## Characterizing and Understanding the Generalization Error of Transfer Learning with Gibbs Algorithm

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#### Abstract

We provide an information-theoretic analysis of the generalization ability of Gibbsbased transfer learning algorithms by focusing on two popular empirical risk minimization (ERM) approaches for transfer learning,  $\alpha$ -weighted-ERM and two-stage-ERM. Our key result is an exact characterization of the generalization behavior using the conditional symmetrized Kullback-Leibler (KL) information between the output hypothesis and the target training samples given the source training samples. Our results can also be applied to provide novel distribution-free generalization error upper bounds on these two aforementioned Gibbs algorithms. Our approach is versatile, as it also characterizes the generalization errors and excess risks of these two Gibbs algorithms in the asymptotic regime, where they converge to the  $\alpha$ -weighted-ERM and two-stage-ERM, respectively. Based on our theoretical results, we show that the benefits of transfer learning can be viewed as a bias-variance trade-off, with the bias induced by the source distribution and the variance induced by the lack of target samples. We believe this viewpoint can guide the choice of transfer learning algorithms in practice.

#### 1 INTRODUCTION

A common assumption in supervised learning is that both the training and test data samples are generated from the same distribution. However, this assumption does not always hold in many applications, as we often have easy access to samples generated from a source distribution, and we want to use the hypothesis trained using source training samples, which can be readily available, on a different target task, from which only limited data is available. Transfer learning and domain adaptation methods are developed to tackle this challenge, and the state-of-the-art transfer learning algorithms based on pre-trained models and fine-tuning have led to significant improvements in various applications such as computer vision, natural language processing, and more (Li et al., 2012; Long et al., 2015; Yosinski et al., 2014; Raffel et al., 2019).

Many works have attempted to explain the empirical success of transfer learning from different perspectives. The first theoretical analysis for domain adaptation is proposed by Ben-David et al. (2007) for binary classification, where the authors provide a VCdimension-based excess risk bound for the zero-one loss in terms of  $d_A$ -distance as a measure of discrepancy between source and target tasks. A new notion of discrepancy measure for transfer learning called transfer-exponent under the covariate-shift assumption is proposed in Hanneke and Kpotufe (2019). A minimax lower bound on the generalization error for transfer learning in neural networks is derived in Kalan and Fabian (2020). Recently, an Empirical Risk Minimization (ERM) algorithm via representation learning is proposed in Tripuraneni et al. (2020), and an upper bound on the excess risk of the new task is provided in terms of Gaussian complexity. Wang et al. (2019) provides an upper bound on excess risk based on instance weighting. Using KL divergence as a measure of similarity between the source and target data-generating distribution, an informationtheoretic generalization error upper bound for transfer learning is proposed in Wu et al. (2020).

However, these upper bounds on excess risk and generalization error may not entirely capture the generalization ability of a transfer learning algorithm. One immediate concern is the tightness issue, as the proposed bounds (Wang et al., 2019) can be loose or even vacuous when evaluated in practice. More importantly, the current definitions of discrepancy metric do not

<sup>\*</sup> Equal contribution. Proceedings of the 25<sup>th</sup> International Conference on Artificial Intelligence and Statistics (AISTATS) 2022, Valencia, Spain. PMLR: Volume 151. Copyright 2022 by the author(s).

fully characterize all the aspects that could influence the performance of a transfer learning approach, e.g., most discrepancy measures are either algorithm independent (KL divergence in Wu et al. (2020)), or only depend on the hypothesis class ( $d_A$ -distance in Ben-David et al. (2007)), or apply only under specific assumptions (the transfer exponent under covariate shift assumption in Hanneke and Kpotufe (2019)). Therefore, our understanding of transfer learning algorithms is still limited.

To overcome these limitations, we study transfer learning approaches using two Gibbs algorithms, i.e.,  $\alpha$ -weighted Gibbs algorithm and two-stage Gibbs algorithm, which can be viewed as randomized versions of two ERM-based transfer learning algorithms, i.e.,  $\alpha$ -weighted-ERM (Ben-David et al., 2010; Zhang et al., 2012) and two-stage-ERM (Tripuraneni et al., 2020; Donahue et al., 2014) by information-theoretic tools.

Our main contributions are as follows:

- We derive exact characterizations of the generalization errors for α-weighted Gibbs algorithm and two-stage Gibbs algorithm in terms of the conditional symmetrized KL information. We also provide novel distribution-free upper bounds, which quantify how the number of samples from the source and target will influence the generalization error of these transfer learning algorithms.
- We further demonstrate how to use our method to characterize the asymptotic behavior of the generalization error for these two Gibbs algorithms under large inverse temperature, where the αweighted Gibbs algorithm and two-stage Gibbs algorithm converge to the α-weighted-ERM and two-stage-ERM, respectively.
- Finally, by studying the excess risk of the α-weighted-ERM and two-stage-ERM algorithms in the asymptotic regime, we show that transfer learning algorithms admit a bias-variance trade-off viewpoint, whereby the choice of a transfer learning algorithm should depend on both the bias induced by the source distribution and the variance caused by the limited target samples.

**Notations:** Throughout the paper, upper-case letters denote random variables (e.g., Z), lower-case letters denote the realizations of random variables (e.g., z), and calligraphic letters denote spaces (e.g., Z). All the logarithms are the natural ones, and all information measure units are in nats.  $\mathcal{N}(\mu, \Sigma)$  denotes a Gaussian distribution with mean  $\mu$  and covariance matrix  $\Sigma$ .

#### 2 PROBLEM FORMULATION

Let  $D_s = \{Z_i^s\}_{i=1}^n$  and  $D_t = \{Z_j^t\}_{j=1}^m$  be the source and target training sets, respectively, where  $Z_i^s$  and  $Z_j^t$  are defined on the same alphabet  $\mathcal{Z}$ . Note that  $D_s$  and  $D_t$  are independent, but neither  $D_s$  nor  $D_t$  is required to be i.i.d generated from the data-generating source or target distributions  $P_z^s$  or  $P_z^t$ . We denote the joint distribution of all source training samples as  $P_{D_s}$  and that of the target training samples as  $P_{D_t}$ . We denote the hypotheses by  $w \in \mathcal{W}$ , where  $\mathcal{W}$  is a hypothesis class. The performance of any hypotheses is measured by a non-negative loss function  $\ell: \mathcal{W} \times \mathcal{Z} \to \mathbb{R}_0^+$ , and we can define the empirical risk and the population risk of a source task for a given source dataset  $d_s$  as

$$L_E(w, d_s) \triangleq \frac{1}{n} \sum_{i=1}^n \ell(w, z_i^s), \tag{1}$$

$$L_P(w, P_{D_s}) \triangleq \mathbb{E}_{P_{D_s}}[L_E(w, D_s)],$$
 (2)

and the empirical risk and the population risk of the target task for a given target dataset  $d_t$ ,

$$L_E(w, d_t) \triangleq \frac{1}{m} \sum_{j=1}^{m} \ell(w, z_j^t), \tag{3}$$

$$L_P(w, P_{D_t}) \triangleq \mathbb{E}_{P_{D_t}}[L_E(w, D_t)]. \tag{4}$$

A transfer learning algorithm can be modeled as a randomized mapping from the source and target training sets  $(D_s, D_t)$  onto a hypothesis  $W \in \mathcal{W}$  according to the conditional distribution  $P_{W|D_s,D_t}$ . Thus, the expected transfer generalization error quantifying the degree of over-fitting on the target training data can be written as

$$\overline{\operatorname{gen}}(P_{W|D_s,D_t}, P_{D_s}, P_{D_t}) \triangleq \mathbb{E}_{P_{W,D_s,D_t}}[L_P(W, P_{D_t}) - L_E(W, D_t)],$$
 (5)

where the expectation is taken over the joint distribution  $P_{W,D_s,D_t} = P_{W|D_s,D_t} \otimes P_{D_s} \otimes P_{D_t}$ .

#### 2.1 Transfer Learning Algorithms

We focus on the following two transfer learning approaches:  $\alpha$ -weighted-ERM and two-stage-ERM.

 $\alpha$ -Weighted-ERM Transfer Learning: We denote the hypothesis by  $w_{\alpha} \in \mathcal{W}$  as the output of  $\alpha$ -weighted-ERM learning algorithm. The hypothesis  $w_{\alpha}$  is typically obtained by minimizing a convex combination of the source and target task empirical risks as in Ben-David et al. (2010), i.e.,

$$L_E(w_{\alpha}, d_s, d_t) = (1 - \alpha)L_E(w_{\alpha}, d_s) + \alpha L_E(w_{\alpha}, d_t), \quad (6)$$

for  $0 \le \alpha \le 1$ .

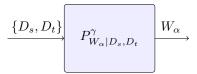


Figure 1:  $\alpha$ -weighted Gibbs Algorithm

Two-stage-ERM Transfer Learning: Suppose that the hypothesis  $w \in \mathcal{W}$  can be written as  $w = (w_{\phi}, w_c)$ , where  $w_{\phi} \in \mathcal{W}_{\phi}$  is the shared hypothesis (parameter) across both source and target tasks, and  $w_c^s \in \mathcal{W}_c$  and  $w_c^t \in \mathcal{W}_c$  denote some task-specific hypothesis (parameter) for the source and target tasks, respectively. In practice,  $w_{\phi}$  aggregates the parameters of the first few layers of a neural network for both tasks (e.g., shared featurizer), and  $w_c^s$ ,  $w_c^t$  collect the remaining parameters for the source and target tasks, respectively. The performance of the pair  $(w_{\phi}, w_c)$  is measured by a non-negative loss function  $\ell : \mathcal{W}_c \times \mathcal{W}_{\phi} \times \mathcal{Z} \to \mathbb{R}_0^+$ . We consider the following two-stage-ERM transfer learning algorithm inspired by Tripuraneni et al. (2020).

First Stage: The algorithm first learns the shared hypothesis  $w_{\phi}$  and the source-specific hypothesis  $w_c^s$  by minimizing the following empirical risk function defined on the source dataset at Stage 1:

$$L_E^{S1}(w_{\phi}, w_c^s, d_s) \triangleq \frac{1}{n} \sum_{i=1}^n \ell(w_{\phi}, w_c^s, z_i^s).$$
 (7)

**Second Stage:** The algorithm fixes the shared hypothesis  $w_{\phi}$  and learns the target-specific hypothesis  $w_{c}^{t}$  by minimizing the following empirical risk function defined on the target dataset at Stage 2:

$$L_E^{S2}(w_\phi, w_c^t, d_t) = \frac{1}{m} \sum_{j=1}^m \ell(w_\phi, w_c^t, z_j^t).$$
 (8)

#### 2.2 Transfer Learning with Gibbs algorithms

Intending to understand the generalization behavior of transfer learning techniques, we now consider the Gibbs counterpart of the aforementioned ERM-based transfer learning algorithms. In particular, the  $(\gamma, \pi(w), f(w, d))$ -Gibbs distribution, which was first proposed by Gibbs (1902) in statistical mechanics, is defined as:

$$P_{W|D}^{\gamma}(w|d) \triangleq \frac{\pi(w)e^{-\gamma f(w,d)}}{V(d,\gamma)}, \quad \gamma \ge 0, \tag{9}$$

where  $\gamma$  is the inverse temperature,  $\pi(w)$  is an arbitrary prior distribution on W, f(w,d) is energy function, and  $V(d,\gamma) \triangleq \int \pi(w)e^{-\gamma f(w,d)}dw$  is the partition function.

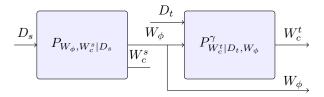


Figure 2: Two-stage Gibbs Algorithm

The  $(\gamma, \pi(w), L_E(w, d_t))$ -Gibbs distribution can be viewed as a randomized version of an ERM algorithm using only target samples if we specify the energy function  $f(w,d) = L_E(w,d_t)$ . Moreover, as the inverse temperature  $\gamma \to \infty$ , the prior distribution  $\pi(w)$  becomes negligible, and the Gibbs algorithm converges to the standard supervised-ERM algorithm.

Similarly, we can immediately define the following  $\alpha$ -weighted Gibbs algorithm and two-stage Gibbs algorithm, which can be viewed as randomized versions of  $\alpha$ -weighted-ERM and two-stage-ERM, respectively.

 $\alpha$ -weighted Gibbs algorithm generalizes the  $\alpha$ -weighted-ERM via a  $(\gamma, \pi(w_{\alpha}), L_E(w_{\alpha}, d_s, d_t))$ -Gibbs algorithm (see, Figure 1)

$$P_{W_{\alpha}|D_s,D_t}^{\gamma}(w_{\alpha}|d_s,d_t) = \frac{\pi(w_{\alpha})e^{-\gamma L_E(w_{\alpha},d_s,d_t)}}{V_{\alpha}(d_s,d_t,\gamma)}. \quad (10)$$

The expected transfer generalization error of the  $\alpha$ -weighted Gibbs algorithm is denoted as

$$\overline{\operatorname{gen}}_{\alpha}(P_{D_s}, P_{D_t}) \triangleq \overline{\operatorname{gen}}(P_{W_{\alpha}|D_s, D_t}^{\gamma}, P_{D_s}, P_{D_t}). \quad (11)$$

Two-stage Gibbs algorithm generalizes the two-stage-ERM via a  $(\gamma, \pi(w_c^t), L_E^{S2}(w_\phi, w_c^t, d_t))$ -Gibbs algorithm algorithm

$$P_{W_c^t|D_t,W_{\phi}}^{\gamma}(w_c^t|d_t,w_{\phi}) = \frac{\pi(w_c^t)e^{-\gamma L_E^{S_2}(w_{\phi},w_c^t,d_t)}}{V_{\beta}(w_{\phi},d_t,\gamma)} \quad (12)$$

in the second stage, where the shared hypothesis  $w_{\phi}$  is the output of the learning algorithm  $P_{W_{\phi},W_c^s|D_s}$  at the first stage. As shown in Figure 2, the two-stage Gibbs algorithm is constructed by concatenating two randomized mappings  $P_{W_c^t|D_t,W_{\phi}}^{\gamma}$  and  $P_{W_{\phi},W_c^s|D_s}$ .

The population risk for the target task is defined as:

$$L_P(w_{\phi}, w_c^t, P_{D_t}) = \mathbb{E}_{P_{D_t}}[L_E^{S2}(w_{\phi}, w_c^t, D_t)], \quad (13)$$

and the expected transfer generalization error under two-stage Gibbs algorithm can be denoted as

$$\overline{\operatorname{gen}}_{\beta}(P_{D_s}, P_{D_t}) \triangleq \tag{14}$$

$$\mathbb{E}_{P_{W_{\phi}},W_{c}^{t},D_{t}}[L_{P}(W_{\phi},W_{c}^{t},P_{D_{t}})-L_{E}^{S2}(W_{\phi},W_{c}^{t},D_{t})],$$

where the expectation is taken over the joint distribution  $P_{W_{\phi},W_{c}^{t},D_{t}} = P_{W_{c}^{t}|D_{t},W_{\phi}}^{\gamma} \otimes P_{W_{\phi}} \otimes P_{D_{t}}$ .

#### 2.3 Information Measures

We will characterize the aforementioned generalization errors using various information measures. If P and Q are probability measures over space  $\mathcal{X}$ , and P is absolutely continuous with respect to Q, the Kullback-Leibler (KL) divergence between P and Q is given by  $D(P||Q) \triangleq \int_{\mathcal{X}} \log\left(\frac{dP}{dQ}\right) dP$ . If Q is absolutely continuous with respect to P, the symmetrized KL divergence (a.k.a., Jeffrey's divergence (Jeffreys, 1946)) is

$$D_{\text{SKL}}(P||Q) \triangleq D(P||Q) + D(Q||P). \tag{15}$$

The mutual information between two random variables X and Y is the KL divergence between the joint distribution and product-of-marginal distribution

$$I(X;Y) \triangleq D(P_{X,Y} || P_X \otimes P_Y)$$

or equivalently, the conditional KL divergence between  $P_{Y|X}$  and  $P_Y$  averaged over  $P_X$ ,  $D(P_{Y|X}||P_Y|P_X) \triangleq \int_{\mathcal{X}} D(P_{Y|X=x}||P_Y) dP_X(x)$ . By swapping the role of  $P_{X,Y}$  and  $P_X \otimes P_Y$  in mutual information, we get the lautum information introduced by Palomar and Verdú (2008).

$$L(X;Y) \triangleq D(P_X \otimes P_Y || P_{X,Y}).$$

Finally, the symmetrized KL information between X and Y is given by Aminian et al. (2015):

$$I_{\text{SKL}}(X;Y) \triangleq (16)$$

$$D_{\text{SKL}}(P_{X,Y} || P_X \otimes P_Y) = I(X;Y) + L(X;Y).$$

The conditional mutual information between two random variables X and Y conditioned on Z is the KL divergence between  $P_{X,Y|Z}$  and  $P_{X|Z} \otimes P_{Y|Z}$  averaged over  $P_Z$ ,

$$I(X;Y|Z) \triangleq \int_{\mathcal{Z}} D(P_{X,Y|Z=z} || P_{Y|Z=z} \otimes P_{X|Z=z}) dP_Z(z).$$

Similarly, we can also define the conditional lautum information L(X;Y|Z), and the conditional symmetrized KL information is given by

$$I_{SKL}(X;Y|Z) \triangleq I(X;Y|Z) + L(X;Y|Z). \tag{17}$$

#### 3 RELATED WORK

Other Interpretations for Gibbs Algorithm: Besides viewing the Gibbs algorithm as a randomized ERM, there are additional interpretations for considering Gibbs algorithm in transfer learning.

**SGLD:** The Stochastic Gradient Langevin Dynamics (SGLD), which can be viewed as noisy version of Stochastic Gradient Descent (SGD), is defined as:

$$W_{k+1} = W_k - \eta \nabla L_E(W_k, d_t) + \sqrt{\frac{2\beta}{\gamma}} \zeta_k, \quad k = 0, 1, \cdots,$$

where  $\zeta_k$  is a standard Gaussian random vector and  $\eta > 0$  is the step size. In Raginsky et al. (2017), it is proved that under some conditions on the loss function, the conditional distribution  $P_{W_k|D_t}$  induced by SGLD algorithm is close to  $(\gamma, \pi(W_0), L_E(w_k, d_t))$ -Gibbs distribution in 2-Wasserstein distance for sufficiently large k.

Information Risk Minimization: The Gibbs algorithm also arises within the information risk minimization framework, where one adopts a conditional KL divergence regularizer to reduce over-fitting. In particular, it is shown in (Xu and Raginsky, 2017; Zhang, 2006; Zhang et al., 2006) that the solution to the regularized ERM problem

$$\begin{split} P_{W|D_t}^{\star} &= \arg\inf_{P_{W|D_t}} \left( \mathbb{E}_{P_{W,D_t}} [L_E(W,D_t)] \right. \\ &+ \frac{1}{\gamma} D(P_{W|D_t} \| \pi(W) | P_{D_t}) \right), \end{split}$$

corresponds to the  $(\gamma, \pi(w), L_E(w, d_t))$ -Gibbs distribution. The inverse temperature  $\gamma$  controls the regularization term and balances between over-fitting and generalization.

#### Supervised Learning with the Gibbs Algorithm:

An exact characterization of the generalization error of the Gibbs algorithm in terms of symmetrized KL information is provided by Aminian et al. (2021). The authors also provide a generalization error upper bound with the rate of  $\mathcal{O}(\alpha/n)$  under the sub-Gaussian assumption. An information-theoretic upper bound with similar rate  $\mathcal{O}(\alpha/n)$  is provided in Raginsky et al. (2016) for the Gibbs algorithm with bounded loss function, and PAC-Bayesian bounds using a variational approximation of Gibbs posteriors are studied in Alquier et al. (2016). Asadi and Abbe (2020); Kuzborskij et al. (2019) both focus on bounding the excess risk of the Gibbs algorithm.

Other Analyses Transfer Learn-In hypothesis transfer learning ing: problem (Kuzborskij and Orabona, 2013), where we only have access to the learned source hypotheses instead of the source training data, an upper bound on the leave-one-out error measured by square loss is provided. An extension of hypothesis transfer learning is studied in Kuzborskij and Orabona (2017), involving an algorithm combining the hypotheses from multiple sources based on regularized ERM principle. There are also works focusing on the theoretical aspects of domain adaptation, see (Ben-David et al., 2007, 2010; Mansour et al., 2009a,b; Germain et al., 2016; David et al., 2010), which are also related to our Note that in domain adaptation, there problem. is no labeled target data and only unlabeled target samples are available. Actually, having access to

target labeled data would improve the performance of the learning algorithm for target task (Mansour et al., 2021; Wang et al., 2019).

Note that we provide an *exact* characterization of the generalization error for these Gibbs algorithms in transfer learning scenarios, which differs from this body of research.

## 4 GENERALIZATION ERROR OF TRANSFER LEARNING ALGORITHM

We now offer exact characterizations of the expected transfer generalization errors in terms of symmetrized KL information for the  $\alpha$ -weighted and two-stage Gibbs algorithms, respectively. Then, combining the exact characterization of expected transfer generalization error for Gibbs algorithms with a conditional mutual information-based generalization error upper bound, we derive novel distribution-free upper bounds for these two Gibbs algorithms. Finally, we provide another exact characterization of the generalization errors in terms of symmetrized KL divergence, which is shown to be useful in the asymptotic analysis.

### 4.1 Exact Characterization of Generalization Error Using Conditional Symmetrized KL Information

One of our main results, which characterizes the exact expected transfer generalization error of the  $\alpha$ -weighted Gibbs algorithm with prior distribution  $\pi(w_{\alpha})$ , is as follows:

**Theorem 1** (Proved in Appendix A). For the  $\alpha$ -weighted Gibbs algorithm,  $0 < \alpha < 1$  and  $\gamma > 0$ ,

$$P_{W_{\alpha}|D_{s},D_{t}}^{\gamma}(w_{\alpha}|d_{s},d_{t}) = \frac{\pi(w_{\alpha})e^{-\gamma L_{E}(w_{\alpha},d_{s},d_{t})}}{V_{\alpha}(d_{s},d_{t},\gamma)}, \quad (18)$$

the expected transfer generalization error is given by

$$\overline{gen}_{\alpha}(P_{D_s}, P_{D_t}) = \frac{I_{SKL}(W_{\alpha}; D_t | D_s)}{\gamma \alpha}.$$
 (19)

We also provide an exact characterization of the expected transfer generalization error for two-stage Gibbs algorithm using conditional symmetrized KL information.

**Theorem 2** (Proved in Appendix A). The expected transfer generalization error of the two-stage Gibbs algorithm in (12) is given by

$$\overline{gen}_{\beta}(P_{D_s}, P_{D_t}) = \frac{I_{\text{SKL}}(W_c^t; D_t | W_{\phi})}{\gamma}.$$
 (20)

To the best of our knowledge, these results are the first exact characterizations of the expected transfer generalization error for the  $\alpha$ -weighted and two-stage Gibbs algorithm. Note that both Theorem 1 and Theorem 2 only assume that the loss function is non-negative and the training set of source and target are independent, and they hold even for non-i.i.d source and target training samples.

The expected transfer generalization errors are non-negative, i.e.,  $\overline{\text{gen}}_{\alpha}(P_{D_s}, P_{D_t}) \geq 0$  and  $\overline{\text{gen}}_{\beta}(P_{D_s}, P_{D_t}) \geq 0$ , which follows by the non-negativity of the conditional symmetrized KL information.

#### 4.2 Example: Mean Estimation

We now consider a simple mean estimation problem, where the symmetrized KL information can be computed exactly, to demonstrate the usefulness of our Theorems. All details are provided in Appendix B.

Consider the problem of learning the mean  $\mu_t \in \mathbb{R}^d$  of the target task using n i.i.d. source samples  $D_s = \{Z_i^s\}_{i=1}^n$  and m i.i.d. target samples  $D_t = \{Z_j^t\}_{j=1}^m$ . We assume that the samples from the source and target tasks satisfying  $\mathbb{E}[Z^s] = \mu_s$ ,  $\operatorname{cov}[Z^s] = \sigma_s^2 I_d$  and  $\mathbb{E}[Z^t] = \mu_t$ ,  $\operatorname{cov}[Z^t] = \sigma_t^2 I_d$ , respectively. We adopt the mean-squared loss  $\ell(\boldsymbol{w}, \boldsymbol{z}) = \|\boldsymbol{z} - \boldsymbol{w}\|_2^2$ , and assume a Gaussian prior for the mean  $\pi(\boldsymbol{w}) = \mathcal{N}(\boldsymbol{\mu}_0, \sigma_0^2 I_d)$ .

For the  $\alpha$ -weighted Gibbs algorithm, if we set the inverse-temperature  $\gamma = \frac{m+n}{2\sigma^2}$  and  $\alpha = \frac{m}{m+n}$ , then the  $(\frac{m+n}{2\sigma^2}, \mathcal{N}(\boldsymbol{\mu}_0, \sigma_0^2 I_d), L_E(\boldsymbol{w}_\alpha, d_s, d_t))$ -Gibbs algorithm is given by the following posterior (Murphy, 2007),

$$P_{W_{\alpha}|D_t,D_s}^{\gamma}(\boldsymbol{w}_{\alpha}|D_s,D_t) \sim \mathcal{N}(\boldsymbol{m}_{\alpha},\sigma_1^2 I_d),$$
 (21)

with  $\boldsymbol{m}_{\alpha} = \frac{\sigma_{1}^{2}}{\sigma_{0}^{2}}\boldsymbol{\mu}_{0} + \frac{\sigma_{1}^{2}}{\sigma^{2}}\left(\sum_{i=1}^{n}Z_{i}^{s} + \sum_{j=1}^{m}Z_{j}^{t}\right)$ , and  $\sigma_{1}^{2} = \frac{\sigma_{0}^{2}\sigma^{2}}{(m+n)\sigma_{0}^{2}+\sigma^{2}}$ . Since  $P_{W_{\alpha}|D_{s},D_{t}}^{\gamma}$  is Gaussian, the conditional symmetrized KL information does not depend on the distribution  $P_{Z^{t}}$  as long as  $\operatorname{cov}[Z^{t}] = \sigma_{t}^{2}I_{d}$ , i.e.,

$$I_{\text{SKL}}(W_{\alpha}; D_t | D_s) = \frac{m d\sigma_0^2 \sigma_t^2}{((m+n)\sigma_0^2 + \sigma^2)\sigma^2}.$$
 (22)

From Theorem 1, the expected transfer generalization error of this algorithm can be computed exactly as:

$$\overline{\text{gen}}_{\alpha}(P_{D_s}, P_{D_t}) = \frac{I_{\text{SKL}}(W_{\alpha}; D_t | D_s)}{\gamma \alpha} 
= \frac{2d\sigma_0^2 \sigma_t^2}{(m+n)(\sigma_0^2 + \frac{1}{2\gamma})}.$$
(23)

For the two-stage Gibbs algorithm, we learn the first  $d_{\phi}$  components  $\boldsymbol{\mu}_{\phi} \in \mathbb{R}^{d_{\phi}}$  using source samples. Then,

we set inverse temperature  $\gamma = \frac{m}{2\sigma^2}$  and use the  $(\frac{m}{2\sigma^2}, \mathcal{N}(\boldsymbol{\mu}_{0,c}, \sigma_0^2 I_{d_c}), L_E^{S2}(\boldsymbol{\mu}_{\phi}, \boldsymbol{w}_c^t, d_t))$ -Gibbs algorithm to learn the remaining  $d_c = d - d_{\phi}$  components. Following similar steps, by Theorem 2, we have

$$\overline{\operatorname{gen}}_{\beta}(P_{D_s}, P_{D_t}) = \frac{I_{\text{SKL}}(W_c^t; D_t | W_{\phi})}{\gamma} 
= \frac{2d_c \sigma_0^2 \sigma_t^2}{m(\sigma_0^2 + \frac{1}{2\gamma})}.$$
(24)

Remark 1 (Comparison with Supervised Learning). It is shown in Aminian et al. (2021) that the generalization error of a supervised Gibbs algorithm for this mean estimation example is

$$\overline{gen}(P_{W|D_t}^{\gamma}, P_{D_t}) = \frac{2d\sigma_0^2 \sigma_t^2}{m(\sigma_0^2 + \frac{1}{2\gamma})}, \tag{25}$$

where  $P_{W|D_t}^{\gamma}$  is  $(\frac{m}{2\sigma^2}, \mathcal{N}(\boldsymbol{\mu}_0, \sigma_0^2 I_d), L_E(w, d_t))$ -Gibbs algorithm. Comparing to the supervised Gibbs algorithm, the  $\alpha$ -weighted Gibbs algorithm reduces the generalization error to  $\mathcal{O}(\frac{d}{m+n})$  by fitting n source samples and m target samples simultaneously, and the two-stage Gibbs algorithm achieves the rate of  $\mathcal{O}(\frac{d_c}{m})$  by only learning  $\boldsymbol{w}_c^t \in \mathbb{R}^{d_c}$  from the target samples  $D_t$ .

Remark 2 (Effect of Source samples). As shown in (23) and (24), the transfer generalization errors of this mean estimation problem do not depend on the distribution of sources samples  $D_s$ . The reason is that the effect of sources samples is cancelled out in generalization error by subtracting the empirical risk from the population risk. Although different source distributions do not change generalization errors, they will influence the population risks and excess risks, and more detailed discussion is provided in Appendix B.

#### 4.3 Distribution-free Upper Bounds

To understand the behavior of expected transfer generalization error, we also provide distribution-free upper bounds in this subsection. These bounds quantify how the generalization errors of the  $\alpha$ -weighted and two-stage Gibbs algorithms depend on the number of target (source) samples m (n), and can be applied when directly computing symmetrized KL information is hard.

We first provide a conditional mutual information based upper bound on the expected transfer generalization error for any general learning algorithm  $P_{W|D_s,D_t}$  under i.i.d and  $\sigma$ -sub-Gaussian assumptions.

**Theorem 3** (Proved in Appendix C). Suppose that the target training samples  $D_t = \{Z_j^t\}_{j=1}^m$  are i.i.d generated from the distribution  $P_Z^t$ , and the non-negative loss function  $\ell(W, Z)$  is  $\sigma$ -sub-Gaussian under the dis-

tribution  $P_Z^t \otimes P_W$ . Then the following upper bound holds

$$|\overline{gen}(P_{W|D_s,D_t}, P_{D_s}, P_{D_t})| \le \sqrt{\frac{2\sigma^2}{m}}I(W; D_t|D_s).$$
 (26)

The following distribution-free upper bound on the expected transfer generalization error for  $\alpha$ -weighted Gibbs algorithm can be obtained by combining the upper bound in Theorem 3 with the exact characterization in Theorem 1.

**Theorem 4** (Proved in Appendix D). Suppose that the target training samples  $D_t = \{Z_j^t\}_{j=1}^m$  are i.i.d generated from the distribution  $P_Z^t$ , and the non-negative loss function  $\ell(W,Z)$  is  $\sigma_{\alpha}$ -sub-Gaussian under the distribution  $P_Z^t \otimes P_{W_{\alpha}}$ . If we further assume  $C_{\alpha} \leq \frac{L(W_{\alpha};D_t|D_s)}{I(W_{\alpha};D_t|D_s)}$  for some  $C_{\alpha} \geq 0$ , then for the  $\alpha$ -weighted Gibbs algorithm and  $0 < \alpha < 1$ ,

$$\overline{gen}_{\alpha}(P_{D_s}, P_{D_t}) \le \frac{2\sigma_{\alpha}^2 \gamma \alpha}{(1 + C_{\alpha})m}.$$
(27)

**Remark 3.** Let  $\alpha = \frac{m}{n+m}$ , then we have

$$\overline{gen}_{\alpha}(P_{D_s}, P_{D_t}) \le \frac{2\sigma_{\alpha}^2 \gamma}{(1 + C_{\alpha})(n + m)}, \qquad (28)$$

which is lower than the distribution-free upper bound for supervised learning under  $(\gamma, \pi(w), L_E(w, d_t))$ -Gibbs algorithm  $P_{W|D_t}^{\gamma}$  provided in (Aminian et al., 2021, Theorem 2), i.e.,  $\overline{gen}_{\alpha}(P_{W|D_t}^{\gamma}, P_{D_t}) \leq \frac{2\sigma^2 \gamma}{(1+C_E)m}$ , if  $C_E = C_{\alpha}$  and  $\sigma^2 = \sigma_{\alpha}^2$ .

Using similar approach, we can obtain a distributionfree upper bound on the expected transfer generalization error for the two-stage Gibbs algorithm.

**Theorem 5** (Proved in Appendix D). Suppose that the target training samples  $D_t = \{Z_j^t\}_{j=1}^m$  are i.i.d generated from the distribution  $P_Z^t$ , and the non-negative loss function  $\ell(W_c, w_\phi, Z)$  is  $\sigma_\beta$ -sub-Gaussian under distribution  $P_Z^t \otimes P_{W_c^t|W_\phi=w_\phi}$  for all  $w_\phi \in W_\phi$ . If we further assume  $C_\beta \leq \frac{L(W_c^t;D_t|W_\phi)}{I(W_c^t;D_t|W_\phi)}$  for some  $C_\beta \geq 0$ , then for the two-stage Gibbs algorithm in (12), we have

$$\overline{gen}_{\beta}(P_{D_s}, P_{D_t}) \le \frac{2\sigma_{\beta}^2 \gamma}{(1 + C_{\beta})m}.$$
 (29)

**Remark 4** (Choice of  $C_{\beta}$  and  $C_{\alpha}$ ). Setting  $C_{\alpha} = 0$  in Theorem 4 and  $C_{\beta} = 0$  in Theorem 5 is always valid since the lautum information is always positive whenever the mutual information is positive.

### 4.4 Exact Characterization of Generalization Error Using Conditional Symmetrized KL Divergence

In this section, we provide exact characterizations of expected transfer generalization errors for  $\alpha$ -weighted

 $<sup>\</sup>begin{array}{ll} ^{1}\text{A random variable } X \quad \text{is} \quad \sigma\text{-sub-Gaussian} \quad \text{if} \\ \log \mathbb{E}[e^{\lambda(X-\mathbb{E}X)}] \leq \frac{\sigma^{2}\lambda^{2}}{2}, \, \forall \lambda \in \mathbb{R}. \end{array}$ 

and two-stage Gibbs algorithms using conditional symmetrized KL divergence by considering the Gibbs algorithm with the population risks as energy functions in (9). Such a result is very useful in the asymptotic analysis Section 5.1.

**Theorem 6** (Proved in Appendix E). The expected transfer generalization error of the  $\alpha$ -weighted Gibbs algorithm in (10) is given by:

$$\overline{gen}_{\alpha}(P_{D_s}, P_{D_t}) =$$

$$D_{SKL}(P_{W_{\alpha}|D_s, D_t}^{\gamma} \| P_{W_{\alpha}|D_s}^{\gamma, L_{\alpha}(w_{\alpha}, d_s, P_{D_t})} | P_{D_s} P_{D_t})$$

 $\frac{D_{\text{SKL}}(P_{W_{\alpha}|D_{s},D_{t}}^{\gamma}\|P_{W_{\alpha}|D_{s}}^{\gamma,L_{\alpha}(w_{\alpha},d_{s},P_{D_{t}})}|P_{D_{s}}P_{D_{t}})}{\gamma\alpha},$ where  $P_{W_{\alpha}|D_{s}}^{\gamma,L_{\alpha}(w_{\alpha},d_{s},P_{D_{t}})}$  is  $(\gamma,\pi(w_{\alpha}),L_{\alpha}(w_{\alpha},d_{s},P_{D_{t}}))$ -Gibbs algorithm with  $L_{\alpha}(w, d_s, P_{D_t}) \triangleq \alpha L_P(w_{\alpha}, P_{D_t}) +$  $(1-\alpha)L_E(w_\alpha,d_s)$ .

A similar result can be obtained for the two-stage Gibbs algorithm.

**Theorem 7** (Proved in Appendix E). The expected transfer generalization error of the two-stage Gibbs algorithm in (12) is given by:

$$\begin{split} \overline{gen}_{\beta}(P_{D_s}, P_{D_t}) &= \\ \frac{D_{\text{SKL}}(P_{W_c^t|D_t, W_{\phi}}^{\gamma} \| P_{W_c^t|W_{\phi}}^{\gamma, L_P(w_{\phi}, w_c^t, P_{D_t})} | P_{D_t} P_{W_{\phi}})}{\gamma}, \\ where & P_{W_c^t|W_{\phi}}^{\gamma, L_P(w_{\phi}, w_c^t, P_{D_t})} & is \ (\gamma, \pi(w_c^t), L_P(w_{\phi}, w_c^t, P_{D_t})) - Collection & (2.11) \end{split}$$

Gibbs algorithm.

More discussions about the connection between the results obtained using symmetrized KL information and those of symmetrized KL divergence are provided in Appendix E.

#### 5 ASYMPTOTIC BEHAVIOR OF GENERALIZATION ERROR AND EXCESS RISK

In this section, we first consider the asymptotic behavior of the generalization error for the two Gibbs algorithms as the inverse temperature  $\gamma \to \infty$ . Note that, in this regime, both Gibbs algorithms converge to the corresponding ERM algorithms, and the distributionfree upper bounds obtained in the previous section become vacuous. Then, we show that such results can be applied to characterize the excess risks of the two ERM algorithms as  $m, n \to \infty$ , leading up to useful intuition about how to select different transfer learning approaches.

#### Generalization Error 5.1

 $\alpha$ -weighted-ERM: We assume that there exists a unique  $W_{\alpha}(D_s, D_t)$  and a unique  $W_{\alpha}(D_s)$  that minimizes the risk  $L_E(w, D_s, D_t)$  and  $L_{\alpha}(w, D_s, P_{D_t})$ , respectively, i.e.,

$$\hat{W}_{\alpha}(D_s, D_t) = \operatorname*{arg\,min}_{w \in \mathcal{W}} L_E(w, D_s, D_t), \tag{32}$$

$$\hat{W}_{\alpha}(D_s) = \operatorname*{arg\,min}_{w \in \mathcal{W}} L_{\alpha}(w, D_s, P_{D_t}). \tag{33}$$

It is shown in Hwang (1980) that if the following Hessian matrices

$$H^*(D_s, D_t) \triangleq \nabla_w^2 L_E(w, D_s, D_t) \big|_{w = \hat{W}_{\alpha}(D_s, D_t)}, (34)$$

$$H^*(D_s) \triangleq \nabla_w^2 L_\alpha(w, D_s, P_{D_t})\big|_{w = \hat{W}_\alpha(D_s)}$$
(35)

are not singular, then, as  $\gamma \to \infty$ 

$$P_{W_{\alpha}|D_{s},D_{t}}^{\gamma} \to \mathcal{N}(\hat{W}_{\alpha}(D_{s},D_{t}), \frac{1}{\gamma}H^{*}(D_{s},D_{t})^{-1}),$$

$$P_{W_{\alpha}|D_{s}}^{\gamma,L_{\alpha}(w_{\alpha},d_{s},P_{D_{t}})} \to \mathcal{N}(\hat{W}_{\alpha}(D_{s}), \frac{1}{\gamma}H^{*}(D_{s})^{-1}). \quad (36)$$

Thus, the conditional symmetrized KL divergence in Theorem 6 can be evaluated directly using Gaussian approximations.

**Proposition 1** (Proved in Appendix F.1). If the Hessian matrices  $H^*(D_s, D_t) = H^*(D_s) = H^*$  are independent of  $D_s$  and  $D_t$ , then the generalization error of the  $\alpha$ -weighted-ERM algorithm is

$$\overline{gen}_{\alpha}(P_{D_t}, P_{D_s}) = \frac{\mathbb{E}_{P_{D_s} \otimes P_{D_t}}[\|\hat{W}_{\alpha}(D_s, D_t) - \hat{W}_{\alpha}(D_s)\|_{H^*}^2]}{\alpha},$$

where  $||W||_H^2 \triangleq W^\top HW$ .

Remark 5. The assumptions that the two Hessian matrices  $H^*(D_s, D_t)$  and  $H^*(D_s)$  coincide and are independent of  $D_s$  and  $D_t$ , are only needed to simplify the expression in Proposition 1. Note that these assumptions are satisfied in the asymptotic regime where  $m, n \to \infty$  in standard maximum likelihood estimates (MLE) setting discussed below.

We can use Proposition 1 to obtain the generalization error of (MLE) in the asymptotic regime  $m, n \to \infty$ . More specifically, suppose that we have m and n i.i.d. samples generated from the target distribution  $P_Z^t$ and source distribution  $P_Z^s$ , respectively. We want to fit the training data with a parametric distribution family  $\{f(z|\boldsymbol{w}_{\alpha})\}$  using the  $\alpha$ -weighted-ERM algorithm, where  $\boldsymbol{w}_{\alpha} \in \mathcal{W} \subset \mathbb{R}^d$  denotes the parameter of the model. Here, the true data-generating distribution may not belong to the parametric family, i.e.,  $P_Z^s, P_Z^t \notin \{f(\cdot|\boldsymbol{w}_\alpha)|\boldsymbol{w}_\alpha \in \mathcal{W}\}.$ 

If we use the log-loss  $\ell(\boldsymbol{w}_{\alpha}, z) = -\log f(z|\boldsymbol{w}_{\alpha})$  in the  $\alpha$ -weighted Gibbs algorithm, and set  $\alpha = \frac{m}{m+n}$ , as  $\gamma \to \infty$ , it converges to the  $\alpha$ -weighted-ERM algorithm, which is equivalent to the following MLE, i.e.,

$$\hat{W}_{\alpha}(D_s, D_t) \tag{37}$$

$$= \arg \max_{\boldsymbol{w}_{\alpha} \in \mathcal{W}} \sum_{i=1}^{n} \log f(Z_{i}^{s} | \boldsymbol{w}_{\alpha}) + \sum_{j=1}^{m} \log f(Z_{j}^{t} | \boldsymbol{w}_{\alpha}).$$

If we further let  $m, n \to \infty$ , under regularization conditions for MLE (details in Appendix F.2) which guarantee that  $\hat{W}_{\alpha}(D_s, D_t)$  and  $\hat{W}_{\alpha}(D_s)$  are unique, we can show that

$$\hat{W}_{\alpha}(D_s, D_t) - \hat{W}_{\alpha}(D_s) \rightarrow \mathcal{N}\left(0, \frac{m\bar{J}(\boldsymbol{w}_{\alpha}^*)^{-1}\bar{\mathcal{I}}(\boldsymbol{w}_{\alpha}^*)\bar{J}(\boldsymbol{w}_{\alpha}^*)^{-1}}{(m+n)^2}\right),$$

where

$$\boldsymbol{w}_{\alpha}^{*} \triangleq \underset{\boldsymbol{w} \in \mathcal{W}}{\operatorname{arg \, min}} nD(P_{Z}^{s} || f(\cdot | \boldsymbol{w})) + mD(P_{Z}^{t} || f(\cdot | \boldsymbol{w})),$$

 $\bar{J}(\boldsymbol{w}_{\alpha}^{*})$  is the weighted expectation of the Hessian matrix, and  $\bar{\mathcal{I}}(\boldsymbol{w}_{\alpha}^{*})$  is the weighted Fisher information matrix. Detailed definitions of  $\bar{J}$  and  $\bar{\mathcal{I}}$  and proofs are provided in Appendix F.3.

In addition, the Hessian matrix  $H^*(D_s, D_t) \to \bar{J}(\boldsymbol{w}_{\alpha}^*)$  as  $m, n \to \infty$ , which is independent of the samples  $D_s, D_t$ . Thus, Proposition 1 gives

$$\overline{\operatorname{gen}}_{\alpha}(P_{D_t}, P_{D_s}) = \frac{\operatorname{tr}(\bar{\mathcal{I}}(\boldsymbol{w}_{\alpha}^*)\bar{J}(\boldsymbol{w}_{\alpha}^*)^{-1})}{n+m}, \quad (38)$$

which scales as  $\mathcal{O}(\frac{d}{m+n})$ .

**Two-stage-ERM:** We assume that there exists one unique  $\hat{W}_c^t(D_t, W_{\phi})$  which minimize the empirical risk of stage 2,

$$\hat{W}_c^t(D_t, W_\phi) \triangleq \underset{w_c \in \mathcal{W}_c}{\arg \min} L_E^{S2}(W_\phi, w_c, D_t), \qquad (39)$$

and there is one unique  $\hat{W}_c^t(W_{\phi})$  which minimize the population risk given a fixed  $W_{\phi}$ ,

$$\hat{W}_c^t(W_\phi) \triangleq \underset{w_c \in \mathcal{W}_c}{\arg \min} L_P(W_\phi, w_c, P_{D_t}). \tag{40}$$

Similarly, if the following Hessian matrices

$$H_c^*(D_t, W_\phi) \triangleq \nabla_{w_c}^2 L_E^{S2}(W_\phi, w_c, D_t) \big|_{w_c = \hat{W}_c^t(D_t, W_\phi)}$$
(41)

$$H_c^*(W_\phi) \triangleq \nabla_{w_c}^2 L_P(W_\phi, w_c, P_{D_t}) \big|_{w_c = \hat{W}_c^t(W_\phi)}$$
 (42)

are not singular, we can obtain the following result by evaluating the conditional symmetrized KL divergence in Proposition 7 using similar Gaussian approximation as in (36).

**Proposition 2** (Proved in Appendix F.1). If Hessian matrices  $H_c^*(D_t, W_\phi) = H_c^*(W_\phi) = H_c^*$  are independent of  $D_s, D_t$ , then the generalization error of the two-stage-ERM algorithm is

$$\overline{gen}_{\beta}(P_{D_t}, P_{D_s}) 
= \mathbb{E}_{P_{D_s, D_t, W_{\phi}}} [\|\hat{W}_c^t(D_t, W_{\phi}) - \hat{W}_c^t(W_{\phi})\|_{H_c^*}^2].$$

Consider a similar MLE setting as we did for the  $\alpha$ -weighted-ERM algorithm, except that now we want to fit data with a parametric distribution family  $\{f(z_j^t|\boldsymbol{w}_{\phi},\boldsymbol{w}_c^t)\}_{j=1}^m$  using the two-stage-ERM algorithm, where  $\boldsymbol{w}_{\phi} \in \mathcal{W}_{\phi} \subset \mathbb{R}^{d_{\phi}}, \boldsymbol{w}_c^t \in \mathcal{W}_c \subset \mathbb{R}^{d_c}$  denote the shared and specific parameters, respectively.

If we use the log-loss  $\ell(\boldsymbol{w}_{\phi}, \boldsymbol{w}_{c}^{t}, z) = -\log f(z|\boldsymbol{w}_{\phi}, \boldsymbol{w}_{c}^{t})$  in the two-stage Gibbs algorithm, as  $\gamma \to \infty$ , it converges to the following two-stage MLE approach,

$$[\hat{W}_{\phi}(D_s), \hat{W}_c^s(D_s)] \triangleq \underset{[\boldsymbol{w}_{\phi}, \boldsymbol{w}_c] \in \mathcal{W}}{\operatorname{arg max}} \sum_{i=1}^n \log f(Z_i^s | \boldsymbol{w}_{\phi}, \boldsymbol{w}_c),$$

$$\hat{W}_{c}^{t}(D_{t}, \hat{W}_{\phi}) \triangleq \underset{\boldsymbol{w}_{c} \in \mathcal{W}_{c}}{\arg \max} \sum_{j=1}^{m} \log f(Z_{j}^{t} | \hat{W}_{\phi}, \boldsymbol{w}_{c}).$$

As  $m, n \to \infty$ , under similar regularization conditions (details in Appendix F.2) which guarantee the uniqueness of these estimates, we can show that

$$\begin{split} &\hat{W}_c^t(D_t, \hat{W}_{\phi}) - \hat{W}_c^t(\hat{W}_{\phi}) \rightarrow \\ &\mathcal{N}\left(0, \frac{J_c^t(\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_c^{st*})^{-1} \mathcal{I}_c^t(\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_c^{st*}) J_c^t(\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_c^{st*})^{-1}}{m}\right), \end{split}$$

where

$$[\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_{c}^{s*}] \triangleq \underset{[\boldsymbol{w}_{\phi}, \boldsymbol{w}_{c}] \in \mathcal{W}}{\arg \min} D(P_{Z^{s}} || f(\cdot | \boldsymbol{w}_{\phi}, \boldsymbol{w}_{c})), \quad (43)$$

$$\boldsymbol{w}_{c}^{st*} \triangleq \underset{\boldsymbol{w}_{c} \in \mathcal{W}_{c}}{\min} D(P_{Z^{t}} || f(\cdot | \boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_{c})),$$
 (44)

and  $J_c^t(\boldsymbol{w}_\phi^{s*}, \boldsymbol{w}_c^{st*})$ ,  $\mathcal{I}_c^t(\boldsymbol{w}_\phi^{s*}, \boldsymbol{w}_c^{st*})$  stands for the expected Hessian matrix and Fisher information matrix over  $\boldsymbol{w}_c$  under target distribution, respectively. Detailed proofs are provided in Appendix F.3. As the Hessian matrix  $H_c^*(D_t, W_\phi) = H_c^*(W_\phi) \rightarrow J_c^t(\boldsymbol{w}_\phi^{s*}, \boldsymbol{w}_c^{st*})$  as  $m, n \rightarrow \infty$ , by Proposition 2, we have

$$\overline{\operatorname{gen}}_{\beta}(P_{D_t}, P_{D_s}) = \mathcal{O}(\frac{d_c}{m}). \tag{45}$$

#### 5.2 Excess Risk in MLE Setting

We further consider the excess risks of the  $\alpha$ -weighted-ERM algorithm and the two-stage-ERM algorithm in the aforementioned MLE setting when  $m, n \to \infty$ , and show that such analyses provide some intuitions in selecting different transfer learning algorithms. All the details are provided in Appendix F.4.

The excess risk (Mohri et al., 2018) is defined as the difference between the population risk achieved by the learning algorithm and that achieved by the optimal hypothesis given the knowledge of the true target distribution  $P_{Z_t}$ , i.e.,

$$\mathcal{E}_{r}(P_{W}) \triangleq \mathbb{E}_{P_{W,D_{s},D_{t}}}[L_{P}(W,P_{D_{t}})] - L_{P}(\boldsymbol{w}_{t}^{*},P_{D_{t}}),$$
with  $\boldsymbol{w}_{t}^{*} \triangleq \underset{\boldsymbol{w} \in \mathcal{W}}{\operatorname{arg min}} L_{P}(\boldsymbol{w},P_{D_{t}}),$  (46)

	Standard ERM	$\alpha$ -weighted-ERM	Two-stage-ERM
Excess risk bias	0	$\ oldsymbol{w}_lpha^* - oldsymbol{w}_t^*\ _{J_t(oldsymbol{w}_t^*)}^2$	$\left\  \left[ \bm{w}_{\phi}^{s*}, \bm{w}_{c}^{st*} \right] - \left[ \bm{w}_{\phi}^{t*}, \bm{w}_{c}^{t*} \right] \right\ _{J_{t}(\bm{w}_{\phi}^{t*}, \bm{w}_{c}^{t*})}^{2}$
Excess risk variance	$\mathcal{O}(rac{d}{m})$ $\mathcal{O}(rac{d}{d})$	$\mathcal{O}(rac{d}{m+n})$	$\mathcal{O}(rac{d}{n}+rac{d_c}{m})$
Generalization error	$\mathcal{O}(\frac{d}{m})$	$\mathcal{O}(\frac{d}{m+n})$	$\mathcal{O}(rac{d_c}{m})$

Table 1: Comparison of different algorithms under MLE setting.

where  $\boldsymbol{w}_t^* = \arg\min_{\boldsymbol{w} \in \mathcal{W}} D(P_Z^t || f(\cdot | w))$  holds in the MLE setting considered here.

 $\alpha$ -weighted-ERM: In general, a proper transfer learning algorithm should have small excess risk  $\mathcal{E}_r$ , which justifies the following approximation of the excess risk

$$\mathcal{E}_r(P_{\hat{W}_{\alpha}(D_s,D_t)}) \approx \frac{1}{2} \mathbb{E}_{P_{D_s,D_t}} \left[ \left\| \hat{W}_{\alpha}(D_s,D_t) - \boldsymbol{w}_t^* \right\|_{J_t(\boldsymbol{w}_t^*)}^2 \right]$$
$$= \frac{1}{2} \|\boldsymbol{w}_{\alpha}^* - \boldsymbol{w}_t^* \|_{J_t(\boldsymbol{w}_t^*)}^2 + \frac{\operatorname{tr} \left( J_t(\boldsymbol{w}_t^*) \operatorname{Cov}(\hat{W}_{\alpha}(D_s,D_t)) \right)}{2}.$$

As we can see from the above expression, the excess risk can be decomposed into squared bias and variance terms. The bias is caused by learning from the mixture of the source and target distributions instead of just the target distribution  $P_Z^t$ . In addition, it can be shown that  $\operatorname{tr}(J_t(\boldsymbol{w}_t^*)\operatorname{Cov}(\hat{W}_\alpha(D_s,D_t))) = \mathcal{O}(\frac{d}{m+n})$ , which has the same order as the generalization error in (38).

**Two-stage-ERM:** In the two-stage algorithm,  $\boldsymbol{w}^{t*}$  can be written as  $\boldsymbol{w}^{t*} = [\boldsymbol{w}_{\phi}^{t*}, \boldsymbol{w}_{c}^{t*}]$ , and using similar approximation, we have

$$\mathcal{E}_{r}(P_{\hat{W}_{\phi}(D_{s}),\hat{W}_{c}^{t}(D_{t},\hat{W}_{\phi})})$$

$$\approx \frac{1}{2} \| [\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_{c}^{st*}] - [\boldsymbol{w}_{\phi}^{t*}, \boldsymbol{w}_{c}^{t*}] \|_{J_{t}(\boldsymbol{w}_{\phi}^{t*}, \boldsymbol{w}_{c}^{t*})}^{2} + \frac{\operatorname{tr}(J_{t}(\boldsymbol{w}_{\phi}^{t*}, \boldsymbol{w}_{c}^{t*})\operatorname{Cov}(\hat{W}_{\phi}(D_{s}), \hat{W}_{c}^{t}(D_{t}, \hat{W}_{\phi})))}{2}. \tag{47}$$

Here the bias is caused by sharing the parameter  $\boldsymbol{w}_{\phi}^{s*}$  learned from the source distribution. If  $\boldsymbol{w}_{\phi}^{t*} = \boldsymbol{w}_{\phi}^{s*}$ , then  $\boldsymbol{w}_{c}^{st*} = \boldsymbol{w}_{c}^{t*}$  and the bias is zero. It can be shown that the variance term scales as  $O(\frac{d}{n} + \frac{d_{c}}{m})$ . When  $n \gg m$ , it reduces to  $O(\frac{d_{c}}{m})$ , which is the same as the generalization error in (45).

In Table 1, we summarize the excess risk, and generalization error results for the two transfer learning algorithms studied in the paper and those of the standard supervised learning under MLE setting (Van der Vaart, 2000) as  $m, n \to \infty$ . The improvement of the excess risk for transfer learning algorithms comes from trading the variance induced by the lack of target samples with the bias introduced by the source distribution, which suggests that the choice of learning

algorithm should depend on both source distribution and the number of samples m, n.

The bias term in the excess risks can be interpreted as another notion of discrepancy measure, which is algorithm-dependent, as  $\boldsymbol{w}_{\alpha}^{*}$  and  $\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_{c}^{s*}$  are defined as the optimal parameters under different algorithms given the knowledge of both source and target distributions. Sometimes, these bias terms are more useful in choosing an algorithm than the discrepancy measure used in the literature. For example, consider the mean estimation example in Section 4.2, if we set  $\mu_s = \mu_t$ ,  $\sigma_s^2 \ll \sigma_t^2$ , and let  $m, n \to \infty$ , then the bias term for both  $\alpha$ -weighted-ERM and two-stage-ERM should be zero, and transfer learning algorithms are preferred over the standard ERM. However, the KL divergence between the source and target distribution, which is proposed as a discrepancy measure in Wu et al. (2020), would be large.

The generalization error can be interpreted as the variance of the excess risk when  $n\gg m$ , and the analysis provided in the paper could help us to find a good balance in the bias and variance trade-off. Our results can be also used in transfer learning algorithm selection in the MLE setting by comparing the sum of the corresponding generalization error term and empirical risk achieved by each algorithm, which generalizes the standard Akaike information criterion (AIC) (Akaike, 1998) used in the supervised learning to transfer learning setting.

#### 6 CONCLUSION

We provide an exact characterization of the generalization error for two Gibbs-based transfer learning algorithms, i.e.,  $\alpha$ -weighted Gibbs algorithm and two-stage-ERM Gibbs algorithm, using conditional symmetrized KL information and divergence. Based on our results, we show that the benefits of transfer learning can be viewed as a bias-variance trade-off, and importantly, the term relating to the bias points to a new discrepancy measure that merits further investigation.

#### Acknowledgements

We thank the anonymous reviewers for their valuable feedback, which helped us to improve the paper greatly. Yuheng Bu is supported, in part, by NSF under Grant CCF-1717610 and by the MIT-IBM Watson AI Lab. Gholamali Aminian is supported by the Royal Society Newton International Fellowship, grant no. NIF\R1\192656.

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## Supplementary Material:

## Characterizing and Understanding the Generalization Error of Transfer Learning with Gibbs Algorithm

# A Exact Characterization of Generalization Error Based on Symmetrized KL Information

#### A.1 $\alpha$ -weighted Gibbs Algorithm

**Theorem 1.** (restated) For the  $\alpha$ -weighted Gibbs algorithm,  $0 < \alpha < 1$  and  $\gamma > 0$ ,

$$P_{W_{\alpha}|D_s,D_t}^{\gamma}(w_{\alpha}|d_s,d_t) = \frac{\pi(w_{\alpha})e^{-\gamma L_E(w_{\alpha},d_s,d_t)}}{V_{\alpha}(d_s,d_t,\gamma)},$$

the expected transfer generalization error is given by

$$\overline{gen}_{\alpha}(P_{D_s}, P_{D_t}) = \frac{I_{SKL}(W_{\alpha}; D_t | D_s)}{\gamma \alpha}.$$

*Proof.* By the definition of conditional symmetrized KL information, we have

$$I_{\text{SKL}}(W_{\alpha}; D_{t}|D_{s}) = \mathbb{E}_{P_{D_{s}}} \left[ \mathbb{E}_{P_{W_{\alpha},D_{t}|D_{s}}} \left[ \log \left( \frac{P_{W_{\alpha}|D_{s},D_{t}}}{P_{W_{\alpha}|D_{s}}} \right) \right] + \mathbb{E}_{P_{W_{\alpha}|D_{s}}} P_{D_{t}|D_{s}} \left[ \log \left( \frac{P_{W_{\alpha}|D_{s}}}{P_{W_{\alpha}|D_{s},D_{t}}} \right) \right] \right]$$

$$= \mathbb{E}_{P_{D_{s}}} \left[ \mathbb{E}_{P_{W_{\alpha},D_{t}|D_{s}}} \left[ \log (P_{W_{\alpha}|D_{s},D_{t}}^{\gamma}) \right] - \mathbb{E}_{P_{W_{\alpha}|D_{s}}} P_{D_{t}|D_{s}} \left[ \log (P_{W_{\alpha}|D_{s},D_{t}}^{\gamma}) \right] \right]. \tag{48}$$

Combining with fact that  $D_s$  and  $D_t$  are independent, and plug in the posterior of  $\alpha$ -weighted Gibbs algorithm, we have

$$I_{\text{SKL}}(W_{\alpha}; D_{t}|D_{s}) = \mathbb{E}_{P_{D_{s}}}[\gamma \mathbb{E}_{P_{W_{\alpha},D_{t}|D_{s}}}[L_{E}(W_{\alpha}, D_{s}, D_{t})] - \gamma \mathbb{E}_{P_{W_{\alpha}|D_{s}}P_{D_{t}}}[L_{E}(W_{\alpha}, D_{s}, D_{t})]]$$

$$= \gamma \mathbb{E}_{P_{D_{s}}}[\mathbb{E}_{P_{W_{\alpha},D_{t}|D_{s}}}[(1 - \alpha)L_{E}(w_{\alpha}, d_{s}) + \alpha L_{E}(w_{\alpha}, d_{t})]]$$

$$- \gamma \mathbb{E}_{P_{D_{s}}}[\mathbb{E}_{P_{W_{\alpha}|D_{s}}P_{D_{t}}}[(1 - \alpha)L_{E}(w_{\alpha}, d_{s}) + \alpha L_{E}(w_{\alpha}, d_{t})]]$$

$$= \gamma \alpha [\mathbb{E}_{P_{W_{\alpha},D_{t},D_{s}}}[L_{E}(w_{\alpha}, d_{t})] - [\mathbb{E}_{P_{W_{\alpha},D_{s}}P_{D_{t}}}[L_{E}(w_{\alpha}, d_{t})]]$$

$$= \gamma \alpha \overline{\text{gen}}_{\alpha}(P_{D_{s}}, P_{D_{s}}).$$

$$(49)$$

Due to the symmetry of the  $\alpha$ -weighted Gibbs algorithm, if we use  $\overline{\text{gen}}_{\alpha}(P_{D_t}, P_{D_s})$  to denote the generalization error of treating  $P_{D_t}$  as source task and  $D_s$  as the target, we can obtain that  $\overline{\text{gen}}_{\alpha}(P_{D_t}, P_{D_s}) = \frac{I_{\text{SKL}}(W_{\alpha}; D_s | D_t)}{\gamma_{\alpha}}$ .

It is also worthwhile to mention that the  $\alpha$ -weighted expected generalization error of both source and target tasks can be characterized in terms of symmetrized KL information as shown in the following Proposition.

**Proposition 3.** For  $(\gamma, \pi(w_{\alpha}), L_E(w_{\alpha}, d_s, d_t))$ -Gibbs algorithm and  $0 < \alpha < 1$ , we have

$$\alpha \overline{gen}_{\alpha}(P_{D_s}, P_{D_t}) + (1 - \alpha) \overline{gen}_{\alpha}(P_{D_t}, P_{D_s}) = \frac{I_{SKL}(W_{\alpha}; D_t, D_s)}{\gamma}.$$
(50)

*Proof.* The symmetrized KL information can be written as

$$I_{\text{SKL}}(W_{\alpha}; D_t, D_s) = \mathbb{E}_{P_{W_{\alpha}, D_t, D_s}} \left[ \log(P_{W_{\alpha}|D_s, D_t}^{\gamma}) \right] - \mathbb{E}_{P_{W_{\alpha}}P_{D_t, D_s}} \left[ \log(P_{W_{\alpha}|D_s, D_t}^{\gamma}) \right]. \tag{51}$$

Plug in the posterior of  $\alpha$ -weighted Gibbs algorithm,

$$I_{SKL}(W_{\alpha}; D_{t}, D_{s})$$

$$= \mathbb{E}_{P_{W_{\alpha}, D_{t}, D_{s}}} \left[ -\gamma L_{E}(w_{\alpha}, d_{s}, d_{t}) \right] + \mathbb{E}_{P_{W_{\alpha}} P_{D_{t}, D_{s}}} \left[ \gamma L_{E}(w_{\alpha}, d_{s}, d_{t}) \right]$$

$$= -\gamma \mathbb{E}_{P_{W_{\alpha}, D_{t}, D_{s}}} \left[ \alpha L_{E}(w_{\alpha}, d_{t}) + (1 - \alpha) L_{E}(w_{\alpha}, d_{s}) \right] + \gamma \mathbb{E}_{P_{W_{\alpha}} P_{D_{t}, D_{s}}} \left[ \alpha L_{E}(w_{\alpha}, d_{t}) + (1 - \alpha) L_{E}(w_{\alpha}, d_{s}) \right]$$

$$= \alpha \gamma \overline{\text{gen}}_{\alpha}(P_{D_{s}}, P_{D_{t}}) + (1 - \alpha) \gamma \overline{\text{gen}}_{\alpha}(P_{D_{t}}, P_{D_{s}}).$$

$$\Box$$

$$(52)$$

Note that the Proposition 3 holds even for dependent source  $D_s$  and target  $D_t$  samples.

#### A.2 Two-stage Gibbs Algrotihm

**Theorem 2.** (restated) The expected transfer generalization error of the two-stage Gibbs algorithm,

$$P_{W_c^t|D_t,W_{\phi}}^{\gamma}(w_c^t|d_t,w_{\phi}) = \frac{\pi(w_c^t)e^{-\gamma L_E^{S_2}(w_{\phi},w_c^t,d_t)}}{V_{\beta}(w_{\phi},d_t,\gamma)},$$

is given by

$$\overline{gen}_{\beta}(P_{D_s}, P_{D_t}) = \frac{I_{SKL}(D_t; W_c^t | W_{\phi})}{\gamma}.$$

*Proof.* In the second stage we freeze the share parameters  $W_{\phi}$ , and we will update the specific target task parameter. Thus,

$$I_{SKL}(W_{c}^{t}; D_{t}|W_{\phi})$$

$$= \mathbb{E}_{P_{W_{\phi}}} \left[ \mathbb{E}_{P_{W_{c}^{t}, D_{t}|W_{\phi}}} \left[ \log(P_{W_{c}^{t}|D_{t}, W_{\phi}}) \right] - \mathbb{E}_{P_{W_{c}^{t}|W_{\phi}}} P_{D_{t}|W_{\phi}} \left[ \log(P_{W_{c}^{t}|D_{s}, W_{\phi}}) \right] \right]$$

$$= \gamma \left( \mathbb{E}_{P_{W_{\phi}}} \left[ \mathbb{E}_{P_{W_{c}^{t}|W_{\phi}}} P_{D_{t}|W_{\phi}} \left[ L_{E}^{S2}(W_{\phi}, W_{c}^{t}, D_{t}) \right] - \mathbb{E}_{P_{W_{c}^{s}, D_{t}|W_{\phi}}} \left[ L_{E}^{S2}(W_{\phi}, W_{c}^{t}, D_{t}) \right] \right] \right)$$

$$= \gamma \overline{\text{gen}}_{\beta} (P_{D_{s}}, P_{D_{t}}).$$

$$(53)$$

#### B Example: Mean Estimation

#### B.1 Symmetrized KL Divergence

The following lemma from Palomar and Verdú (2008) characterizes the mutual and lautum information for the Gaussian channel.

Lemma 1. (Palomar and Verdú, 2008, Theorem 14) Consider the following model

$$Y = AX + N_{G}, (54)$$

where  $\mathbf{X} \in \mathbb{R}^{d_X}$  denotes the input random vector with zero mean (not necessarily Gaussian),  $\mathbf{A} \in \mathbb{R}^{d_Y \times d_X}$  denotes the linear transformation undergone by the input,  $\mathbf{Y} \in \mathbb{R}^{d_Y}$  is the output vector, and  $\mathbf{N}_G \in \mathbb{R}^{d_Y}$  is a Gaussian noise vector independent of  $\mathbf{X}$ . The input and the noise covariance matrices are given by  $\mathbf{\Sigma}$  and  $\mathbf{\Sigma}_{N_G}$ . Then, we have

$$I(\boldsymbol{X}; \boldsymbol{Y}) = \frac{1}{2} \operatorname{tr} \left( \boldsymbol{\Sigma}_{N_{G}}^{-1} \boldsymbol{A} \boldsymbol{\Sigma} \boldsymbol{A}^{\top} \right) - D(P_{\boldsymbol{Y}} || P_{N_{G}}),$$
 (55)

$$L(\boldsymbol{X}; \boldsymbol{Y}) = \frac{1}{2} \operatorname{tr} \left( \boldsymbol{\Sigma}_{N_{G}}^{-1} \boldsymbol{A} \boldsymbol{\Sigma} \boldsymbol{A}^{\top} \right) + D(P_{\boldsymbol{Y}} \| P_{N_{G}}).$$
 (56)

In the  $\alpha$ -weighted Gibbs algorithm, the output  $W_{\alpha}$  can be written as

$$W_{\alpha} = \frac{\sigma_1^2}{\sigma_0^2} \mu_0 + \frac{\sigma_1^2}{\sigma^2} \left( \sum_{i=1}^n Z_i^s + \sum_{i=1}^m Z_j^t \right) + N = \frac{\sigma_1^2}{\sigma^2} \sum_{i=1}^m (Z_j^t - \mu_t) + \frac{\sigma_1^2}{\sigma_0^2} \mu_0 + \frac{m\sigma_1^2}{\sigma^2} \mu_t + \frac{\sigma_1^2}{\sigma^2} \sum_{i=1}^n Z_i^s + N, \tag{57}$$

where  $N \sim \mathcal{N}(0, \sigma_1^2 I_d)$ , and  $\sigma_1^2 = \frac{\sigma_0^2 \sigma^2}{(m+n)\sigma_0^2 + \sigma^2}$ . For fixed sources training sample  $d_s$ , we can set  $P_{N_{\rm G}} \sim \mathcal{N}(\frac{\sigma_1^2}{\sigma_0^2} \boldsymbol{\mu}_0 + \frac{m\sigma_1^2}{\sigma^2} \boldsymbol{\mu}_t + \frac{\sigma_1^2}{\sigma^2} \sum_{i=1}^n z_i^s, \sigma_1^2 I_d)$  and  $\boldsymbol{\Sigma} = \sigma_t^2 I_{nd}$  in Lemma 1 gives

$$I_{\text{SKL}}(W_{\alpha}; D_t | D_s = d_s) = \text{tr}\left(\mathbf{\Sigma}_{N_G}^{-1} \mathbf{A} \mathbf{\Sigma} \mathbf{A}^{\top}\right) = \text{tr}\left(\frac{\sigma_t^2}{\sigma_1^2} \mathbf{A} \mathbf{A}^{\top}\right).$$
(58)

Noticing that  $\mathbf{A}\mathbf{A}^{\top} = \frac{m\sigma_1^4}{\sigma^4}I_d$  and taking expectation over  $P_S$ , we have

$$I_{\text{SKL}}(W_{\alpha}; D_t | D_s) = \frac{m d\sigma_0^2 \sigma_t^2}{((m+n)\sigma_0^2 + \sigma^2)\sigma^2}.$$
(59)

For the two-stage Gibbs algorithm, the output  $W_c^t$  can be written as

$$W_c^t = \frac{\sigma_c^2}{\sigma_0^2} \boldsymbol{\mu}_{0,c} + \frac{\sigma_c^2}{\sigma^2} \sum_{i=1}^m Z_{j,c}^t + N_c = \frac{\sigma_c^2}{\sigma^2} \sum_{i=1}^m (Z_{j,c}^t - \boldsymbol{\mu}_{t,c}) + \frac{\sigma_c^2}{\sigma_0^2} \boldsymbol{\mu}_{0,c} + \frac{n\sigma_c^2}{\sigma^2} \boldsymbol{\mu}_{t,c} + N_c, \tag{60}$$

where  $N_c \sim \mathcal{N}(0, \sigma_c^2 I_{d_c})$ ,  $\sigma_c^2 = \frac{\sigma_0^2 \sigma^2}{m \sigma_0^2 + \sigma^2}$ , and subscript c stands for the task-specific component of the parameters. Since  $W_c^t$  is independent of the source samples, setting  $P_{N_{\rm G}} \sim \mathcal{N}(\frac{\sigma_c^2}{\sigma_0^2} \boldsymbol{\mu}_{0,c} + \frac{n \sigma_c^2}{\sigma^2} \boldsymbol{\mu}_{t,c}, \sigma_c^2 I_{d_c})$  and  $\boldsymbol{\Sigma} = \sigma_t^2 I_{nd_c}$  in Lemma 1 gives

$$I_{\text{SKL}}(W_c^t; D_t | W_\phi) = \text{tr}\left(\mathbf{\Sigma}_{N_{\text{G}}}^{-1} \mathbf{A} \mathbf{\Sigma} \mathbf{A}^\top\right) = \text{tr}\left(\frac{\sigma_t^2}{\sigma_c^2} \mathbf{A} \mathbf{A}^\top\right) = \frac{m d_c \sigma_0^2 \sigma_t^2}{(m \sigma_0^2 + \sigma^2) \sigma^2},\tag{61}$$

where the last step follows due to the fact  $AA^{\top} = \frac{m\sigma_c^4}{\sigma^4}I_{d_c}$  in this case.

#### B.2 Effect of Source samples

As shown in (23) and (24), the transfer generalization errors of this mean estimation problem only depend on the number of samples of  $D_s$ , and do not depend on the distribution  $P_{D_s}$ . In this subsection, we will show that, though different sources samples (distribution) do not change generalization error, they will influence the population risks and excess risks.

In this mean estimation example, the population risk of any W can be decomposed into

$$L_P(W, P_{D_t}) = \mathbb{E}_{Z_t}[\|W - Z_t\|_2^2] = \mathbb{E}_{Z_t}[\|W - \mathbb{E}[W] + \mathbb{E}[W] - \boldsymbol{\mu}_t + \boldsymbol{\mu}_t - Z_t\|_2^2]$$

$$= \|\mathbb{E}[W] - \boldsymbol{\mu}_t\|_2^2 + \operatorname{tr}(\operatorname{Cov}[W]) + d\sigma_t^2,$$
(62)

where the first term,  $\|\mathbb{E}[W] - \boldsymbol{\mu}_t\|_2^2$ , is the squared bias, and the second term,  $\operatorname{tr}(\operatorname{Cov}[W])$ , is the variance. It is easy to verify that the optimal  $\boldsymbol{w}^* = \arg\min L_P(W, P_{D_t})$  is just the target mean  $\boldsymbol{\mu}_t$ , and  $L_P(\boldsymbol{w}^*, P_{D_t}) = d\sigma_t^2$ , then the excess risk defined in (46) can be written as,

$$\mathcal{E}_r(P_W) = \|\mathbb{E}[W] - \boldsymbol{\mu}_t\|_2^2 + \operatorname{tr}(\operatorname{Cov}[W]). \tag{63}$$

For the  $\alpha$ -weighted Gibbs algorithm in (60), it can be shown that

Bias = 
$$\mathbb{E}[W_{\alpha}] - \mu_t = \frac{\sigma^2(\mu_0 - \mu_t) + n\sigma_0^2(\mu_s - \mu_t)}{(m+n)\sigma_0^2 + \sigma^2},$$
 (64)

$$\operatorname{tr}(\operatorname{Cov}[W_{\alpha}]) = \frac{d\sigma_1^4}{\sigma^4}(n\sigma_s^2 + m\sigma_t^2) + d\sigma_1^2.$$
(65)

The Bias term will be zero if  $\mu_0 = \mu_s = \mu_t$ . Thus, the excess risk of  $\alpha$ -weighted Gibbs algorithm will be minimized when  $\mu_s = \mu_t$  and  $\sigma_s^2 = 0$ , which is equivalent to the case that the target mean  $\mu_t$  is known.

For the two-stage Gibbs algorithm, if we learn the first  $d_{\phi}$  components  $\boldsymbol{\mu}_{\phi} \in \mathbb{R}^{d_{\phi}}$  using the  $(\frac{n}{2\sigma^2}, \mathcal{N}(\boldsymbol{\mu}_{1,\phi}, \sigma_0^2 I_{d_{\phi}}), L_E^{S1}(\boldsymbol{w}_{\phi}, \boldsymbol{w}_c^s, d_s))$ -Gibbs algorithm, and use the  $(\frac{m}{2\sigma^2}, \mathcal{N}(\boldsymbol{\mu}_{2,c}, \sigma_0^2 I_{d_c}), L_E^{S2}(\boldsymbol{\mu}_{\phi}, \boldsymbol{w}_c^t, d_t))$ -Gibbs

algorithm to learn the remain  $d_c$  components in the second stage, it can be shown that

$$Bias_{\phi} = \mathbb{E}[W_{\phi}] - \mu_{t,\phi} = \frac{\sigma^2(\mu_{1,\phi} - \mu_{t,\phi}) + n\sigma_0^2(\mu_{s,\phi} - \mu_{t,\phi})}{n\sigma_0^2 + \sigma^2},$$
(66)

$$Bias_c = \mathbb{E}[W_c^t] - \mu_{t,c} = \frac{\sigma^2(\mu_{2,c} - \mu_{t,c})}{m\sigma_0^2 + \sigma^2},$$
(67)

$$\operatorname{tr}(\operatorname{Cov}[W_{\phi}]) = \frac{nd_{\phi}\sigma_{\phi}^{4}\sigma_{s}^{2}}{\sigma^{4}} + d_{\phi}\sigma_{\phi}^{2},\tag{68}$$

$$\operatorname{tr}(\operatorname{Cov}[W_c^t]) = \frac{md_c\sigma_c^4\sigma_t^2}{\sigma^4} + d_c\sigma_c^2, \tag{69}$$

with  $\sigma_{\phi}^2 = \frac{\sigma_0^2 \sigma^2}{n \sigma_0^2 + \sigma^2}$  and  $\sigma_c^2 = \frac{\sigma_0^2 \sigma^2}{m \sigma_0^2 + \sigma^2}$ . The excess risk of the two-stage Gibbs algorithm will be minimized when  $\mu_{s,\phi} = \mu_{t,\phi}$  and  $\sigma_s^2 = 0$ , i.e., the optimal shared parameter  $\mu_{t,\phi}$  is known.

## C Expected Transfer Generalization Error Upper Bound for General Learning Algorithm

#### C.1 Preliminaries

We first provide some preliminaries for our proofs in this section by introducing the notion of cumulant generating function, which characterizes different tail behaviors of random variables.

**Definition 1.** The cumulant generating function (CGF) of a random variable X is defined as

$$\Lambda_X(\lambda) \triangleq \log \mathbb{E}[e^{\lambda(X - \mathbb{E}X)}]. \tag{70}$$

Assuming  $\Lambda_X(\lambda)$  exists, it can be verified that  $\Lambda_X(0) = \Lambda_X'(0) = 0$ , and that it is convex.

**Definition 2.** For a convex function  $\psi$  defined on the interval [0,b), where  $0 < b \le \infty$ , its Legendre dual  $\psi^*$  is defined as

$$\psi^{\star}(x) \triangleq \sup_{\lambda \in [0,b)} (\lambda x - \psi(\lambda)). \tag{71}$$

The following lemma characterizes a useful property of the Legendre dual and its inverse function.

**Lemma 2.** (Boucheron et al., 2013, Lemma 2.4) Assume that  $\psi(0) = \psi'(0) = 0$ . Then  $\psi^*(x)$  defined above is a non-negative convex and non-decreasing function on  $[0,\infty)$  with  $\psi^*(0) = 0$ . Moreover, its inverse function  $\psi^{*-1}(y) = \inf\{x \geq 0 : \psi^*(x) \geq y\}$  is concave, and can be written as

$$\psi^{\star - 1}(y) = \inf_{\lambda \in [0, b)} \left( \frac{y + \psi(\lambda)}{\lambda} \right), \quad b > 0.$$
 (72)

We consider the distributions with the following tail behaviors in the appendices:

• Sub-Gaussian: A random variable X is  $\sigma$ -sub-Gaussian, if  $\psi(\lambda) = \frac{\sigma^2 \lambda^2}{2}$  is an upper bound on  $\Lambda_X(\lambda)$ , for  $\lambda \in \mathbb{R}$ . Then by Lemma 2,

$$\psi^{\star - 1}(y) = \sqrt{2\sigma^2 y}.$$

• Sub-Exponential: A random variable X is  $(\sigma_e^2, b)$ -sub-Exponential, if  $\psi(\lambda) = \frac{\sigma_e^2 \lambda^2}{2}$  is an upper bound on  $\Lambda_X(\lambda)$ , for  $0 \le |\lambda| \le \frac{1}{b}$  and b > 0. Using Lemma 2, we have

$$\psi^{\star - 1}(y) = \begin{cases} \sqrt{2\sigma_e^2 y}, & \text{if } y \le \frac{\sigma_e^2}{2b}; \\ by + \frac{\sigma_e^2}{2b}, & \text{otherwise.} \end{cases}$$

• Sub-Gamma: A random variable X is  $\Gamma(\sigma_s^2, c_s)$ -sub-Gamma (Zhang and Chen, 2020), if  $\psi(\lambda) = \frac{\lambda^2 \sigma_s^2}{2(1-c_s|\lambda|)}$  is an upper bound on  $\Lambda_X(\lambda)$ , for  $0 < |\lambda| < \frac{1}{c_s}$  and  $c_s > 0$ . Using Lemma 2, we have

$$\psi^{\star - 1}(y) = \sqrt{2\sigma_s^2 y} + c_s y.$$

#### C.2 Proof of Theorem 3

We prove a more general form of Theorem 3 as follows:

**Theorem 8.** Suppose that the target training samples  $D_t = \{Z_j^t\}_{j=1}^m$  are i.i.d generated from the distribution  $P_Z^t$  and the loss function  $\ell(W,Z)$  satisfies  $\Lambda_{\ell(W,Z)}(\lambda) \leq \psi(-\lambda)$ , for  $\lambda \in (-b,0)$  and  $\Lambda_{\ell(W,Z)}(\lambda) \leq \psi(\lambda)$ , for  $\lambda \in (0,b)$  and b > 0 under the distribution  $P_Z^t \otimes P_W$ . The following upper bound holds:

$$|\overline{gen}(P_{W|D_s,D_t}, P_{D_s}, P_{D_t})| \le \psi^{\star - 1}\left(\frac{I(W; D_t|D_s)}{m}\right). \tag{73}$$

*Proof.* The generalization error can be written as

$$|\overline{\text{gen}}(P_{W|D_s,D_t}, P_{D_s}, P_{D_t})| \le \frac{1}{m} \sum_{i=1}^m |\mathbb{E}_{P_{W,Z_i^t}}[\ell(W, Z_i^t)] - \mathbb{E}_{P_W \otimes P_Z^t}[\ell(W, Z^t)]|.$$
 (74)

Using the Donsker-Varadhan variational representation (Boucheron et al., 2013), for all  $\lambda \in (-b, +b)$ ,

$$D(P_{W,Z_i^t|d_s} || P_{W|d_s} \otimes P_Z^t) \ge \mathbb{E}_{P_{W,Z_i^t|d_s}} [\lambda \ell(W, Z_i^t)] - \log(\mathbb{E}_{P_{W|d_s} \otimes P_Z^t} [e^{\lambda \ell(W, Z^t)}]).$$
 (75)

Taking expectation respect to  $D_s$  over both sides, then we have

$$I(W; Z_i^t | D_s) \ge \mathbb{E}_{P_{W, Z_i^t}} [\lambda \ell(W, Z_i^t)] - \mathbb{E}_{P_{D_s}} [\log(\mathbb{E}_{P_{W | D_s} \otimes P_Z^t} [e^{\lambda \ell(W, Z^t)}])]$$

$$\ge \mathbb{E}_{P_{W, Z_i^t}} [\lambda \ell(W, Z_i^t)] - \log(\mathbb{E}_{P_W \otimes P_Z^t} [e^{\lambda \ell(W, Z^t)}])$$

$$\ge \lambda (\mathbb{E}_{P_{W, Z_i^t}} [\ell(W, Z_i^t)] - \mathbb{E}_{P_W \otimes P_Z^t} [\ell(W, Z^t)]) - \psi(\lambda). \tag{76}$$

Using similar approach as in (Bu et al., 2020, Theorem 1),

$$|\mathbb{E}_{P_{W,Z^t}}[\ell(W, Z_i^t)] - \mathbb{E}_{P_W \otimes P_Z^t}[\ell(W, Z^t)]| \le \psi^{\star - 1}(I(W; Z_i^t | D_s)).$$
(77)

Now by combining (74) and (77), we have:

$$|\overline{\text{gen}}(P_{W|D_s,D_t}, P_{D_s}, P_{D_t})| \leq \frac{1}{m} \sum_{i=1}^m \psi^{\star - 1}(I(W; Z_i^t | D_s))$$

$$\leq \psi^{\star - 1} \left(\frac{1}{m} \sum_{i=1}^m I(W; Z_i^t | D_s)\right)$$

$$\leq \psi^{\star - 1} \left(\frac{I(W, D_t | D_s)}{m}\right), \tag{78}$$

where the inequality follows due to the concavity of  $\psi^{\star-1}$  function and the Independence between  $Z_i^t$ .

**Theorem 3.** (restated) Suppose that the target training samples  $D_t = \{Z_j^t\}_{j=1}^m$  are i.i.d generated from the distribution  $P_Z^t$ , and the non-negative loss function  $\ell(W, Z)$  is  $\sigma$ -sub-Gaussian under the distribution  $P_Z^t \otimes P_W$ . Then, the following upper bound holds

$$|\overline{\operatorname{gen}}(P_{W|D_s,D_t},P_{D_s},P_{D_t})| \leq \sqrt{\frac{2\sigma^2}{m}I(W;D_t|D_s)}.$$

*Proof.* For  $\sigma$ -subgaussian assumption, we have  $\psi^{\star-1}(y) = \sqrt{2\sigma^2 y}$  in Theorem 8 and this completes the proof.  $\Box$ 

Remark 6. Similar upper bound on the expected transfer generalization error in Theorem 3 holds by considering a different assumption that the loss function  $\ell(w, Z)$  is  $\sigma$ -sub-Gaussian under the distribution  $P_Z^t$  for all  $w \in \mathcal{W}$ .

#### C.3 Other Tail Distributions

Using Theorem 8, we can also provide upper bounds on the expected transfer generalization error for any general learning algorithms under sub-Exponential and sub-Gamma assumptions.

Corollary 1 (Sub-Exponential). Suppose that the target training samples  $D_t = \{Z_j^t\}_{j=1}^m$  are i.i.d generated from the distribution  $P_Z^t$ , and the non-negative loss function  $\ell(W,Z)$  ( $\sigma_e^2, b$ )-sub-Exponential under distribution  $P_Z^t \otimes P_W$ . Then the following upper bound holds

$$|\overline{gen}(P_{W|D_s,D_t},P_{D_s},P_{D_t})| \le \begin{cases} \sqrt{2\sigma_e^2 \frac{I(W;D_t|D_s)}{m}}, & if \frac{I(W;D_t|D_s)}{m} \le \frac{\sigma_e^2}{2b}; \\ b\frac{I(W;D_t|D_s)}{m} + \frac{\sigma_e^2}{2b}, & otherwise. \end{cases}$$
(79)

Corollary 2 (Sub-Gamma). Suppose that the target training samples  $D_t = \{Z_j^t\}_{j=1}^m$  are i.i.d generated from the distribution  $P_Z^t$ , and the non-negative loss function  $\ell(W, Z)$  is  $\Gamma(\sigma_s^2, c_s)$ -sub-Gamma under distribution  $P_Z^t \otimes P_W$ . Then, the following upper bound holds

$$|\overline{gen}(P_{W|D_s,D_t}, P_{D_s}, P_{D_t})| \le \sqrt{2\sigma_s^2 \frac{I(W; D_t|D_s)}{m}} + c_s \frac{I(W; D_t|D_s)}{m}.$$
 (80)

### D Distribution-free Upper Bound on Generalization Error

**Theorem 4.** (restated) Suppose that the target training samples  $D_t = \{Z_j^t\}_{j=1}^m$  are i.i.d generated from the distribution  $P_Z^t$ , and the non-negative loss function  $\ell(W,Z)$  is  $\sigma_{\alpha}$ -sub-Gaussian under the distribution  $P_Z^t \otimes P_{W_{\alpha}}$ . If we further assume  $C_{\alpha} \leq \frac{L(W_{\alpha};D_t|D_s)}{I(W_{\alpha};D_t|D_s)}$  for some  $C_{\alpha} \geq 0$ , then for the  $\alpha$ -weighted Gibbs algorithm and  $0 < \alpha < 1$ ,

$$\overline{gen}_{\alpha}(P_{D_s}, P_{D_t}) \leq \frac{2\sigma_{\alpha}^2 \gamma \alpha}{(1 + C_{\alpha})m}.$$

*Proof.* By equation (26) in Theorem 3, we have

$$\overline{\operatorname{gen}}_{\alpha}(P_{D_s}, P_{D_t}) = \frac{I_{\text{SKL}}(W_{\alpha}; D_t | D_s)}{\gamma \alpha} \\
\leq \sqrt{\frac{2\sigma^2 I(W_{\alpha}; D_t | D_s)}{m}}.$$
(81)

As we have  $I(W_{\alpha}; D_t|D_s)(1+C_{\alpha}) \leq I_{SKL}(W_{\alpha}; D_t|D_s)$  in the assumption, the following upper bound holds:

$$\frac{I(W_{\alpha}; D_t|D_s)(1+C_{\alpha})}{\gamma \alpha} \le \sqrt{\frac{2\sigma_{\alpha}^2 I(W_{\alpha}; D_t|D_s)}{m}},\tag{82}$$

which implies that

$$I(W_{\alpha}; D_t | D_s) \le \frac{2\sigma_{\alpha}^2 \gamma^2 \alpha^2}{(1 + C_{\alpha})^2 m}.$$
(83)

Combining (83) with (81) completes the proof.

**Theorem 5.** (restated) Suppose that the target training samples  $D_t = \{Z_j^t\}_{j=1}^m$  are i.i.d generated from the distribution  $P_Z^t$ , and the non-negative loss function  $\ell(W_c, w_\phi, Z)$  is  $\sigma_\beta$ -sub-Gaussian under distribution  $P_Z^t \otimes P_{W_c^t|W_\phi=w_\phi}$  for all  $w_\phi \in \mathcal{W}_\phi$ . If we further assume  $C_\beta \leq \frac{L(W_c^t;D_t|W_\phi)}{I(W_c^t;D_t|W_\phi)}$  for some  $C_\beta \geq 0$ , then for the two-stage Gibbs algorithm,

$$P_{W_c^t|D_t,W_{\phi}}^{\gamma}(w_c^t|d_t,w_{\phi}) = \frac{\pi(w_c^t)e^{-\gamma L_E^{S_2}(w_{\phi},w_c^t,d_t)}}{V_{\beta}(w_{\phi},d_t,\gamma)},$$

we have

$$\overline{gen}_{\beta}(P_{D_s}, P_{D_t}) \le \frac{2\sigma_{\beta}^2 \gamma}{(1 + C_{\beta})m}.$$

*Proof.* Using Theorem 3 by considering  $W = (W_C^t, W_\phi)$ ,

$$|\overline{\operatorname{gen}}_{\beta}(P_{D_s}, P_{D_t})| \le \sqrt{\frac{2\sigma^2}{m}I(W_c^t, W_{\phi}; D_t|D_s)}.$$

Now, based on chain rule for mutual information we have

$$I(W_c^t, W_{\phi}; D_t | D_s) = I(W_{\phi}; D_t | D_s) + I(W_c^t; D_t | D_s, W_{\phi})$$
  
=  $I(W_c^t; D_t | W_{\phi})$ ,

where  $I(W_{\phi}; D_t | D_s) = 0$  due to the fact that  $W_{\phi}$  is independent from  $D_t$  given  $D_s$ , and  $I(W_c^t; D_t | W_{\phi}, D_s) = I(W_c^t; D_t | W_{\phi})$  since  $D_s \perp (W_c^t, D_t) | W_{\phi}$ .

Using Theorem 2, it can be shown that

$$\overline{\operatorname{gen}}_{\beta}(P_{D_s}, P_{D_t}) = \frac{I_{\text{SKL}}(D_t; W_c^t | W_{\phi})}{\gamma} \le \sqrt{\frac{2\sigma_{\beta}^2}{m}} I(W_c^t; D_t | W_{\phi}). \tag{84}$$

As we have  $I(W_c^t; D_t|W_\phi)(1+C_\beta) \leq I_{SKL}(W_c^t; D_t|W_\phi)$ , the following bound holds:

$$\frac{I(W_c^t; D_t|W_\phi)(1+C_\beta)}{\gamma} \le \sqrt{\frac{2\sigma_\beta I(W_c^t; D_t|W_\phi)}{m}},\tag{85}$$

which implies that

$$I(W_c^t; D_t|W_\phi) \le \frac{2\sigma_\beta^2 \gamma^2}{(1 + C_\beta)^2 m}.$$
(86)

Combining (86) with (84) completes the proof.

We could provide distribution-free upper bounds under sub-Exponential and sub-Gamma assumption using similar approach as in Theorem 4 and Theorem 5 for  $\alpha$ -weighted Gibbs algorithm and two-stage Gibbs algorithm, respectively.

sub-Exponential: For α-weighted Gibbs algorithm, we assume that the loss function is  $(\sigma_{\alpha,e}^2, b_{\alpha})$ -sub-Exponential under distribution  $P_Z^t \otimes P_{W_{\alpha}}$ . And for two-stage Gibbs algorithm, we assume that the loss function is  $(\sigma_{\beta,e}^2, b_{\beta})$ -sub-Exponential under distribution  $P_Z^t \otimes P_{W_c^t|W_{\phi}=w_{\phi}}$  for all  $w_{\phi} \in \mathcal{W}_{\phi}$ . We provide the results in Table 2. Denote  $B_{\alpha} \triangleq \lceil \frac{\gamma \alpha b_{\alpha}}{1+C_{\alpha}} \rceil$ ,  $B_{\beta} \triangleq \lceil \frac{\gamma b_{\beta}}{1+C_{\beta}} \rceil$ ,  $I_{\alpha} \triangleq \frac{2b_{\alpha}I(W_{\alpha};D_t|D_s)}{\sigma_{\alpha,e}^2}$  and  $I_{\beta} \triangleq \frac{2b_{\beta}I(W_c^t;D_t|W_{\phi})}{\sigma_{\beta,e}^2}$  in Table 2.

**sub-Gamma:** For  $\alpha$ -weighted Gibbs algorithm, we assume that the loss function is  $\Gamma(\sigma_{\alpha,s}^2, c_{\alpha,s})$ -sub-Gamma under distribution  $P_Z^t \otimes P_{W_{\alpha}}$  and  $m > \frac{\gamma \alpha c_{\alpha,s}}{(1+C_{\alpha})}$ . For two-stage Gibbs algorithm, we assume that the loss function is  $\Gamma(\sigma_{\beta,s}^2, c_{\beta,s})$ -sub-Gamma under distribution  $P_Z^t \otimes P_{W_c^t|W_{\phi}=w_{\phi}}$  for all  $w_{\phi} \in \mathcal{W}_{\phi}$  and  $m > \frac{\gamma c_{\beta,s}}{(1+C_{\beta})}$ . We provide the results in Table 2.

Table 2: Distribution-free Upper Bounds under different Tail Distributions.

	sub-Exponential		sub-Gamma
$\alpha$ -weighted Gibbs Algorithm	$\begin{cases} \frac{2\sigma_{\alpha,e}^2\gamma\alpha}{m(1+C_\alpha)},\\ \frac{\sigma_{\alpha,e}^2}{2b_\alpha}\Big(\frac{\gamma\alpha b_\alpha}{(m(1+C_\alpha)-\gamma\alpha b_\alpha)}+1\Big), \end{cases}$	$if \ m \ge I_{\alpha};$ $if \ B_{\alpha} < m < I_{\alpha}$	$\frac{2\sigma_{\alpha,s}^2\gamma\alpha}{(1+C_\alpha)m-\gamma\alpha c_{\alpha,s}}\left(1+\frac{\gamma\alpha c_{\alpha,s}}{(1+C_\alpha)m-\gamma\alpha c_{\alpha,s}}\right)$
Two-stage Gibbs Algorithm	$ \begin{pmatrix} \frac{2\sigma_{\beta,e}^2\gamma}{m(1+C_{\beta})}, & \\ \frac{\sigma_{\beta,e}^2}{2b_{\beta}} \left(\frac{\gamma b_{\beta}}{(m(1+C_E)-\gamma b_{\beta})} + 1\right), & \end{pmatrix} $	$if \ m \ge I_{\beta};$ $if \ B_{\beta} < m < I_{\beta}$	$\frac{2\sigma_{\beta,s}^2\gamma}{(1+C_{\beta})m-\gamma c_{\beta,s}} \left(1 + \frac{\gamma c_{\beta,s}}{(1+C_{\beta})m-\gamma c_{\beta,s}}\right)$

## E Exact Characterization of Generalization Error Based on Symmetrized KL divergence

We first present the following Lemma to prove the results related to symmetrized KL divergence.

**Lemma 3.** Denote the  $(\gamma, \pi(w), L_E(w, d_t))$ -Gibbs algorithm as  $P_{W|D_t}^{\gamma}$  and the  $(\gamma, \pi(w), L_P(w, P_{D_t}))$ -Gibbs algorithm as  $P_W^{\gamma, L_{P_{D_t}}}$ . Then, the following equality holds for these two Gibbs distributions with the same inverse temperature and prior distribution

$$\mathbb{E}_{\Delta(P_{W|D_{t}=d_{t}}^{\gamma}, P_{W}^{\gamma, L_{P_{D_{t}}}})}[L_{P}(W, P_{D_{t}}) - L_{E}(W, d_{t})] = \frac{D_{SKL}(P_{W|D_{t}=d_{t}}^{\gamma} \| P_{W}^{\gamma, L_{P_{D_{t}}}})}{\gamma}, \tag{87}$$

$$where \ \mathbb{E}_{\Delta(P_{W|D_t=d_t}^{\gamma},P_W^{\gamma,L_{P_{D_t}}})}[f(W)] = \mathbb{E}_{P_{W|D_t=d_t}^{\gamma}}[f(W)] - \mathbb{E}_{P_W^{\gamma,L_{P_{D_t}}}}[f(W)].$$

Proof.

$$D_{SKL}(P_{W|D_{t}=d_{t}}^{\gamma} \| P_{W}^{\gamma, L_{P_{D_{t}}}}) = \int_{\mathcal{W}} (P_{W|D_{t}=d_{t}}^{\gamma} - P_{W}^{\gamma, L_{P_{D_{t}}}}) \log \left( \frac{P_{W|D_{t}=d_{t}}^{\gamma}}{P_{W}^{\gamma, L_{P_{D_{t}}}}} \right) dw$$

$$= \int_{\mathcal{W}} (P_{W|D_{t}=d_{t}}^{\gamma} - P_{W}^{\gamma, L_{P_{D_{t}}}}) \log(e^{-\gamma(L_{E}(w, d_{t}) - L_{P}(w, P_{D_{t}}))}) dw$$

$$= \gamma \mathbb{E}_{\Delta(P_{W|D_{t}=d_{t}}^{\gamma, L_{P_{D_{t}}}})} [L_{P}(W, P_{D_{t}}) - L_{E}(W, d_{t})].$$

$$\square$$
(88)

Using Lemma 3, we provide different characterizations of  $\alpha$ -weighted Gibbs algorithm and two-stage Gibbs algorithm using symmetrized KL divergence.

#### E.1 $\alpha$ -weighted Gibbs Algorithm

**Theorem 6.** (restated) The expected transfer generalization error of the  $\alpha$ -weighted Gibbs algorithm in (10) is given by:

$$\overline{gen}_{\alpha}(P_{D_s}, P_{D_t}) = \frac{D_{\text{SKL}}(P_{W_{\alpha}|D_s, D_t}^{\gamma} || P_{W_{\alpha}|D_s}^{\gamma, L_{\alpha}(w_{\alpha}, d_s, P_{D_t})} || P_{D_s} P_{D_t})}{\gamma \alpha}, \tag{89}$$

where  $P_{W_{\alpha}|D_s}^{\gamma,L_{\alpha}(w_{\alpha},d_s,P_{D_t})}$  is the  $(\gamma,\pi(w_{\alpha}),L_{\alpha}(w_{\alpha},d_s,P_{D_t}))$ -Gibbs algorithm with  $L_{\alpha}(w,d_s,P_{D_t}) \triangleq \alpha L_P(w_{\alpha},P_{D_t}) + (1-\alpha)L_E(w_{\alpha},d_s)$ .

*Proof.* Applying Lemma 3 to the  $\alpha$ -weighted Gibbs algorithm and  $(\gamma, \pi(w_{\alpha}), L_{\alpha}(w, d_s, P_{D_t}))$ -Gibbs algorithm gives

$$\frac{D_{\text{SKL}}(P_{W_{\alpha}|D_{s}=d_{s},D_{t}=d_{t}}^{\gamma} \|P_{W_{\alpha}|D_{s}=d_{s}}^{\gamma,L_{\alpha}(w_{\alpha},d_{s},P_{D_{t}})})}{\gamma} \\
= \mathbb{E}_{\Delta\left(P_{W_{\alpha}|D_{s}=d_{s},D_{t}=d_{t}}^{\gamma},P_{W_{\alpha}|D_{s}=d_{s}}^{\gamma,L_{\alpha}(w_{\alpha},d_{s},P_{D_{t}})}\right)} \left[L_{\alpha}(W_{\alpha},d_{s},P_{D_{t}}) - L_{E}(W_{\alpha},d_{s},d_{t})\right] \\
= \alpha \mathbb{E}_{\Delta\left(P_{W_{\alpha}|D_{s}=d_{s},D_{t}=d_{t}}^{\gamma},P_{W_{\alpha}|D_{s}=d_{s}}^{\gamma,L_{\alpha}(w_{\alpha},d_{s},P_{D_{t}})}\right)} \left[L_{P}(W_{\alpha},P_{D_{t}}) - L_{E}(W_{\alpha},d_{t})\right].$$

Notice the fact that

$$\mathbb{E}_{P_{W_{\alpha}|D_s=d_s}^{\gamma,L_{\alpha}(w_{\alpha},d_s,P_{D_t})}}[L_P(W_{\alpha},P_{D_t})] = \mathbb{E}_{P_{D_t}}\big[\mathbb{E}_{P_{W_{\alpha}|D_s=d_s}^{\gamma,L_{\alpha}(w_{\alpha},d_s,P_{D_t})}}[L_E(W_{\alpha},D_t)]\big],$$

and taking expectation over  $D_s$  and  $D_t$ , we have

$$\begin{split} D_{\text{SKL}}(P_{W_{\alpha}|D_{s},D_{t}}^{\gamma}\|P_{W_{\alpha}|D_{s}}^{\gamma,L_{\alpha}(w_{\alpha},d_{s},P_{D_{t}})}|P_{D_{s}}P_{D_{t}}) &= \mathbb{E}_{P_{D_{s}}P_{D_{t}}}[D_{\text{SKL}}(P_{W_{\alpha}|d_{s},d_{t}}^{\gamma}\|P_{W_{\alpha}|d_{s}}^{\gamma,L_{\alpha}(w_{\alpha},d_{s},P_{D_{t}})})], \\ &= \gamma \alpha \overline{\text{gen}}_{\alpha}(P_{D_{s}},P_{D_{t}}). \end{split}$$

In the following, we provide an explanation for the existence of two different characterizations of the expected transfer generalization error, i.e., Theorem 6 and Theorem 1.

For an arbitrary conditional distribution on hypothesis space  $Q_{W_{\alpha}|D_s}$ , we can write

$$I(W_{\alpha}; D_t | D_s) = D(P_{W_{\alpha}, D_t | D_s} || Q_{W_{\alpha} | D_s} \otimes P_{D_t} | P_{D_s}) - D(P_{W_{\alpha} | D_s} || Q_{W_{\alpha} | D_s} || P_{D_s}), \tag{91}$$

$$L(W_{\alpha}; D_t | D_s) = \mathbb{E}_{P_{D_s}} \left[ \mathbb{E}_{P_{D_t} \otimes P_{W_{\alpha} | D_s}} [\log(Q_{W_{\alpha} | D_s} / P_{W_{\alpha} | D_t, D_s})] \right] + D(P_{W_{\alpha} | D_s} | Q_{W_{\alpha} | D_s} | P_{D_s}). \tag{92}$$

Thus, the symmetrized KL information can be written as

$$I_{SKL}(W_{\alpha}; D_{t}|D_{s}) = I(W_{\alpha}; D_{t}|D_{s}) + L(W_{\alpha}; D_{t}|D_{s})$$

$$= D(P_{W_{\alpha},D_{t}|D_{s}} \|Q_{W_{\alpha}|D_{s}} \otimes P_{D_{t}}|P_{D_{s}}) + \mathbb{E}_{P_{D_{s}}} [\mathbb{E}_{P_{D_{t}} \otimes P_{W_{\alpha}|D_{s}}} [\log(Q_{W_{\alpha}|D_{s}}/P_{W_{\alpha}|D_{t},D_{s}})]], \quad (93)$$

which holds for all  $Q_{W_{\alpha}|D_s}$ . We compare this expression with the following representation:

$$D(P_{W_{\alpha},D_{t}|D_{s}}||Q_{W_{\alpha}|D_{s}}\otimes P_{D_{t}}||P_{D_{s}}) + D(Q_{W_{\alpha}|D_{s}}\otimes P_{D_{t}}||P_{W_{\alpha},D_{t}|D_{s}}||P_{D_{s}}).$$
(94)

The difference between these two expressions is as follows:

$$I_{SKL}(W_{\alpha}; D_{t}|D_{s}) - \left(D(P_{W_{\alpha},D_{t}|D_{s}} \| Q_{W_{\alpha}|D_{s}} \otimes P_{D_{t}} | P_{D_{s}}) + D(Q_{W_{\alpha}|D_{s}} \otimes P_{D_{t}} \| P_{W_{\alpha},D_{t}|D_{s}} | P_{D_{s}})\right)$$

$$= \mathbb{E}_{P_{D_{s}}} \left[\mathbb{E}_{P_{D_{t}} \otimes P_{W_{\alpha}|D_{s}}} \left[\log(Q_{W_{\alpha}|D_{s}}/P_{W|D_{t},D_{s}})\right] - D(Q_{W_{\alpha}|D_{s}} \otimes P_{D_{t}} \| P_{W_{\alpha},D_{t}|D_{s}} | P_{D_{s}})\right]$$

$$= \mathbb{E}_{P_{D_{s}}} \left[\mathbb{E}_{P_{D_{t}} \otimes P_{W_{\alpha}|D_{s}}} \left[\log(Q_{W_{\alpha}|D_{s}}/P_{W_{\alpha}|D_{t},D_{s}})\right] - \mathbb{E}_{P_{D_{t}} \otimes Q_{W_{\alpha}|D_{s}}} \left[\log(Q_{W_{\alpha}|D_{s}}/P_{W_{\alpha}|D_{t},D_{s}})\right]\right]$$

$$= \mathbb{E}_{P_{D_{s}}} \left[\mathbb{E}_{\Delta(P_{W_{\alpha}|D_{s}},Q_{W_{\alpha}|D_{s}})} \left[\mathbb{E}_{P_{D_{t}}} \left[\log(Q_{W_{\alpha}|D_{s}}/P_{W_{\alpha}|D_{t},D_{s}})\right]\right]\right]. \tag{95}$$

Thus, if  $Q_{W_{\alpha}|D_s}$  satisfies the following condition

$$\mathbb{E}_{\Delta(P_{W_{\alpha}|D_{s}} - Q_{W_{\alpha}|D_{s}})}[\mathbb{E}_{P_{D_{t}}}[\log(Q_{W_{\alpha}|D_{s}}/P_{W_{\alpha}|D_{t},D_{s}})]] = 0, \tag{96}$$

then we have

$$I_{SKL}(W_{\alpha}; D_t) = D(P_{W_{\alpha}, D_t | D_s} || Q_{W_{\alpha} | D_s} \otimes P_{D_t} || P_{D_s}) + D(Q_{W_{\alpha} | D_s} \otimes P_{D_t} || P_{W_{\alpha}, D_t | D_s} || P_{D_s}). \tag{97}$$

Now, if we set  $(\gamma, \pi(w), L_E(w, d_s, d_t))$ -Gibbs algorithm as  $P_{W_{\alpha}|D_t,D_s}$ , then it can be verified that using  $(\gamma, \pi(w), L_{\alpha}(w_{\alpha}, d_s, P_{D_t}))$ -Gibbs algorithm as  $Q_{W_{\alpha}|D_s}$  would satisfy the condition in (96). Thus, we can represent the expected transfer generalization error using both symmetrized KL information and divergence.

#### E.2 Two-stage Gibbs Algorithm

**Theorem 7.** (restated) The expected transfer generalization error of the two-stage Gibbs algorithm in (12) is given by:

$$\overline{gen}_{\beta}(P_{D_s}, P_{D_t}) = \frac{D_{\text{SKL}}(P_{W_c^t|D_t, W_{\phi}}^{\gamma} \|P_{W_c^t|W_{\phi}}^{\gamma, L_P(w_{\phi}, w_c^t, P_{D_t})} | P_{D_t} P_{W_{\phi}})}{\gamma},$$

where  $P_{W_c^t|W_\phi}^{\gamma,L_P(w_\phi,w_c^t,P_{D_t})}$  is the  $(\gamma,\pi(w_c^t),L_P(w_\phi,w_c^t,P_{D_t}))$ -Gibbs algorithm.

*Proof.* Applying Lemma 3 to the two-stage Gibbs algorithm and  $(\gamma, \pi(w_c^t), L_P(w_\phi, w_c^t, P_{D_t}))$ -Gibbs algorithm, we have

$$\frac{D_{\text{SKL}}(P_{W_{c}^{t}|D_{t}=d_{t},W_{\phi}=w_{\phi}}^{\gamma} \|P_{W_{c}^{t}|W_{\phi}=w_{\phi}}^{\gamma,L_{P}(w_{\phi},W_{c}^{t},P_{D_{t}})})}{\gamma} \\
= \mathbb{E}_{\Delta\left(P_{W_{c}^{t}|D_{t}=d_{t},W_{\phi}=w_{\phi}}^{\gamma,L_{P}(w_{\phi},w_{c}^{t},P_{D_{t}})}\right)} \left[L_{P}(W_{c}^{t},w_{\phi},P_{D_{t}}) - L_{E}(W_{c}^{t},w_{\alpha},d_{t})\right].$$
(98)

Notice the fact that

$$\mathbb{E}_{P^{\gamma,L_{P}(w_{\phi},w_{c}^{t},P_{D_{t}})}_{W^{t}_{c}|W_{\phi}=w_{\phi}}}[L_{P}(W^{t}_{c},w_{\phi},P_{D_{t}})] = \mathbb{E}_{P_{D_{t}}}\big[\mathbb{E}_{P^{\gamma,L_{P}(w_{\phi},w_{c}^{t},P_{D_{t}})}_{W^{t}_{c}|W_{\phi}=w_{\phi}}}[L_{E}(W^{t}_{c},w_{\phi},d_{t})]\big],$$

and taking expectation over  $W_{\phi}$  and  $D_t$  completes the proof.

## F Asymptotic Behavior of Generalization Error for Gibbs Algorithm

We first provide a summary of different variables used in the Appendix F in Table 3.

Notation	Definition
$  W  _H^2$	$W^{\top}HW$
$\hat{W}_{\alpha}(D_s, D_t)$	$\operatorname{argmin}_{w \in \mathcal{W}} L_E(w, D_s, D_t)$
$\hat{W}_{\alpha}(D_s)$	$\operatorname{argmin}_{w \in \mathcal{W}} L_{\alpha}(w, D_s, P_{D_t})$
$\boldsymbol{w}_{\alpha}^{*}$	$\operatorname{argmin}_{\boldsymbol{w} \in \mathcal{W}} nD(P_Z^s    f(\cdot   \boldsymbol{w})) + mD(P_Z^t    f(\cdot   \boldsymbol{w}))$
$\hat{W}_c^t(D_t, W_\phi)$	$\operatorname{argmin}_{w_c \in \mathcal{W}_c} L_E^{S2}(W_{\phi}, w_c, D_t)$
$\hat{W}_c^t(W_\phi)$	$\arg\min_{w_c \in \mathcal{W}_c} L_P(W_\phi, w_c, P_{D_t})$
$[oldsymbol{w}_{\phi}^{s*}, oldsymbol{w}_{c}^{s*}]$	$rg \min_{[oldsymbol{w}_{\phi}, oldsymbol{w}_c] \in \mathcal{W}} D(P_{Z^s} \  f(\cdot   oldsymbol{w}_{\phi}, oldsymbol{w}_c))$
$oldsymbol{w}_c^{st*}$	$\arg\min_{\boldsymbol{w}_c \in \mathcal{W}_c} D(P_{Z^t} \  f(\cdot   \boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_c))$

Table 3: Notations and Definitions

#### F.1 Generalization Error

**Proposition 1.** (restated) If the Hessian matrices  $H^*(D_s, D_t) = H^*(D_s) = H^*$  are independent of  $D_s$  and  $D_t$ , then the generalization error of the  $\alpha$ -weighted-ERM algorithm is

$$\overline{gen}_{\alpha}(P_{D_t},P_{D_s}) = \frac{\mathbb{E}_{P_{D_s,D_t}}[\|\hat{W}_{\alpha}(D_s,D_t) - \hat{W}_{\alpha}(D_s)\|_{H^*}^2]}{\alpha}.$$

*Proof.* It is shown in Hwang (1980) that if the following Hessian matrices

$$H^*(D_s, D_t) \triangleq \nabla_w^2 L_E(w, D_s, D_t) \big|_{w = \hat{W}_{\alpha}(D_s, D_t)}, \tag{99}$$

$$H^*(D_s) \triangleq \nabla_w^2 L_\alpha(w, D_s, P_{D_t})\big|_{w=\hat{W}_\alpha(D_s)} \tag{100}$$

are not singular, then, as  $\gamma \to \infty$ 

$$P_{W_{\alpha}|D_{s},D_{t}}^{\gamma} \to \mathcal{N}(\hat{W}_{\alpha}(D_{s},D_{t}), \frac{1}{\gamma}H^{*}(D_{s},D_{t})^{-1}),$$
and 
$$P_{W_{\alpha}|D_{s}}^{\gamma,L_{\alpha}} \to \mathcal{N}(\hat{W}_{\alpha}(D_{s}), \frac{1}{\gamma}H^{*}(D_{s})^{-1}),$$
(101)

and we use  $P_{W_\alpha|D_s}^{\gamma,L_\alpha}$  to denote  $P_{W_\alpha|D_s}^{\gamma,L_\alpha(w_\alpha,d_s,P_{D_t})}$ 

Thus, the conditional symmetrized KL divergence in Theorem 6 can be evaluated directly using Gaussian ap-

proximations under the assumption that  $H^*(D_s, D_t) = H^*(D_s) = H^*$ ,

$$D_{SKL}(P_{W_{\alpha}|D_{s},D_{t}}^{\gamma}||P_{W_{\alpha}|D_{s}}^{\gamma,L_{\alpha}}|P_{D_{s}}P_{D_{t}})$$

$$= \mathbb{E}_{P_{D_{t},D_{s}}} \left[ \mathbb{E}_{P_{W_{\alpha}|D_{s},D_{t}}} \left[ \log \frac{P_{W_{\alpha}|D_{s},D_{t}}^{\gamma}}{P_{W_{\alpha}|D_{s}}^{\gamma,L_{\alpha}}} \right] - \mathbb{E}_{P_{W_{\alpha}|D_{s}}^{\gamma,L_{\alpha}}} \left[ \log \frac{P_{W_{\alpha}|D_{s},D_{t}}^{\gamma}}{P_{W_{\alpha}|D_{s}}^{\gamma,L_{\alpha}}} \right] \right]$$

$$= \mathbb{E}_{P_{D_{t},D_{s}}} \left[ \mathbb{E}_{\Delta(P_{W_{\alpha}|D_{s},D_{t}}^{\gamma},P_{W_{\alpha}|D_{s}}^{\gamma,L_{\alpha}})} \left[ -\frac{\gamma}{2} (W_{\alpha} - \hat{W}_{\alpha}(D_{s},D_{t}))^{\top} H^{*}(W_{\alpha} - \hat{W}_{\alpha}(D_{s},D_{t})) + \frac{\gamma}{2} (W_{\alpha} - \hat{W}_{\alpha}(D_{s}))^{\top} H^{*}(W_{\alpha} - \hat{W}_{\alpha}(D_{s})) \right] \right]$$

$$= \gamma \mathbb{E}_{P_{D_{t},D_{s}}} \left[ \mathbb{E}_{\Delta(P_{W_{\alpha}|D_{s},D_{t}}^{\gamma},P_{W_{\alpha}|D_{s}}^{\gamma,L_{\alpha}})} \left[ W_{\alpha}^{\top} H^{*} \hat{W}_{\alpha}(D_{s},D_{t}) - W_{\alpha}^{\top} H^{*} \hat{W}_{\alpha}(D_{s}) \right] \right]$$

$$= \gamma \mathbb{E}_{P_{D_{t},D_{s}}} \left[ \hat{W}_{\alpha}(D_{s},D_{t})^{\top} H^{*} \hat{W}_{\alpha}(D_{s},D_{t}) - \hat{W}_{\alpha}(D_{s})^{\top} H^{*} \hat{W}_{\alpha}(D_{s}) \right]$$

$$= \gamma \mathbb{E}_{P_{D_{t},D_{s}}} \left[ (\hat{W}_{\alpha}(D_{s},D_{t}) - \hat{W}_{\alpha}(D_{s}))^{\top} H^{*} (\hat{W}_{\alpha}(D_{s},D_{t}) - \hat{W}_{\alpha}(D_{s})) \right]. \tag{102}$$

Thus,

$$\overline{\operatorname{gen}}_{\alpha}(P_{D_s}, P_{D_t}) = \frac{D_{\operatorname{SKL}}(P_{W_{\alpha}|D_s,D_t}^{\gamma} \| P_{W_{\alpha}|D_s}^{\gamma,L_{\alpha}} | P_{D_s} P_{D_t})}{\gamma \alpha} = \frac{\mathbb{E}_{P_{D_s,D_t}}[\| \hat{W}_{\alpha}(D_s, D_t) - \hat{W}_{\alpha}(D_s) \|_{H^*}^2]}{\alpha}.$$

**Proposition 2.** (restated) If Hessian matrices  $H_c^*(D_t, W_\phi) = H_c^*(W_\phi) = H_c^*$  are independent of  $D_s, D_t$ , then the generalization error of the two-stage-ERM algorithm is

$$\overline{gen}_{\beta}(P_{D_t}, P_{D_s}) = \mathbb{E}_{D_s, D_t, W_{\phi}}[\|\hat{W}_c^t(D_t, W_{\phi}) - \hat{W}_c^t(W_{\phi})\|_{H^*}^2].$$

*Proof.* It is shown in Hwang (1980) that if the following Hessian matrices

$$H_c^*(D_t, W_\phi) \triangleq \nabla_{w_c}^2 L_E^{S2}(W_\phi, w_c, D_t) \Big|_{w_c = \hat{W}_c^t(D_t, W_\phi)}$$
(103)

$$H_c^*(W_\phi) \triangleq \nabla_{w_c}^2 L_P(W_\phi, w_c, P_{D_t})\big|_{w_c = \hat{W}_c^t(W_\phi)}$$
 (104)

are not singular, then, as  $\gamma \to \infty$ 

$$P_{W_c^t|D_t,W_{\phi}}^{\gamma} \to \mathcal{N}(\hat{W}_c^t(D_t,W_{\phi}), \frac{1}{\gamma}H_c^*(D_t,W_{\phi})^{-1}),$$

$$P_{W_c^t|W_{\phi}}^{\gamma,L_P} \to \mathcal{N}(\hat{W}_c^t(W_{\phi}), \frac{1}{\gamma}H^*(D_s)^{-1}),$$
(105)

where we use  $P_{W_c^t|W_{\phi}}^{\gamma,L_P}$  to denote  $P_{W_c^t|W_{\phi}}^{\gamma,L_P(w_{\phi},w_c^t,P_{D_t})}$ . Thus, the conditional symmetrized KL divergence in Theorem 7 can be evaluated directly using Gaussian approximations under the assumption that  $H_c^*(D_t,W_{\phi})=H_c^*(W_{\phi})=H_c^*$ .

$$\begin{split} &D_{\text{SKL}}(P_{W_{c}^{l}|D_{t},W_{\phi}}^{\gamma}\|P_{W_{c}^{l}|W_{\phi}}^{\gamma,L_{P}}|P_{D_{t}}P_{W_{\phi}}) \\ &= \mathbb{E}_{P_{D_{t},W_{\phi}}} \left[ \mathbb{E}_{P_{W_{c}^{l}|D_{t},W_{\phi}}} \left[ \log \frac{P_{W_{c}^{l}|D_{t},W_{\phi}}^{\gamma}}{P_{W_{c}^{l}|W_{\phi}}^{\gamma,L_{P}}} \right] - \mathbb{E}_{P_{W_{c}^{l}|W_{\phi}}^{\gamma,L_{P}}} \left[ \log \frac{P_{W_{c}^{l}|D_{t},W_{\phi}}^{\gamma}}{P_{W_{c}^{l}|W_{\phi}}^{\gamma,L_{P}}} \right] \right] \\ &= \mathbb{E}_{P_{D_{t},W_{\phi}}} \left[ \mathbb{E}_{\Delta(P_{W_{c}^{l}|D_{t},W_{\phi}}^{\gamma},P_{W_{c}^{l}|W_{\phi}}^{\gamma,L_{P}})} \left[ -\frac{\gamma}{2} (W_{c}^{t} - \hat{W}_{c}^{t}(D_{t},W_{\phi}))^{\top} H_{c}^{*} (W_{c}^{t} - \hat{W}_{c}^{t}(D_{t},W_{\phi})) \right] \\ &+ \frac{\gamma}{2} (W_{c}^{t} - \hat{W}_{c}^{t}(W_{\phi}))^{\top} H_{c}^{*} (W_{c}^{t} - \hat{W}_{c}^{t}(W_{\phi})) \right] \right] \\ &= \gamma \mathbb{E}_{P_{D_{t},W_{\phi}}} \left[ \mathbb{E}_{\Delta(P_{W_{c}^{l}|D_{t},W_{\phi}}^{\gamma},P_{W_{c}^{l}|W_{\phi}}^{\gamma,L_{P}})} \left[ (W_{c}^{t})^{\top} H_{c}^{*} \hat{W}_{c}^{t}(D_{t},W_{\phi}) - (W_{c}^{t})^{\top} H_{c}^{*} \hat{W}_{c}^{t}(W_{\phi}) \right] \right] \\ &= \gamma \mathbb{E}_{P_{D_{t},W_{\phi}}} \left[ \hat{W}_{c}^{t}(D_{t},W_{\phi})^{\top} H_{c}^{*} \hat{W}_{c}^{t}(D_{t},W_{\phi}) - \hat{W}_{c}^{t}(D_{t},W_{\phi})^{\top} H_{c}^{*} \hat{W}_{c}^{t}(W_{\phi}) \right] \\ &= \gamma \mathbb{E}_{P_{D_{t},W_{\phi}}} \left[ (\hat{W}_{c}^{t}(D_{t},W_{\phi}) - \hat{W}_{c}^{t}(W_{\phi}))^{\top} H_{c}^{*} (\hat{W}_{c}^{t}(D_{t},W_{\phi}) - \hat{W}_{c}^{t}(W_{\phi})) \right]. \end{split}$$

Thus,

$$\overline{\operatorname{gen}}_{\beta}(P_{D_{t}}, P_{D_{s}}) = \frac{D_{\operatorname{SKL}}(P_{W_{c}^{t}|D_{t}, W_{\phi}}^{\gamma} \|P_{W_{c}^{t}|W_{\phi}}^{\gamma, L_{P}} | P_{D_{t}} P_{W_{\phi}})}{\gamma} = \mathbb{E}_{D_{t}, W_{\phi}}[\|\hat{W}_{c}^{t}(D_{t}, W_{\phi}) - \hat{W}_{c}^{t}(W_{\phi})\|_{H_{c}^{*}}^{2}]. \qquad \Box$$

#### F.2 Regularity Conditions for MLE

In this section, we present the regularity conditions required by the asymptotic normality (Van der Vaart, 2000) of maximum likelihood estimates.

#### Assumption 1. Regularity Conditions for MLE:

- 1.  $f(z|\mathbf{w}) \neq f(z|\mathbf{w}')$  for  $\mathbf{w} \neq \mathbf{w}'$ .
- 2. W is an open subset of  $\mathbb{R}^d$ .
- 3. The function  $\log f(z|\mathbf{w})$  is three times continuously differentiable with respect to  $\mathbf{w}$ .
- 4. There exist functions  $F_1(z): \mathcal{Z} \to \mathbb{R}$ ,  $F_2(z): \mathcal{Z} \to \mathbb{R}$  and  $M(z): \mathcal{Z} \to \mathbb{R}$ , such that

$$\mathbb{E}_{Z \sim f(z|\boldsymbol{w})}[M(Z)] < \infty,$$

and the following inequalities hold for any  $\mathbf{w} \in \mathcal{W}$ ,

$$\left| \frac{\partial \log f(z|\boldsymbol{w})}{\partial w_i} \right| < F_1(z), \qquad \left| \frac{\partial^2 \log f(z|\boldsymbol{w})}{\partial w_i \partial w_j} \right| < F_1(z),$$

$$\left| \frac{\partial^3 \log f(z|\boldsymbol{w})}{\partial w_i \partial w_j \partial w_k} \right| < M(z), \qquad i, j, k = 1, 2, \dots, d.$$

5. The following inequality holds for an arbitrary  $\mathbf{w} \in \mathcal{W}$ ,

$$0 < \mathbb{E}_{Z \sim f(z|\boldsymbol{w})} \left[ \frac{\partial \log f(z|\boldsymbol{w})}{\partial w_i} \frac{\partial \log f(z|\boldsymbol{w})}{\partial w_j} \right] < \infty, \quad i, j = 1, 2, \cdots, d.$$

#### F.3 Generalization error in MLE

 $\alpha$ -weighted ERM: We use the following notations to denote the expectation of the Hessian matrices and the Fisher information matrices,

$$J_{s}(\boldsymbol{w}_{\alpha}) \triangleq \mathbb{E}_{P_{Z}^{s}} \left[ -\nabla_{\boldsymbol{w}_{\alpha}}^{2} \log f(Z|\boldsymbol{w}_{\alpha}) \right], \quad J_{t}(\boldsymbol{w}_{\alpha}) \triangleq \mathbb{E}_{P_{Z}^{t}} \left[ -\nabla_{\boldsymbol{w}_{\alpha}}^{2} \log f(Z|\boldsymbol{w}_{\alpha}) \right],$$

$$\mathcal{I}_{s}(\boldsymbol{w}_{\alpha}) \triangleq \mathbb{E}_{P_{Z}^{s}} \left[ \nabla_{\boldsymbol{w}_{\alpha}} \log f(Z|\boldsymbol{w}_{\alpha}) \nabla_{\boldsymbol{w}_{\alpha}} \log f(Z|\boldsymbol{w}_{\alpha})^{\top} \right], \quad \mathcal{I}_{t}(\boldsymbol{w}_{\alpha}) \triangleq \mathbb{E}_{P_{Z}^{t}} \left[ \nabla_{\boldsymbol{w}_{\alpha}} \log f(Z|\boldsymbol{w}_{\alpha}) \nabla_{\boldsymbol{w}_{\alpha}} \log f(Z|\boldsymbol{w}_{\alpha})^{\top} \right],$$

$$\bar{J}(\boldsymbol{w}_{\alpha}) = \frac{n}{m+n} J_{s}(\boldsymbol{w}_{\alpha}) + \frac{m}{m+n} J_{t}(\boldsymbol{w}_{\alpha}), \quad \bar{\mathcal{I}}(\boldsymbol{w}_{\alpha}) = \frac{n}{m+n} \mathcal{I}_{s}(\boldsymbol{w}_{\alpha}) + \frac{m}{m+n} \mathcal{I}_{t}(\boldsymbol{w}_{\alpha}).$$

**Lemma 4.** Under Assumption 1, for any fixed source samples  $d_s$ , if we let  $m \to \infty$ , then the  $\alpha$ -weighted ERM satisfies

$$\sqrt{m} (\hat{W}_{\alpha}(d_s, D_t) - \hat{W}_{\alpha}(d_s)) \to \mathcal{N}(0, \alpha^2 \tilde{J}(\hat{W}_{\alpha}(d_s))^{-1} \mathcal{I}_t(\hat{W}_{\alpha}(d_s)) \tilde{J}(\hat{W}_{\alpha}(d_s))^{-1}), \tag{107}$$

where  $\widetilde{J}(\hat{W}_{\alpha}(d_s)) \triangleq \alpha J_t(\hat{W}_{\alpha}(d_s)) + (1 - \alpha) \nabla_w^2 L_E(w, d_s) \big|_{w = \hat{W}_{\alpha}(d_s)}$ , and  $\mathcal{I}_t(\hat{W}_{\alpha}(d_s))$  is the covariance matrix of  $\nabla_w \log f(Z^t | \hat{W}_{\alpha}(d_s))$ .

*Proof.* By using a Taylor expansion of the first derivative of the weighted log-likelihood  $L_E(\hat{W}_{\alpha}(d_s, D_t), d_s, D_t)$  around  $\hat{W}_{\alpha}(d_s)$ , we obtain

$$0 = \nabla_w L_E(w, d_s, D_t) \big|_{w = \hat{W}_{\alpha}(d_s, D_t)}$$

$$\approx \nabla_w L_E(w, d_s, D_t) \big|_{w = \hat{W}_{\alpha}(d_s)} + \nabla_w^2 L_E(w, d_s, D_t) \big|_{w = \hat{W}_{\alpha}(d_s)} (\hat{W}_{\alpha}(d_s, D_t) - \hat{W}_{\alpha}(d_s)).$$
(108)

From the Taylor series expansion formula, the following approximation can be obtained

$$-\nabla_{w}^{2} L_{E}(w, d_{s}, D_{t})\big|_{w = \hat{W}_{\alpha}(d_{s})} (\hat{W}_{\alpha}(d_{s}, D_{t}) - \hat{W}_{\alpha}(d_{s})) \approx \nabla_{w} L_{E}(w, d_{s}, D_{t})\big|_{w = \hat{W}_{\alpha}(d_{s})}.$$
(109)

By the law of large numbers, when  $m \to \infty$ , it can be shown that

$$-\nabla_w^2 L_E(\hat{W}_{\alpha}(d_s), D_t) = \frac{1}{m} \sum_{i=1}^m \nabla_w^2 \log f(Z_i^t | \hat{W}_{\alpha}(d_s)) \to -J_t(\hat{W}_{\alpha}(d_s)).$$
 (110)

Thus, the LHS of (109) can be written as

$$\nabla_{w}^{2} L_{E}(w, d_{s}, D_{t}) \Big|_{w = \hat{W}_{\alpha}(d_{s})} = \nabla_{w}^{2} \left[ \alpha L_{E}(w, D_{t}) + (1 - \alpha) L_{E}(w, d_{s}) \right] \Big|_{w = \hat{W}_{\alpha}(d_{s})} \to \widetilde{J}(\hat{W}_{\alpha}(d_{s})), \tag{111}$$

where  $\widetilde{J}(\hat{W}_{\alpha}(d_s)) = \alpha J_t(\hat{W}_{\alpha}(d_s)) + (1 - \alpha) \nabla_w^2 L_E(w, d_s) \Big|_{w = \hat{W}_{\alpha}(d_s)}$ .

As for the RHS of (109), note that

$$\sqrt{m}\nabla_w L_E(w, D_t)\big|_{w=\hat{W}_\alpha(d_s)} = -\frac{1}{\sqrt{m}} \sum_{i=1}^m \nabla_w \log f(Z_i^t | \hat{W}_\alpha(d_s)), \tag{112}$$

by multivariate central limit theorem

$$\frac{1}{\sqrt{m}} \sum_{i=1}^{n} \left( -\nabla_w \log f(Z_i^t | \hat{W}_{\alpha}(d_s)) + \mathbb{E}_{Z^t} [\nabla_w \log f(Z^t | \hat{W}_{\alpha}(d_s))] \right) \to \mathcal{N}(0, \mathcal{I}_t(\hat{W}_{\alpha}(d_s))), \tag{113}$$

where  $\mathcal{I}_t(\hat{W}_{\alpha}(d_s))$  is the covariance matrix of  $\nabla_w \log f(Z^t | \hat{W}_{\alpha}(d_s))$ .

Due to the definition of  $\hat{W}_{\alpha}(d_s)$ , we have  $\nabla_w L_E(w, d_s, P_{D_t})\big|_{w=\hat{W}_{\alpha}(d_s)} = 0$ , i.e.,

$$(1 - \alpha)\nabla_w L_E(\hat{W}_\alpha(d_s), d_s) = \alpha \mathbb{E}_{Z^t}[\nabla_w \log f(Z^t | \hat{W}_\alpha(d_s))]. \tag{114}$$

Thus, the RHS of (109) will converge to

$$\sqrt{m}\nabla_w L_E(w, D_s, D_t)\big|_{w=\hat{W}_\alpha(D_s)} \to \mathcal{N}\big(0, \alpha^2 \mathcal{I}_t(\hat{W}_\alpha(d_s))\big). \tag{115}$$

Combining with (110), when  $m \to \infty$ , we obtain

$$\sqrt{m} (\hat{W}_{\alpha}(d_s, D_t) - \hat{W}_{\alpha}(d_s)) \to \mathcal{N}(0, \alpha^2 \tilde{J}(\hat{W}_{\alpha}(d_s))^{-1} \mathcal{I}_t(\hat{W}_{\alpha}(d_s)) \tilde{J}(\hat{W}_{\alpha}(d_s))^{-1}). \tag{116}$$

In the main body of the paper, we further let  $n \to \infty$ , then  $\hat{W}_{\alpha}(d_s) \to \boldsymbol{w}_{\alpha}^*$ , and  $\tilde{J}(\hat{W}_{\alpha}(d_s)) \to \bar{J}(\boldsymbol{w}_{\alpha}^*)$ ,  $\mathcal{I}_t(\hat{W}_{\alpha}(d_s)) \to \mathcal{I}_t(\boldsymbol{w}_{\alpha}^*)$ . For  $\alpha = \frac{m}{m+n}$ , using Lemma 4, we can show that

$$\hat{W}_{\alpha}(D_s, D_t) - \hat{W}_{\alpha}(D_s) \to \mathcal{N}\left(0, \frac{m}{(m+n)^2} \bar{J}(\boldsymbol{w}_{\alpha}^*)^{-1} \mathcal{I}_t(\boldsymbol{w}_{\alpha}^*) \bar{J}(\boldsymbol{w}_{\alpha}^*)^{-1}\right). \tag{117}$$

In addition, the Hessian matrix  $H^*(D_s, D_t) \to \bar{J}(\boldsymbol{w}_{\alpha}^*)$  as  $m, n \to \infty$ , which is independent of the samples  $D_s, D_t$ . Proposition 1 gives

$$\overline{\operatorname{gen}}_{\alpha}(P_{D_t}, P_{D_s}) = \frac{\operatorname{tr}(\mathcal{I}_t(\boldsymbol{w}_{\alpha}^*) \bar{J}(\boldsymbol{w}_{\alpha}^*)^{-1})}{n+m} = \mathcal{O}(\frac{d}{m+n}).$$

#### Two-stage ERM:

We use the following notations to denote the expectation of the Hessian matrix and the Fisher information matrix with respect to  $w_c$ ,

$$J_c^t(\boldsymbol{w}_{\phi}, \boldsymbol{w}_c) \triangleq \mathbb{E}_{P_Z^t} \left[ -\nabla_{\boldsymbol{w}_c}^2 \log f(Z|[\boldsymbol{w}_{\phi}, \boldsymbol{w}_c]) \right],$$
  
$$\mathcal{I}_c^t(\boldsymbol{w}_{\phi}, \boldsymbol{w}_c) \triangleq \mathbb{E}_{P_Z^t} \left[ \nabla_{\boldsymbol{w}_c} \log f(Z|[\boldsymbol{w}_{\phi}, \boldsymbol{w}_c)]) \nabla_{\boldsymbol{w}_c}^{\top} \log f(Z|[\boldsymbol{w}_{\phi}, \boldsymbol{w}_c]) \right].$$

**Lemma 5.** Under Assumption 1, for any fixed  $\hat{\mathbf{w}}_{\phi}$ , if we let  $m \to \infty$ , then the two-stage ERM satisfies

$$\sqrt{m} \left( (\hat{W}_c^t(D_t, \hat{\boldsymbol{w}}_{\phi}) - \hat{\boldsymbol{w}}_c^t(\hat{\boldsymbol{w}}_{\phi})) \right) \to \mathcal{N} \left( 0, J_c^t(\hat{\boldsymbol{w}}_{\phi}, \hat{\boldsymbol{w}}_c^t(\hat{\boldsymbol{w}}_{\phi}))^{-1} \mathcal{I}_c^t(\hat{\boldsymbol{w}}_{\phi}, \hat{\boldsymbol{w}}_c^t(\hat{\boldsymbol{w}}_{\phi})) J_c^t(\hat{\boldsymbol{w}}_{\phi}, \hat{\boldsymbol{w}}_c^t(\hat{\boldsymbol{w}}_{\phi}))^{-1} \right). \tag{118}$$

*Proof.* For any fixed  $\hat{\boldsymbol{w}}_{\phi}$ , using a Taylor expansion of the gradient with respect to  $\boldsymbol{w}_{c}$  of the log-likelihood  $L_{E}^{S2}(\hat{\boldsymbol{w}}_{\phi}, \hat{W}_{c}^{t}(D_{t}, \hat{\boldsymbol{w}}_{\phi}), D_{t})$  around  $\hat{\boldsymbol{w}}_{c}^{t}(\hat{\boldsymbol{w}}_{\phi})$ , we obtain

$$0 = \nabla_{\boldsymbol{w}_{c}} L_{E}^{S2}(\hat{\boldsymbol{w}}_{\phi}, \hat{W}_{c}^{t}(D_{t}, \hat{\boldsymbol{w}}_{\phi}), D_{t})$$

$$\approx \nabla_{\boldsymbol{w}_{c}} L_{E}^{S2}(\hat{\boldsymbol{w}}_{\phi}, \hat{\boldsymbol{w}}_{c}^{t}(\hat{\boldsymbol{w}}_{\phi}), D_{t}) + \nabla_{\boldsymbol{w}_{c}}^{2} L_{E}^{S2}(\hat{\boldsymbol{w}}_{\phi}, \hat{\boldsymbol{w}}_{c}^{t}(\hat{\boldsymbol{w}}_{\phi}), D_{t}) (\hat{W}_{c}^{t}(D_{t}, \hat{\boldsymbol{w}}_{\phi}) - \hat{\boldsymbol{w}}_{c}^{t}(\hat{\boldsymbol{w}}_{\phi})).$$

From the Taylor series expansion formula, the following approximation can be obtained

$$-\nabla_{\boldsymbol{w}_{c}}^{2} L_{E}^{S2}(\hat{\boldsymbol{w}}_{\phi}, \hat{\boldsymbol{w}}_{c}^{t}(\hat{\boldsymbol{w}}_{\phi}), D_{t})(\hat{W}_{c}^{t}(D_{t}, \hat{\boldsymbol{w}}_{\phi}) - \hat{\boldsymbol{w}}_{c}^{t}(\hat{\boldsymbol{w}}_{\phi})) \approx \nabla_{\boldsymbol{w}_{c}} L_{E}^{S2}(\hat{\boldsymbol{w}}_{\phi}, \hat{\boldsymbol{w}}_{c}^{t}(\hat{\boldsymbol{w}}_{\phi}), D_{t}). \tag{119}$$

By the law of large numbers, when  $m \to \infty$ , it can be shown that

$$-\nabla_{\boldsymbol{w}_{c}}^{2} L_{E}^{S2}(\hat{\boldsymbol{w}}_{\phi}, \hat{\boldsymbol{w}}_{c}^{t}(\hat{\boldsymbol{w}}_{\phi}), D_{t}) = \frac{1}{m} \sum_{i=1}^{m} \nabla_{\boldsymbol{w}_{c}}^{2} \log f(Z_{i}^{t} | [\hat{\boldsymbol{w}}_{\phi}, \hat{\boldsymbol{w}}_{c}^{t}(\hat{\boldsymbol{w}}_{\phi})]) \to -J_{c}^{t}(\hat{\boldsymbol{w}}_{\phi}, \hat{\boldsymbol{w}}_{c}^{t}(\hat{\boldsymbol{w}}_{\phi})).$$
(120)

As for the RHS of (119), note that  $\mathbb{E}_{P_Z^t}[\nabla_{\boldsymbol{w}_c} \log f(Z|[\hat{\boldsymbol{w}}_{\phi}, \hat{\boldsymbol{w}}_c^t(\hat{\boldsymbol{w}}_{\phi})])] = 0$  due to the definition of  $\hat{\boldsymbol{w}}_c^t(\hat{\boldsymbol{w}}_{\phi})$ , by multivariate central limit theorem, we have

$$\frac{1}{\sqrt{m}} \sum_{i=1}^{n} \left( -\nabla_{\boldsymbol{w}_c} \log f(Z_i^t | [\hat{\boldsymbol{w}}_{\phi}, \hat{\boldsymbol{w}}_c^t(\hat{\boldsymbol{w}}_{\phi})]) \right) \to \mathcal{N}(0, \mathcal{I}_c^t(\hat{\boldsymbol{w}}_{\phi}, \hat{\boldsymbol{w}}_c^t(\hat{\boldsymbol{w}}_{\phi}))), \tag{121}$$

where  $\mathcal{I}_c^t(\hat{\boldsymbol{w}}_{\phi}, \hat{\boldsymbol{w}}_c^t(\hat{\boldsymbol{w}}_{\phi})) = \mathbb{E}_{P_Z^t}[\nabla_{\boldsymbol{w}_c} \log f(Z|[\hat{\boldsymbol{w}}_{\phi}, \hat{\boldsymbol{w}}_c^t(\hat{\boldsymbol{w}}_{\phi})])\nabla_{\boldsymbol{w}_c}^{\top} \log f(Z|[\hat{\boldsymbol{w}}_{\phi}, \hat{\boldsymbol{w}}_c^t(\hat{\boldsymbol{w}}_{\phi})])].$ 

Thus, the RHS of (119) will converge to

$$\sqrt{m}\nabla_{\boldsymbol{w}_{c}}L_{E}^{S2}(\hat{\boldsymbol{w}}_{\phi},\boldsymbol{w}_{c},D_{t})\big|_{\boldsymbol{w}_{c}=\hat{\boldsymbol{w}}_{c}^{t}(\hat{\boldsymbol{w}}_{\phi})} \to \mathcal{N}\big(0,\mathcal{I}_{c}^{t}(\hat{\boldsymbol{w}}_{\phi},\hat{\boldsymbol{w}}_{c}^{t}(\hat{\boldsymbol{w}}_{\phi}))\big). \tag{122}$$

When  $m \to \infty$ , we obtain

$$\sqrt{m} \left( (\hat{W}_c^t(D_t, \hat{\boldsymbol{w}}_{\phi}) - \hat{\boldsymbol{w}}_c^t(\hat{\boldsymbol{w}}_{\phi})) \right) \to \mathcal{N} \left( 0, J_c^t(\hat{\boldsymbol{w}}_{\phi}, \hat{\boldsymbol{w}}_c^t(\hat{\boldsymbol{w}}_{\phi}))^{-1} \mathcal{I}_c^t(\hat{\boldsymbol{w}}_{\phi}, \hat{\boldsymbol{w}}_c^t(\hat{\boldsymbol{w}}_{\phi})) J_c^t(\hat{\boldsymbol{w}}_{\phi}, \hat{\boldsymbol{w}}_c^t(\hat{\boldsymbol{w}}_{\phi}))^{-1} \right). \tag{123}$$

In the main body of the paper, we further let  $n \to \infty$ , then  $\hat{\boldsymbol{w}}_{\phi} \to \boldsymbol{w}_{\phi}^{s*}$ , and  $\hat{\boldsymbol{w}}_{c}^{t}(\hat{\boldsymbol{w}}_{\phi}) \to \boldsymbol{w}_{c}^{s**}$ . Using Lemma 5, we can show that

$$\hat{W}_{c}^{t}(D_{t}, \hat{W}_{\phi}) - \hat{W}_{c}^{t}(\hat{W}_{\phi}) \to \mathcal{N}\left(0, \frac{J_{c}^{t}(\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_{c}^{st*})^{-1}\mathcal{I}_{c}^{t}(\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_{c}^{st*})J_{c}^{t}(\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_{c}^{st*})^{-1}}{m}\right).$$

As the Hessian matrix  $H_c^*(D_t, W_\phi) = H_c^*(W_\phi) \to J_c^t(\boldsymbol{w}_\phi^{s*}, \boldsymbol{w}_c^{s**})$  as  $m, n \to \infty$ . By Proposition 2, we have

$$\overline{\operatorname{gen}}_{\beta}(P_{D_t}, P_{D_s}) = \frac{\operatorname{tr}\left(\mathcal{I}_c^t(\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_c^{st*})J_c^t(\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_c^{st*})^{-1}\right)}{m} = \mathcal{O}(\frac{d_c}{m}). \tag{124}$$

#### F.4 Excess risk

 $\alpha$ -weighted ERM: In the following lemma, we characterize the variance of the  $\alpha$ -weighted ERM algorithm.

**Lemma 6.** Under Assumption 1, if we let  $m, n \to \infty$ , then the  $\alpha$ -weighted ERM satisfies

$$\sqrt{m+n}(\hat{W}_{\alpha}(D_s, D_t) - \boldsymbol{w}_{\alpha}^*) \to \mathcal{N}(0, \bar{J}(\boldsymbol{w}_{\alpha}^*)^{-1}\bar{\mathcal{I}}_t(\boldsymbol{w}_{\alpha}^*)\bar{J}(\boldsymbol{w}_{\alpha}^*)^{-1}). \tag{125}$$

*Proof.* By using a Taylor expansion of the first derivative of the weighted log-likelihood  $L_E(\hat{W}_{\alpha}(D_s, D_t), D_s, D_t)$  around  $\boldsymbol{w}_{\alpha}^*$ , we obtain

$$0 = \nabla_w L_E(w, D_s, D_t)\big|_{w = \hat{W}_{\alpha}(D_s, D_t)} \approx \nabla_w L_E(w, D_s, D_t)\big|_{w = \boldsymbol{w}_{\alpha}^*} + \nabla_w^2 L_E(w, D_s, D_t)\big|_{w = \boldsymbol{w}_{\alpha}^*} (\hat{W}_{\alpha}(D_s, D_t) - \boldsymbol{w}_{\alpha}^*).$$

From the Taylor series expansion formula, the following approximation can be obtained

$$-\nabla_w^2 L_E(w, D_s, D_t)\big|_{w=\boldsymbol{w}_{\alpha}^*} (\hat{W}_{\alpha}(D_s, D_t) - \boldsymbol{w}_{\alpha}^*) \approx \nabla_w L_E(w, D_s, D_t)\big|_{w=\boldsymbol{w}_{\alpha}^*}.$$
 (126)

By the law of large numbers, when  $m, n \to \infty$ , it can be shown that

$$-\nabla_w^2 L_E(\boldsymbol{w}_{\alpha}^*, D_t) = \frac{1}{m} \sum_{i=1}^m \nabla_w^2 \log f(Z_i^t | \boldsymbol{w}_{\alpha}^*) \to -J_t(\boldsymbol{w}_{\alpha}^*), \tag{127}$$

$$-\nabla_w^2 L_E(\boldsymbol{w}_{\alpha}^*, D_s) = \frac{1}{n} \sum_{i=1}^n \nabla_w^2 \log f(Z_i^s | \boldsymbol{w}_{\alpha}^*) \to -J_s(\boldsymbol{w}_{\alpha}^*).$$
(128)

Thus, the LHS of (126) converges to

$$\nabla_w^2 L_E(w, D_s, D_t) \Big|_{w = \boldsymbol{w}_{\alpha}^*} \to \bar{J}(\boldsymbol{w}_{\alpha}^*), \tag{129}$$

where  $\bar{J}(\boldsymbol{w}_{\alpha}^*) \triangleq \alpha J_t(\boldsymbol{w}_{\alpha}^*) + (1-\alpha)J_t(\boldsymbol{w}_{\alpha}^*).$ 

As for the RHS of (126), by multivariate central limit theorem

$$\frac{1}{\sqrt{m}} \sum_{i=1}^{n} \left( -\nabla_{w} \log f(Z_{i}^{t} | \boldsymbol{w}_{\alpha}^{*}) + \mathbb{E}_{Z^{t}} [\nabla_{w} \log f(Z^{t} | \boldsymbol{w}_{\alpha}^{*})] \right) \to \mathcal{N}(0, \mathcal{I}_{t}(\boldsymbol{w}_{\alpha}^{*})), \tag{130}$$

$$\frac{1}{\sqrt{n}} \sum_{i=1}^{n} \left( -\nabla_w \log f(Z_i^s | \boldsymbol{w}_{\alpha}^*) + \mathbb{E}_{Z^s} [\nabla_w \log f(Z^s | \boldsymbol{w}_{\alpha}^*)] \right) \to \mathcal{N}(0, \mathcal{I}_s(\boldsymbol{w}_{\alpha}^*)), \tag{131}$$

where  $\mathcal{I}_t(\boldsymbol{w}_{\alpha}^*)$  and  $\mathcal{I}_s(\boldsymbol{w}_{\alpha}^*)$  are the covariance matrix of  $\nabla_w \log f(Z^t | \boldsymbol{w}_{\alpha}^*)$  and  $\nabla_w \log f(Z^s | \boldsymbol{w}_{\alpha}^*)$ , respectively.

Due to the definition of  $\boldsymbol{w}_{\alpha}^{*}$ , we have

$$(1 - \alpha)\mathbb{E}_{Z^s}[\nabla_w \log f(Z^s | \boldsymbol{w}_{\alpha}^*)] + \alpha \mathbb{E}_{Z^t}[\nabla_w \log f(Z^t | \boldsymbol{w}_{\alpha}^*)] = 0. \tag{132}$$

Thus, the RHS of (126) will converge to

$$\nabla_w L_E(w, D_s, D_t)\big|_{w=\boldsymbol{w}_{\alpha}^*} \to \mathcal{N}\big(0, \frac{\alpha^2}{m} \mathcal{I}_t(\boldsymbol{w}_{\alpha}^*) + \frac{(1-\alpha)^2}{n} \mathcal{I}_s(\boldsymbol{w}_{\alpha}^*)\big). \tag{133}$$

When  $m, n \to \infty$ , we obtain

$$\left(\hat{W}_{\alpha}(D_s, D_t) - \boldsymbol{w}_{\alpha}^*\right) \to \mathcal{N}\left(0, \bar{J}(\boldsymbol{w}_{\alpha}^*)^{-1}\left(\frac{\alpha^2}{m}\mathcal{I}_t(\boldsymbol{w}_{\alpha}^*) + \frac{(1-\alpha)^2}{n}\mathcal{I}_s(\boldsymbol{w}_{\alpha}^*)\right)\bar{J}(\boldsymbol{w}_{\alpha}^*)^{-1}\right). \tag{134}$$

For  $\alpha = \frac{m}{m+n}$ , if we denote  $\bar{\mathcal{I}}(\boldsymbol{w}_{\alpha}) = \frac{n}{m+n}\mathcal{I}_s(\boldsymbol{w}_{\alpha}) + \frac{m}{m+n}\mathcal{I}_t(\boldsymbol{w}_{\alpha})$ , we have

$$\left(\hat{W}_{\alpha}(D_s, D_t) - \boldsymbol{w}_{\alpha}^*\right) \to \mathcal{N}\left(0, \frac{1}{m+n}\bar{J}(\boldsymbol{w}_{\alpha}^*)^{-1}\bar{\mathcal{I}}(\boldsymbol{w}_{\alpha}^*)\bar{J}(\boldsymbol{w}_{\alpha}^*)^{-1}\right). \tag{135}$$

Thus, the variance term in the excess risk can be computed as

$$\operatorname{tr}(J_{t}(\boldsymbol{w}_{t}^{*})\operatorname{Cov}(\hat{W}_{\alpha}(D_{s}, D_{t}))) = \frac{\operatorname{tr}(J_{t}(\boldsymbol{w}_{t}^{*})\bar{J}(\boldsymbol{w}_{\alpha}^{*})^{-1}\bar{\mathcal{I}}(\boldsymbol{w}_{\alpha}^{*})\bar{J}(\boldsymbol{w}_{\alpha}^{*})^{-1})}{m+n} = \mathcal{O}(\frac{d}{m+n}). \tag{136}$$

**Two-stage ERM:** We use the following notations to denote the expectation of the Hessian matrix and the Fisher information matrix with respect to  $\boldsymbol{w}_{\phi}$ ,

$$\begin{split} J_{c,\phi}^t(\boldsymbol{w}_{\phi}, \boldsymbol{w}_c) &\triangleq \mathbb{E}_{P_Z^t} \Big[ - \nabla_{\boldsymbol{w}_c, \boldsymbol{w}_{\phi}}^2 \log f(Z|[\boldsymbol{w}_{\phi}, \boldsymbol{w}_c]) \Big], \\ J_{\phi}^s(\boldsymbol{w}_{\phi}) &\triangleq \mathbb{E}_{P_Z^s} \Big[ - \nabla_{\boldsymbol{w}_{\phi}}^2 \log f(Z|[\boldsymbol{w}_{\phi}, \boldsymbol{w}_c]) \Big], \\ \mathcal{I}_{\phi}^s(\boldsymbol{w}_{\phi}, \boldsymbol{w}_c) &\triangleq \mathbb{E}_{P_Z^s} [\nabla_{\boldsymbol{w}_{\phi}} \log f(Z|[\boldsymbol{w}_{\phi}, \boldsymbol{w}_c])] \nabla_{\boldsymbol{w}_{\phi}}^{\top} \log f(Z|[\boldsymbol{w}_{\phi}, \boldsymbol{w}_c]) \Big]. \end{split}$$

In the following lemma, we characterize the variance of the two-stage ERM algorithm.

**Lemma 7.** Under Assumption 1, if we let  $m, n \to \infty$ , then the two-stage ERM satisfies

$$\left(\hat{W}_{c}^{t}(\hat{W}_{\phi}, D_{t}) - \boldsymbol{w}_{c}^{st*}\right) \to \mathcal{N}\left(0, J_{c}^{t}(\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_{c}^{st*})^{-1} \right) \\
\left(\frac{1}{m}\mathcal{I}_{c}^{t}(\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_{c}^{st*}) + \frac{1}{n}J_{c,\phi}^{t}(\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_{c}^{st*})J_{\phi}^{s}(\boldsymbol{w}_{\phi}^{s*})^{-1}\mathcal{I}_{\phi}^{s}(\boldsymbol{w}_{\phi}^{s*})J_{\phi}^{s}(\boldsymbol{w}_{\phi}^{s*})^{-1}J_{c,\phi}^{t}(\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_{c}^{st*})\right)J_{c}^{t}(\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_{c}^{st*})^{-1}\right).$$
(137)

*Proof.* By using a Taylor expansion of the gradient with respect to  $\boldsymbol{w}_c$  of the log-likelihood  $L_E^{S2}(\hat{W}_{\phi}(D_s), \hat{W}_c^t(\hat{W}_{\phi}, D_t), D_t)$  around  $[\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_c^{st*}]$ , we obtain

$$0 = \nabla_{\boldsymbol{w}_{c}} L_{E}^{S2}(\hat{W}_{\phi}(D_{s}), \hat{W}_{c}^{t}(\hat{W}_{\phi}, D_{t}), D_{t})$$

$$\approx \nabla_{\boldsymbol{w}_{c}} L_{E}^{S2}(\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_{c}^{st*}, D_{t}) + \nabla_{\boldsymbol{w}_{c}, \boldsymbol{w}_{\phi}}^{S2} L_{E}^{S2}(\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_{c}^{st*}, D_{t})(\hat{W}_{\phi}(D_{s}) - \boldsymbol{w}_{\phi}^{s*})$$

$$+ \nabla_{\boldsymbol{w}_{c}}^{S2} L_{E}^{S2}(\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_{c}^{st*}, D_{t})(\hat{W}_{c}^{t}(\hat{W}_{\phi}, D_{t}) - \boldsymbol{w}_{c}^{st*}).$$

From the Taylor series expansion formula, the following approximation can be obtained

$$-\nabla_{\boldsymbol{w}_{c}}^{2} L_{E}^{S2}(\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_{c}^{st*}, D_{t})(\hat{W}_{c}^{t}(\hat{W}_{\phi}, D_{t}) - \boldsymbol{w}_{c}^{st*})$$

$$\approx \nabla_{\boldsymbol{w}_{c}} L_{E}^{S2}(\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_{c}^{st*}, D_{t}) + \nabla_{\boldsymbol{w}_{c}, \boldsymbol{w}_{\phi}}^{2} L_{E}^{S2}(\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_{c}^{st*}, D_{t})(\hat{W}_{\phi}(D_{s}) - \boldsymbol{w}_{\phi}^{s*}). \tag{138}$$

By the law of large numbers, when  $m \to \infty$ , it can be shown that

$$-\nabla_{\boldsymbol{w}_{c}}^{2} L_{E}^{S2}(\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_{c}^{st*}, D_{t}) = \frac{1}{m} \sum_{i=1}^{m} \nabla_{\boldsymbol{w}_{c}}^{2} \log f(Z_{i}^{t} | [\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_{c}^{st*}]) \to -J_{c}^{t}(\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_{c}^{st*}),$$
(139)

$$-\nabla_{\boldsymbol{w}_{c},\boldsymbol{w}_{\phi}}^{2}L_{E}^{S2}(\boldsymbol{w}_{\phi}^{s*},\boldsymbol{w}_{c}^{st*},D_{t}) = \frac{1}{m}\sum_{i=1}^{m}\nabla_{\boldsymbol{w}_{c},\boldsymbol{w}_{\phi}}^{2}\log f(Z_{i}^{t}|[\boldsymbol{w}_{\phi}^{s*},\boldsymbol{w}_{c}^{st*}]) \to -J_{c,\phi}^{t}(\boldsymbol{w}_{\phi}^{s*},\boldsymbol{w}_{c}^{st*}).$$
(140)

As for the first term in the RHS of (138), note that  $\mathbb{E}_{P_Z^t}[\nabla_{\boldsymbol{w}_c} \log f(Z|[\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_c^{st*}])] = 0$ , by multivariate central limit theorem, we have

$$\frac{1}{\sqrt{m}} \sum_{i=1}^{n} \left( -\nabla_{\boldsymbol{w}_{c}} \log f(Z_{i}^{t} | [\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_{c}^{st*}]) \right) \to \mathcal{N}(0, \mathcal{I}_{c}^{t}(\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_{c}^{st*})). \tag{141}$$

When  $n \to \infty$ , due to the asymptotic normality of maximum likelihood estimate, we have

$$\sqrt{n}(\hat{W}_{\phi}(D_s) - \boldsymbol{w}_{\phi}^{s*}) \to \mathcal{N}(0, J_{\phi}^{s}(\boldsymbol{w}_{\phi}^{s*})^{-1}\mathcal{I}_{\phi}^{s}(\boldsymbol{w}_{\phi}^{s*})J_{\phi}^{s}(\boldsymbol{w}_{\phi}^{s*})^{-1}), \tag{142}$$

where  $\mathcal{I}_{\phi}^{s}(\boldsymbol{w}_{\phi}^{s*}) = \mathbb{E}_{P_{Z}^{s}}[\nabla_{\boldsymbol{w}_{\phi}}\log f(Z|[\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_{c}^{s*}])\nabla_{\boldsymbol{w}_{\phi}}^{\top}\log f(Z|[\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_{c}^{s*}])].$ 

Thus, the RHS of (138) converges to

$$\mathcal{N}\left(0, \ \frac{1}{m}\mathcal{I}_{c}^{t}(\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_{c}^{st*}) + \frac{1}{n}J_{c,\phi}^{t}(\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_{c}^{st*})J_{\phi}^{s}(\boldsymbol{w}_{\phi}^{s*})^{-1}\mathcal{I}_{\phi}^{s}(\boldsymbol{w}_{\phi}^{s*})J_{\phi}^{s}(\boldsymbol{w}_{\phi}^{s*})^{-1}J_{c,\phi}^{t}(\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_{c}^{st*})\right)$$
(143)

when  $m, n \to \infty$ .

Thus, we obtain

$$\left(\hat{W}_{c}^{t}(\hat{W}_{\phi}, D_{t}) - \boldsymbol{w}_{c}^{st*}\right) \rightarrow \mathcal{N}\left(0, J_{c}^{t}(\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_{c}^{st*})^{-1}\right) \\
\left(\frac{1}{m}\mathcal{I}_{c}^{t}(\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_{c}^{st*}) + \frac{1}{n}J_{c,\phi}^{t}(\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_{c}^{st*})J_{\phi}^{s}(\boldsymbol{w}_{\phi}^{s*})^{-1}\mathcal{I}_{\phi}^{s}(\boldsymbol{w}_{\phi}^{s*})J_{\phi}^{s}(\boldsymbol{w}_{\phi}^{s*})^{-1}J_{c,\phi}^{t}(\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_{c}^{st*})\right)J_{c}^{t}(\boldsymbol{w}_{\phi}^{s*}, \boldsymbol{w}_{c}^{st*})^{-1}\right).$$

Note that  $Cov(\hat{W}_{\phi}(D_s))$  can be characterized by the asymptotic normality of maximum likelihood estimate. Thus, the variance term in the excess risk can be computed as:

$$\operatorname{tr}\left(J_{t}(\boldsymbol{w}_{\phi}^{t*}, \boldsymbol{w}_{c}^{t*})\operatorname{Cov}(\hat{W}_{\phi}(D_{s}), \hat{W}_{c}^{t}(D_{t}, \hat{W}_{\phi}))\right) = \mathcal{O}(\frac{d_{c}}{m} + \frac{d}{n}). \tag{145}$$