $\widetilde{C}_{m,u} \triangleq \sqrt{\log(4mu/(m+u))/d}$, with probability at least $1 - \sqrt{(m+u)/4mu}$ we have

$$\begin{aligned}
\|\boldsymbol{\epsilon}\|_2^2 \le& d\sigma^2 + 2\sigma^2\sqrt{d\log(\sqrt{4mu/(m+u)})} + \sigma^2\log(4mu/(m+u)) \\
\le& d\sigma^2 + 2\sigma^2\sqrt{d\log(4mu/(m+u))} + \sigma^2\log(4mu/(m+u)) \\
=& \sigma^2 d\left(1 + \sqrt{\frac{\log(4mu/(m+u))}{d}}\right)^2 = \sigma^2 d\left(1 + \widetilde{C}_{m,u}\right)^2 \triangleq \rho^2,
\end{aligned} \tag{65}$$

Denote by $A = \{\|\boldsymbol{\epsilon}\|_2^2 \leq \rho^2\}$ the event that the Euclidean norm of $\boldsymbol{\epsilon}$ is not larger than ρ, with probability at least $1-\delta$:

$$
\begin{aligned}
&R_u(\mathbf{w}, Z) \\
\leq&\mathbb{E}_{\boldsymbol{\epsilon}\sim\mathcal{N}(\mathbf{0},\sigma^2\mathbf{I})}\left[R_u(\mathbf{w}+\boldsymbol{\epsilon}, Z)\right] \\
=&\mathbb{P}\{A\}\mathbb{E}_{\boldsymbol{\epsilon}\sim\mathcal{N}(\mathbf{0},\sigma^2\mathbf{I})}\left[R_u(\mathbf{w}+\boldsymbol{\epsilon}, Z)|A\right] + \mathbb{P}\{\bar{A}\}\mathbb{E}_{\boldsymbol{\epsilon}\sim\mathcal{N}(\mathbf{0},\sigma^2\mathbf{I})}\left[R_u(\mathbf{w}+\boldsymbol{\epsilon}, Z)|\bar{A}\right] \\
=&\left(1-\sqrt{\frac{m+u}{4mu}}\right)\mathbb{E}_{\boldsymbol{\epsilon}\sim\mathcal{N}(\mathbf{0},\sigma^2\mathbf{I})}\left[R_u(\mathbf{w}+\boldsymbol{\epsilon}, Z)|A\right] + \sqrt{\frac{m+u}{4mu}}\mathbb{E}_{\boldsymbol{\epsilon}\sim\mathcal{N}(\mathbf{0},\sigma^2\mathbf{I})}\left[R_u(\mathbf{w}+\boldsymbol{\epsilon}, Z)|\bar{A}\right] \\
\leq&\mathbb{E}_{\boldsymbol{\epsilon}\sim\mathcal{N}(\mathbf{0},\sigma^2\mathbf{I})}\left[R_u(\mathbf{w}+\boldsymbol{\epsilon}, Z)|A\right] + \sqrt{\frac{m+u}{4mu}} \\
\leq&\mathbb{E}_{W\sim Q}R_m(W, Z) + \sqrt{\frac{m+u}{4mu}} \\
&+\sqrt{\frac{C_{m,u}}{2}\left(\frac{1}{m}+\frac{1}{u}\right)\left(\frac{1}{2}\left[1+d\log\left(1+\frac{\|\mathbf{w}\|_2^2}{d\sigma^2}\right)\right]+\log\left(\frac{1}{6\delta}\right)+2\log\left(\pi j^*\right)\right)} \\
\leq&\max_{\|\boldsymbol{\epsilon}\|_2\leq\rho} R_m(\mathbf{w}+\boldsymbol{\epsilon}, Z) \\
&+\sqrt{C_{m,u}\left(\frac{1}{m}+\frac{1}{u}\right)\left(1+\frac{d}{2}\log\left(1+\frac{\|\mathbf{w}\|_2^2}{\rho^2}\left(1+\widetilde{C}_{m,u}\right)^2\right)+\log\left(\frac{1}{6\delta}\right)+2\log\left(\pi j^*\right)\right)}.
\end{aligned}
\tag{66}
$$

Here we use the assumption to obtain the first inequality, and the second line is due to law of total expectation. The second inequality is due to the fact that $R_u(\mathbf{w}, Z) \leq 1$ for any $\mathbf{w}$ and Z since the loss is 0-1 loss. We use the fact $\sqrt{a}+\sqrt{a+b} \leq \sqrt{2(2a+b)}$ in the last inequality. The remaining step is to specify the value of c. Note that if

$$
\|\mathbf{w}\|_2^2 \geq \frac{\rho^2}{(1+\widetilde{C}_{m,u})^2}\left(\exp\left\{\frac{2mu}{(m+u)d}\right\}-1\right), \tag{67}
$$

the slack term in Eq. (66) will exceed 1 and the inequality holds trivially. Therefore, we only need to consider the case that

$$
\|\mathbf{w}\|_2^2 < \frac{\rho^2}{(1+\widetilde{C}_{m,u})^2}\left(\exp\left\{\frac{2mu}{(m+u)d}\right\}-1\right). \tag{68}
$$

which implies that

$$
\sigma^2 + \frac{\|\mathbf{w}\|_2^2}{d} < \frac{\rho^2}{(1+\widetilde{C}_{m,u})^2 d}\exp\left\{\frac{2mu}{(m+u)d}\right\} = \sigma^2\exp\left\{\frac{2mu}{(m+u)d}\right\} \triangleq c. \tag{69}
$$

Here we have used Eq. (65) since we only need to consider the case that $\|\boldsymbol{\epsilon}\|_2^2 \leq \rho^2$. One can verify that j^* is an valid integer under this definition. Note that

$$
\begin{aligned}
\log(j^*) &\leq \log\left(1+d\log\left(\frac{c}{\sigma^2+\|\mathbf{w}\|_2^2/d}\right)\right) \\
&\leq \log\left(1+d\log\left(\frac{c}{\sigma^2}\right)\right) = \log\left(1+\frac{2mu}{(m+u)}\right) \\
&\leq \log\left(\frac{4mu}{(m+u)}\right).
\end{aligned}
\tag{70}
$$

Plugging Eq. (70) into Eq. (66), with probability at least $1-\delta$ over the randomness of Z:

$$
\begin{aligned}
&R_u(\mathbf{w}, Z) \\
\leq&\max_{\|\boldsymbol{\epsilon}\|_2\leq\rho} R_m(\mathbf{w}+\boldsymbol{\epsilon}, Z) \\
&+\sqrt{\frac{C_{m,u}(m+u)\left(2+d\log\left(1+\frac{\|\mathbf{w}\|_2^2}{\rho^2}\left(1+\widetilde{C}_{m,u}\right)^2\right)+2\log\left(\frac{1}{6\delta}\right)+4\log\left(\frac{4\pi mu}{m+u}\right)\right)}{2mu}}.
\end{aligned}
\tag{71}
$$

I Proof of Theorem 5

This proof is inspired by [74, 113]. Since $\mathbb{E}\left[R_u(w_T+U_T,Z)-R_u(w_T,Z)\right]\geq 0$ holds for any realization of $W_T=w_T$ we have

$$\begin{aligned}&\mathbb{E}_{Z,W_T,U_T}\left[R_u(\widetilde{W}_T,Z)-R_u(W_T,Z)\right]\\=&\int_{w_T}\left[\mathbb{E}_{Z,U_T}\left[R_u(w_T+U_T,Z)-R_u(w_T,Z)|W_T=w_T\right]\right]\mathrm{d}P_{W_T}(w_T)\geq 0.\end{aligned}\tag{72}$$

Therefore, the transductive generalization error can be bounded by

$$\begin{aligned}&\mathbb{E}_{Z,W_T}\left[R_u(W_T,Z)-R_m(W_T,Z)\right]\\=&\mathbb{E}_{Z,W_T,U_T}\left[R_m(\widetilde{W}_T,Z)-R_m(W_T,Z)\right]-\mathbb{E}_{Z,W_T,U_T}\left[R_u(\widetilde{W}_T,Z)-R_u(W_T,Z)\right]\\&+\mathbb{E}_{Z,W_T,U_T}\left[R_u(\widetilde{W}_T,Z)-R_m(\widetilde{W}_T,Z)\right]\\\leq&\mathbb{E}_{Z,W_T,U_T}\left[R_m(\widetilde{W}_T,Z)-R_m(W_T,Z)\right]+\sqrt{\frac{C_{m,u}}{2}\left(\frac{1}{m}+\frac{1}{u}\right)I(Z;\widetilde{W}_T)}.\end{aligned}\tag{73}$$

Now the last step is to provide a upper bound for $I(Z;\widetilde{W}_T)$. Following [113], the mutual information term is decomposed by

$$\begin{aligned}&I(Z;\widetilde{W}_T)\\=&I\left(Z;\widetilde{W}_{T-1}-\frac{\eta}{\sqrt{v_T}+\epsilon}\odot g(W_{T-1},B_T(Z))+N_T\right)\\\leq&I\left(Z;\widetilde{W}_{T-1},-\frac{\eta}{\sqrt{v_T}+\epsilon}\odot g(W_{T-1},B_T(Z))+N_T\right)\\=&I(Z;\widetilde{W}_{T-1})+I\left(-\frac{\eta}{\sqrt{v_T}+\epsilon}\odot g(W_{T-1},B_T(Z))+N_T;Z\middle|\widetilde{W}_{T-1}\right)\end{aligned}$$

Recursively repeating the above process, we obtain

$$\begin{aligned}I(Z;\widetilde{W}_T)\leq&\sum_{t=1}^{T}I\left(-\frac{\eta}{\sqrt{v_t}+\epsilon}\odot g(W_{t-1},B_t(Z))+N_t;Z\middle|\widetilde{W}_{t-1}\right)\\=&\sum_{t=1}^{T}I\left(-\frac{\eta}{\sqrt{v_t}+\epsilon}\odot g(\widetilde{W}_{t-1}-U_{t-1},B_t(Z))+N_t;Z\middle|\widetilde{W}_{t-1}\right)\end{aligned}\tag{74}$$

Then we need to provide a upper bound for the conditional mutual information. Let V,X,U be random variables that are independent of $N\sim\mathcal{N}(\mathbf{0},\mathbf{I}_d)$. Define Ψ as a function of random variables U,V,X,Y. Denote by $h(\cdot)$ the differential entropy, then

$$\begin{aligned}&I(\Psi(V,y-U,X)+\sigma N;X|Y=y)\\=&h(\Psi(V,y-U,X)+\sigma N|Y=y)-h(\Psi(V,y-U,X)+\sigma N|X,Y=y)\end{aligned}\tag{75}$$

For the first term, using the fact that Gaussian minimizes entropy, we have

$$\begin{aligned}&h(\Psi(V,y-U,X)+\sigma N|Y=y)\\\leq&\frac{d}{2}\log\left(2\pi e\frac{\mathbb{E}\left[\|\Psi(V,X,y-U)+\sigma N\|_2^2|Y=y\right]}{d}\right)\\=&\frac{d}{2}\log\left(2\pi e\frac{\mathbb{E}\left[\|\Psi(U,V,X,y-U)\|_2^2|Y=y\right]+\sigma^2\mathbb{E}\left[\|N\|_2^2\right]}{d}\right)\\=&\frac{d}{2}\log\left(2\pi e\frac{\mathbb{E}\left[\|\Psi(V,X,y-U)\|^2|Y=y\right]+d\sigma^2}{d}\right).\end{aligned}\tag{76}$$

For the second term, we have:

$$\begin{aligned}&h(\Psi(V,y-U,X)+\sigma N|X,Y=y)\geq h(\Psi(V,y-U,X)+\sigma N|U,V,X,Y=y)\\=&h(\sigma N)=\frac{d}{2}\log 2\pi e\sigma^2.\end{aligned}\tag{77}$$

Let $V = W^{[t-2]} \triangleq (W_0, \ldots, W_{t-2})$, $X = Z$, $Y = \widetilde{W}_{t-1}$, $U = U_{t-1}$ and

$$\begin{aligned}&\Psi(V, y-U, X) = \Psi(W^{[t-2]}, \widetilde{w}_{t-1} - U_{t-1}, Z)\\ =&-\frac{\eta}{\sqrt{v_t(W^{[t-2]}, \widetilde{w}_{t-1}-U_{t-1})}+\epsilon} \odot g(\widetilde{w}_{t-1}-U_{t-1}, B_t(Z)),\end{aligned}$$

plugging Eqs. (76,77) into Eq. (75), we have

$$\begin{aligned}&I\left(\Psi(W^{[t-2]}, \widetilde{w}_{t-1}-U_{t-1}, Z)+N_t; Z\middle|\widetilde{W}_{T-1}=\widetilde{w}_{t-1}\right)\\ =&I\left(\Psi(W^{[t-2]}, \widetilde{w}_{t-1}-U_{t-1}, Z)+N_t; Z\middle|\widetilde{W}_{t-1}=\widetilde{w}_{t-1}\right)\\ \le&\frac{d}{2}\log\left(\frac{1}{d\sigma_t^2}\mathbb{E}\left[\left\|\Psi(W^{[t-2]}, \widetilde{w}_{t-1}-U_{t-1}, Z)\right\|_2^2\middle|\widetilde{W}_{t-1}=\widetilde{w}_{t-1}\right]+1\right),\end{aligned}$$

which implies that

$$\begin{aligned}&I\left(\Psi(W^{[t-2]}, \widetilde{w}_{t-1}-U_{t-1}, Z)+N_t; Z\middle|\widetilde{W}_{t-1}\right)\\ \le&\int_{\widetilde{w}_{t-1}}\frac{d}{2}\log\left(\frac{1}{d\sigma_t^2}\mathbb{E}\left[\left\|\Psi(W^{[t-2]}, \widetilde{w}_{t-1}-U_{t-1}, Z)\right\|_2^2\middle|\widetilde{W}_{t-1}=\widetilde{w}_{t-1}\right]+1\right)\mathrm{d}P_{\widetilde{W}_{T-1}}(\widetilde{w}_{T-1})\\ \le&\frac{d}{2}\log\left(\frac{1}{d\sigma_t^2}\mathbb{E}\left[\left\|\Psi(W^{[t-2]}, \widetilde{W}_{t-1}-U_{t-1}, Z)\right\|_2^2\right]+1\right).\end{aligned}\tag{78}$$

Let $w^{[k]} \triangleq (w_1, \ldots, w_k)$ and

$$\zeta(W^{[t-2]}, \widetilde{W}_{t-1}-U_{t-1}, Z) \triangleq \left\|\Psi(W^{[t-2]}, \widetilde{W}_{t-1}-U_{t-1}, Z)+\mathbb{E}\left[g(\widetilde{W}_{t-1}-U_{t-1}, B_t(Z))\right]\right\|_2^2,$$

we have

$$\begin{aligned}&\mathbb{E}_{W^{[t-2]}, \widetilde{W}_{t-1}, U_{t-1}, Z}\left[\zeta(W^{[t-2]}, \widetilde{W}_{t-1}-U_{t-1}, Z)\right]\\ =&\int_z\int_{w^{[t-2]}}\int_{\widetilde{w}_{t-1}}\int_u \zeta(w^{[t-2]}, \widetilde{w}_{t-1}-u, z)\,\mathrm{d}P_{W_{t-1}|Z,W_{t-2}}(\widetilde{w}_{t-1}-u)\,\mathrm{d}P_{U_{t-1}}(u)\,\mathrm{d}P_{W^{[t-2]}|Z}(w^{[t-2]})\,\mathrm{d}P_Z(z)\\ =&\int_z\int_{w^{[t-2]}}\int_{\widetilde{w}_{t-1}}\int_{w_{t-1}} \zeta(w^{[t-2]}, w_{t-1}, z)\,\mathrm{d}P_{W_{t-1}|Z,W_{t-2}}(w_{t-1})\,\mathrm{d}P_{U_{t-1}}(\widetilde{w}_{t-1}-w_{t-1})\,\mathrm{d}P_{W^{[t-2]}|Z}(w^{[t-2]})\,\mathrm{d}P_Z(z)\\ =&\int_z\int_{w^{[t-2]}}\int_{w_{t-1}} \zeta(w^{[t-2]}, w_{t-1}, z)\,\mathrm{d}P_{W_{t-1}|Z,W_{t-2}}(w_{t-1})\,\mathrm{d}P_{W^{[t-2]}|Z}(w^{[t-2]})\,\mathrm{d}P_Z(z)\\ =&\int_z\int_{w^{[t-1]}} \zeta(w^{[t-2]}, w_{t-1}, z)\,\mathrm{d}P_{W^{[t-1]},Z}(w^{[t-1]}, z)\\ =&\mathbb{E}_{W^{[t-1]},Z}[\zeta(W^{[t-1]}, Z)].\end{aligned}\tag{79}$$

Here the first inequality is due to the convolution formulation, and we use $w_{t-1} \triangleq \widetilde{w}_{t-1} - u$ to obtain the second inequality. Plugging Eqs. (78, 79) into Eq. (74), we have

$$\begin{aligned}&I(Z; \widetilde{W}_T)\\ \le&\sum_{t=1}^T\frac{d}{2}\log\left(\frac{1}{d\sigma_t^2}\mathbb{E}\left[\left\|\Psi(W^{[t-2]}, W_{t-1}, Z)+\mathbb{E}\left[g(W_{t-1}, B_t(Z))\right]\right\|_2^2\right]+1\right)\\ =&\sum_{t=1}^T\frac{d}{2}\log\left(\frac{1}{d\sigma_t^2}\mathbb{E}\left[\left\|\frac{\eta}{\sqrt{v_t(W^{[t-1]})}+\epsilon}\odot g(W_{t-1}, B_t(Z))-\mathbb{E}\left[g(W_{t-1}, B_t(Z))\right]\right\|_2^2\right]+1\right).\end{aligned}\tag{80}$$

Combining Eq. (80) with Eq. (73), we have

$$\begin{aligned}&\mathbb{E}_{Z,W_T}\left[R_u(W_T, Z)-R_m(W_T, Z)\right]\\ \le&\sum_{t=1}^T\frac{d}{2}\log\left(\frac{1}{d\sigma_t^2}\mathbb{E}\left[\left\|\frac{\eta}{\sqrt{v_t(W^{[t-1]})}+\epsilon}\odot g(W_{t-1}, B_t(Z))-\mathbb{E}\left[g(W_{t-1}, B_t(Z))\right]\right\|_2^2\right]+1\right)\\ &+\mathbb{E}_{Z,W_T,U_T}\left[R_m(W_T+U_T, Z)-R_m(W_T, Z)\right]\end{aligned}\tag{81}$$

Now we discuss how to extend this result to Adam optimization algorithm. For $t \in [T]$, the update rule of Adam is

$$\begin{aligned}&m_t = \beta_1 m_{t-1} + (1-\beta_1)g(W_{t-1}, B_t(Z)),\\ &v_t = \beta_2 v_{t-1} + (1-\beta_2)g(W_{t-1}, Z)\odot g(W_{t-1}, B_t(Z)),\\ &\hat{v}_t = \frac{1}{1-\beta_2^t}v_t, W_t = W_{t-1} - \frac{\eta m_t}{\sqrt{\hat{v}_t}+\epsilon}.\end{aligned}$$

Note that

$$W_t = W_{t-1} - \frac{\eta m_t}{\sqrt{\hat{v}_t}+\epsilon} = W_{t-1} - \sum_{\tau=0}^{t-1} \beta_1^{t-\tau-1} \frac{(1-\beta_1)\eta}{\sqrt{\hat{v}_t}+\epsilon} \odot g(W_\tau, B_{\tau+1}(Z)) \\ \triangleq W_{t-1} - \Psi(W^{[t-1]}, Z).$$

Similarly, we construct the weight process as

$$\widetilde{W}_0 = W_0, \widetilde{W}_t = \widetilde{W}_{t-1} - \Psi(W^{[t-1]}, Z) + N_t.$$

By the same technique, one can find that

$$\begin{aligned} & I(Z; \widetilde{W}_T) \\ \leq & \sum_{t=1}^{T} \frac{d}{2} \log \left(\frac{1}{d\sigma_t^2} \mathbb{E} \left[\left\| \Psi(W^{[t-2]}, W_{t-1}, Z) + \mathbb{E}\left[g(W_{t-1}, B_t(Z)) \right] \right\|_2^2 \right] + 1 \right) \\ = & \sum_{t=1}^{T} \frac{d}{2} \log \left(\frac{1}{d\sigma_t^2} \mathbb{E} \left[\left\| \sum_{\tau=0}^{t-1} \beta_1^{t-\tau-1} \frac{(1-\beta_1)\eta}{\sqrt{\hat{v}_t}+\epsilon} \odot g(W_\tau, B_{\tau+1}(Z)) \right\|_2^2 \right] + 1 \right). \end{aligned} \tag{82}$$

Then the upper bound is given by

$$\begin{aligned} & \mathbb{E}_{Z,W_T}\left[R_u(W_T, Z) - R_m(W_T, Z) \right] \\ \leq & \sum_{t=1}^{T} \frac{d}{2} \log \left(\frac{1}{d\sigma_t^2} \mathbb{E} \left[\left\| \sum_{\tau=0}^{t-1} \beta_1^{t-\tau-1} \frac{(1-\beta_1)\eta}{\sqrt{\hat{v}_t}+\epsilon} \odot g(W_\tau, B_{\tau+1}(Z)) \right\|_2^2 \right] + 1 \right) \\ & + \mathbb{E}_{Z,W_T,U_T}\left[R_m(W_T + U_T, Z) - R_m(W_T, Z) \right]. \end{aligned} \tag{83}$$

J Proof of Proposition 2

First we have

$$\begin{aligned} & \mathbb{E}_{D_m, D_u^X, W} \left[\frac{1}{u} \sum_{i=m+1}^{m+u} \ell(W, (X_i, Y_i)) - \frac{1}{m} \sum_{i=1}^{m} \ell(W, (X_i, Y_i)) \right] \\ = & \mathbb{E}_{D_{m+u}} \mathbb{E}_{Z,W|D_{m+u}} \left[R_u(W, Z) - R_m(W, Z) \right]. \end{aligned} \tag{84}$$

By the proof of Theorem 1, the following inequality holds for any realization of $W = w$:

$$\mathbb{E}_{Z|D_{m+u}=d_{m+u}} \left[\exp\left\{ \lambda(R_u(w, Z) - R_m(w, Z)) \right\} \right] \leq \exp\left\{ \frac{\lambda^2 (m+u) C_{m,u}}{8mu} \right\}. \tag{85}$$

Let Z' be the independent copy of Z. By Donsker-Varadhan's variational formula, for any $\lambda \in \mathbb{R}$:

$$\begin{aligned} & \mathrm{D_{KL}}(P_{Z,W|D_{m+u}=d_{m+u}} || P_{Z',W|D_{m+u}=d_{m+u}}) \\ \geq & \mathbb{E}_{Z,W|D_{m+u}=d_{m+u}} \left[\lambda(R_u(W, Z) - R_m(W, Z)) \right] - \log \mathbb{E}_{Z',W|D} \left[\exp\left\{ \lambda(R_u(W, Z') - R_m(W, Z')) \right\} \right] \\ \geq & \mathbb{E}_{Z,W|D=d} \left[\lambda(R_u(W, Z) - R_m(W, Z)) \right] - \frac{\lambda^2 C_{m,u}}{8} \left(\frac{1}{m} + \frac{1}{u} \right), \end{aligned} \tag{86}$$

which implies that

$$\left| \mathbb{E}_{Z,W|D=d} \left[\lambda(R_u(W, Z) - R_m(W, Z)) \right] \right| \leq \sqrt{\frac{C_{m,u}}{2} \left(\frac{1}{m} + \frac{1}{u} \right) I(Z, W|D=d)}. \tag{87}$$

Taking expectation on both side and plugging into Eq. (84) we have

$$\begin{aligned} & \left| \mathbb{E}_{S_m, S_u^X, W} \left[\frac{1}{u} \sum_{i=m+1}^{m+u} \ell(W, (X_i, Y_i)) - \frac{1}{m} \sum_{i=1}^{m} \ell(W, (X_i, Y_i)) \right] \right| \\ = & \left| \mathbb{E}_{S_{m+u}} \mathbb{E}_{Z,W|S_{m+u}} \left[R_u(W, Z) - R_m(W, Z) \right] \right| \\ \leq & \mathbb{E}_{S_{m+u}} \left| \mathbb{E}_{Z,W|S_{m+u}} \left[\lambda(R_u(W, Z) - R_m(W, Z)) \right] \right| \\ \leq & \mathbb{E}_{S_{m+u}} \sqrt{\frac{C_{m,u}}{2} \left(\frac{1}{m} + \frac{1}{u} \right) I(Z, W|S_{m+u})}. \end{aligned} \tag{88}$$

This finishes the first part. For the second part, define $R_\mu(W) \triangleq \mathbb{E}_{(X,Y)\sim\mu}\ell(W,(X,Y))$, then we have

$$\begin{aligned}
&\mathbb{E}_{S_m,S_u^X,W}R(W,S_{m+u}) = \mathbb{E}_{S_{m+u},Z,W}R(W,S_{m+u})\\
=&\mathbb{E}_{S_{m+u}}\mathbb{E}_{Z,W|S_{m+u}}\left[\frac{m}{m+u}R_m(W,Z)+\frac{u}{m+u}R_u(W,Z)\right]\\
\leq&\mathbb{E}_{S_{m+u}}\left[\mathbb{E}_{Z,W|S_{m+u}}[R_m(W,Z)]+\frac{u}{m+u}\sqrt{\frac{C_{m,u}}{2}\left(\frac{1}{m}+\frac{1}{u}\right)I(Z,W|S_{m+u})}\right]\\
=&\frac{1}{m}\sum_{i=1}^m\ell(W,(X_i,Y_i))+\mathbb{E}_{S_{m+u}}\sqrt{\frac{C_{m,u}I(Z,W|S_{m+u})}{2m(m/u+1)}}.
\end{aligned} \tag{89}$$

By Donsker-Varadhan's variational formula,

$$\begin{aligned}
&\mathrm{D}_{\mathrm{KL}}(P,||P_{Z',W|D=d})\\
\geq&\mathbb{E}_{S_{m+u},Z,W}\left[\lambda(R_\mu(W)-R(W,S_{m+u}))\right]-\log\mathbb{E}_{S'_{m+u},Z',W}\left[\exp\left\{\lambda(R_\mu(W)-R(W,S_{m+u}))\right\}\right]\\
=&\mathbb{E}_{S_m,S_u^X,W}\left[\lambda(R_\mu(W)-R(W,S_{m+u}))\right]-\log\mathbb{E}_{S'_{m+u},Z',W}\left[\exp\left\{\lambda(R_\mu(W)-R(W,S_{m+u}))\right\}\right]\\
\geq&\mathbb{E}_{S_m,S_u^X,W}\left[\lambda(R_\mu(W)-R(W,S_{m+u}))\right]-\frac{\lambda^2B^2}{2(m+u)}.
\end{aligned} \tag{90}$$

Therefore, we have

$$\begin{aligned}
&\mathbb{E}_{S_m,S_u^X,W}R_\mu(W)\\
\leq&\mathbb{E}_{S_m,S_u^X,W}R(W,S_{m+u})+\sqrt{\frac{2I(S_{m+u},Z;W)}{m+u}}\\
\leq&\frac{1}{m}\sum_{i=1}^m\ell(W,(X_i,Y_i))+\mathbb{E}_{S_{m+u}}\sqrt{\frac{C_{m,u}I(Z,W|S_{m+u})}{2m(m/u+1)}}+\sqrt{\frac{2I(S_{m+u},Z;W)}{m+u}}.
\end{aligned} \tag{91}$$

Also, we have

$$\begin{aligned}
&\left|\mathbb{E}_{S_m,S_u^X,W}\left[\frac{1}{u}\sum_{i=m+1}^{m+u}\ell(W,(X_i,Y_i))-\frac{1}{m}\sum_{i=1}^m\ell(W,(X_i,Y_i))\right]\right|\\
=&\left|\mathbb{E}_{S_{m+u}}\mathbb{E}_{Z,W|S_{m+u}}\left[R_u(W,Z)-R_m(W,Z)\right]\right|\\
=&\left|\mathbb{E}_{S_{m+u}}\mathbb{E}_{\widetilde{Z},U,W|S_{m+u}}\left[R_u(W,Z)-R_m(W,Z)\right]\right|\\
\leq&\frac{1}{m}\sum_{i=1}^m\mathbb{E}_{S_{m+u}}\mathbb{E}_{\widetilde{Z}|S_{m+u}}\left|\mathbb{E}_{U,W|\widetilde{Z},S_{m+u}}\left[\ell(W,\widetilde{Z}_{i,S_i})-\ell(W,\widetilde{Z}_{i,1-S_i})\right]\right|\\
=&\frac{1}{m}\sum_{i=1}^m\mathbb{E}_{S_{m+u}}\mathbb{E}_{\widetilde{Z}|S_{m+u}}\left|\mathbb{E}_{F_i,U_i|\widetilde{Z},S_{m+u}}\left[g(F_i,S_i,\widetilde{Y}_i)\right]\right|.
\end{aligned} \tag{92}$$