

# HIGH-DIMENSIONAL ASYMPTOTICS OF TRANSFERRING FROM DIFFERENT DOMAINS IN LINEAR REGRESSION

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Hard parameter sharing for multi-task learning is widely used in empirical research despite the fact that its generalization properties have not been well established in many cases. This paper studies its generalization properties in a fundamental setting: How does hard parameter sharing work given multiple linear regression tasks? We develop new techniques and establish a number of new results in the high-dimensional setting, where the sample size and feature dimension increase at a fixed ratio. First, we show a sharp bias-variance decomposition of hard parameter sharing, given multiple tasks with the same features. Second, we characterize the asymptotic bias-variance limit for two tasks, even when they have arbitrarily different sample size ratios and covariate shifts. We also demonstrate that these limiting estimates for the empirical loss are incredibly accurate in moderate dimensions. Finally, we explain an intriguing phenomenon where increasing one task's sample size helps another task initially by reducing variance but hurts eventually due to increasing bias. This suggests progressively adding data for optimizing hard parameter sharing, and we validate its efficiency in text classification tasks.

**1. Introduction.** Hard parameter sharing (HPS) for multi-task learning is widely used in empirical research and goes back to the seminal work of [12]. Recent work has revived interests in this approach because it improves performance and reduces the cost of collecting labeled data [34]. It is generally applied by sharing the feature layers between all tasks while keeping an output layer for every task. Often, hard parameter sharing offers two critical advantages if successfully applied. First, it reduces model parameters since all tasks use the same feature space. Second, it reduces the amount of labeled data needed from each task by augmenting the entire training dataset.

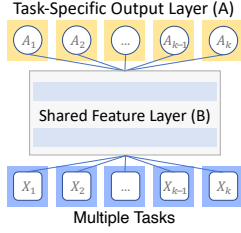
Hard parameter sharing works as an inductive transfer mechanism and a regularizer that reduces overfitting, both of which have great intuitive appeal [34]. For example, by restricting the shared space's size, HPS encourages information sharing among multiple tasks [21]. Another source of inductive bias comes from the tasks and depends on datasets' properties such as sample sizes and task covariances [40]. However, how these dataset properties impact HPS has not been well established. Part of the challenge may be that HPS' generalization performance depends intricately on the sample size ratios and covariate shifts between tasks, and is not amenable to standard concentration results. Previous results based on Rademacher complexity or VC dimensions have considered cases where all tasks' sample sizes are equal to logarithmic factors of the feature dimension [8, 27], and when all tasks' sample sizes increase simultaneously [2, 26].

This paper presents new techniques to study hard parameter sharing and establishes a number of new results. We consider regression analysis, which is arguably one of the most fundamental problems in statistics and machine learning. We are interested in the *high-dimensional* setting, where each dataset's sample size and feature dimension grow linearly

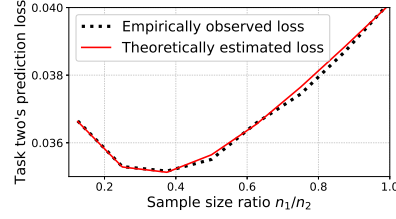
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(a) A hard parameter sharing architecture



(b) Varying sample size ratio

Fig 1: Left: an illustrative picture of HPS. Right: an illustrative example of using HPS for two tasks  $X_1, Y_1$  and  $X_2, Y_2$  with sample size  $n_1, n_2$ , respectively. Increasing  $n_1/n_2$  decreases task two's prediction loss initially but increase afterward. This phenomenon occurs due to different bias-variance tradeoffs as  $n_1/n_2$  increases. Our result provides an estimated loss (solid line) that accurately matches the empirical loss (dotted line). See Section ?? for the precise setting.

instead of logarithmically. This setting captures the fact that a single task's sample size is usually insufficient for accurate learning in many applications. For example, if a dataset's sample size is only a constant factor of dimension in linear regression, the variance is also constant (cf. Fact 3.7). The high-dimensional setting is challenging but is crucial for understanding how datasets' sample sizes impact generalization performance.

**1.1. Setup and definitions.** Consider the transfer learning setting with two data sets. We denote their sample sizes by  $n_1$  and  $n_2$ . For  $i = 1, 2$ , Let  $X^{(i)} \in \mathbb{R}^{n_i \times p}$  denote dataset  $i$ 's feature covariates. We assume that the label vector  $Y^{(i)} \in \mathbb{R}^{n_i}$  for  $X^{(i)}$  follows a linear model plus random noise:

$$Y^{(i)} = X^{(i)}\beta^{(i)} + \varepsilon^{(i)}, \quad i = 1, 2.$$

In this paper, we make the following assumptions on feature covariates  $X^{(i)}$  and the noise vectors  $\varepsilon^{(i)}$ . We remark that all these assumptions are natural in high-dimensional statistics.

We assume that the row vectors of  $X^{(i)}$  are i.i.d. centered random vectors with population covariance matrix  $\Sigma^{(i)}$ . More precisely, let

$$(1.1) \quad X^{(i)} = Z^{(i)}(\Sigma^{(i)})^{1/2} \in \mathbb{R}^{n_i \times p}, \quad i = 1, 2,$$

where each  $\Sigma^{(1)}$  and  $\Sigma^{(2)}$  are  $p \times p$  deterministic positive definite symmetric matrices, and  $Z^{(1)} = (z_{ij}^{(1)})$  and  $Z^{(2)} = (z_{ij}^{(2)})$  are  $n_1 \times p$  and  $n_2 \times p$  random matrices with real i.i.d. entries satisfying

$$(1.2) \quad \mathbb{E}z_{ij}^{(1)} = \mathbb{E}z_{ij}^{(2)} = 0, \quad \mathbb{E}|z_{ij}^{(1)}|^2 = \mathbb{E}|z_{ij}^{(2)}|^2 = 1,$$

Another commonly used transfer learning estimator is defined as the minimizer of the total loss function [7, 23]:

$$\hat{\beta}^{\text{TL}} := \arg \min \left[ \|X^{(1)}\beta - Y^{(1)}\|^2 + \|X^{(2)}\beta - Y^{(2)}\|^2 \right].$$

Given a solution from minimizing  $f(A, B)$ , denoted by  $(\hat{A}, \hat{B})$  (which we will specify below), let  $\hat{\beta}_i^{\text{HPS}} = \hat{B}\hat{A}_i$  denote the HPS estimator for task  $i$ . The critical questions are: (i) How well does the estimator work? In particular, how does the performance of the estimator scale with sample size? (ii) For datasets with different sample sizes and covariate shifts, how do they affect the estimator?

1.2. *Main results.* Our first result (Theorem 5.1) applies to multi-label prediction settings where all datasets have the same features (and sample size), and we want to make several predictions for every input (cf. examples in [18]). We analyze the global minimizer of  $f(A, B)$ , and provide a sharp bias-variance decomposition of its (out-of-sample) prediction loss for any task. This setting is tractable even though in general,  $f(A, B)$  is non-convex in  $A$  and  $B$  (e.g. matrix completion is a special case for suitably designed  $X^{(i)}, Y^{(i)}$ ). Our result implies that when all tasks have the same features but different labels, for any task, HPS helps reduce the task’s variance compared to single-task learning but increases bias.

Our second result (Theorem 2.4) applies to two tasks with arbitrarily different sample size ratios and covariate shifts. While we can no longer characterize  $f(A, B)$ ’s global minimum because of non-convexity, we can still provide a sharp bias-variance tradeoff of any local minimizer’s prediction loss for both tasks. Despite being a simple setting, we observe several non-trivial phenomena by varying sample size ratios and covariate shifts between the two tasks. See Figure 1b for an illustration of the former. Consequently, using our precise loss estimates, we observe several qualitative properties of HPS for varying dataset properties.

- *Sample efficiency (Example 3.8):* One advantage of combining multiple datasets is that the requirement for labeled data reduces compared to single-task learning, a phenomenon that [42] has observed empirically. Our results further imply that HPS’s sample efficiency depends on model-specific variances across tasks vs. the noise variance and is generally high when the latter is large.
- *Sample size ratio (Example 3.4):* Increasing one task’s sample size does not always reduce another task’s loss. In a simplified setting, we find that the task loss either decreases first before increasing afterward or decreases monotonically depending on how fast the bias grows. These two trends result from different bias-variance tradeoffs. This result is surprising because previous generalization bounds in multi-task learning typically scale down as all tasks’ sample sizes increase, thus do not apply for different sample size ratios.
- *Covariate shift (Example 3.1):* In addition to sample sizes, variance also scales with two datasets’ covariate shifts. For a large sample size ratio, HPS’s variance is smallest when there is no covariate shift. Counterintuitively, for a small sample size ratio, having covariate shifts reduces variance through a complementary spectrum. We achieve this result through a novel characterization on the inverse of the sum of two sample covariance matrices with arbitrary covariate shifts. See our discussion of proof techniques below for details.

Finally, we discuss the practical implications of our work. Our sample size ratio study implies a concrete progressive training procedure that gradually adds more data until performance drops. For example, in the setting of Figure 1b, this procedure will stop right at the minimum of the local basin. We conduct further studies of this procedure on six text classification datasets and observe that it reduces the computational cost by 65% compared to a standard round-robin training procedure while keeping the average accuracy of all tasks simultaneously.

**Proof techniques.** There are two main ideas in our analysis. The proof of our first result uses a geometric intuition that hard parameter sharing finds a “rank- $r$ ” approximation of the datasets. We carefully keep track of the concentration error between the global minimizer of  $f(A, B)$  and its population version (cf. equation (5.5)). The proof of our second result is significantly more involved because of different sample sizes and covariate shifts. We show that the inverse of the sum of two sample covariance matrices with arbitrary covariate shifts converges to a deterministic diagonal matrix asymptotically (cf. Theorem 2.4). We use recently developed techniques from random matrix theory to show a sharp convergence rate. One limitation of our analysis is that in Example 3.4, there is an error term that can result in vacuous bounds for

very small  $n_1$  (cf. equation (??)). We believe our result has provided significant initial insights, and it is an interesting question to tighten our result. See Section 6 for more discussions of the technical challenge.

**1.3. Related Work.** There is a large body of classical and recent works on multi-task learning. We focus our discussion on theoretical results and refer interested readers to several excellent surveys for general references [29, 43, 38]. The early work of [8, 10, 26] studied multi-task learning from a theoretical perspective, often using uniform convergence or Rademacher complexity based techniques. An influential paper by [9] provides uniform convergence bounds that combine multiple datasets in certain settings. One limitation of uniform convergence based techniques is that the results often assume that all tasks have the same sample size, see e.g. [8, 27]. Moreover, these techniques do not apply to the high-dimensional setting because the results usually require a sample size of at least  $p \log p$ .

Our proof techniques use the so-called local law of random matrices [16], a recent development in the random matrix theory literature. In the single-task case, [11] first proved such a local law for sample covariance matrices with isotropic covariance. [20] later extended this result to arbitrary covariance matrices. These techniques provide almost sharp convergence rates to the asymptotic limit compared to other methods such as free probability [28]. To the best of our knowledge, we are not aware of any previous results in the multi-task case, even for two tasks (with arbitrary covariate shifts). [«HZ notes: can you please add a discussion of the related work from RMT?»»](#)

The problem we study here is also related to high-dimensional prediction in transfer learning [23, 7] and distributed learning [15]. For example, [23] provide minimax-optimal rates to predict a target regression task given multiple sparse regression tasks. One closely related work is [40], which studied hard parameter sharing for two linear regression tasks. However, their results only apply to sample size regimes at least logarithmic factors of dimension.

**1.4. Organizations.** The rest of this paper is organized as follows. In Section 5, we present the bias-variance decomposition for hard parameter sharing. In Section 2.2, we describe how varying sample sizes and covariate shifts impact hard parameter sharing using random matrix theory. In Sections ??, we validate our results in simulations. In Section 6, we summarize our work and discuss future work. Section ?? describes our study on text classification tasks. Section C, F, and D present proofs of our results.

**Notations.** For an  $n \times p$  matrix  $X$ , let  $\lambda_{\min}(X)$  denote its smallest singular value and  $\|X\|$  denote its largest singular value. Let  $\lambda_1(X), \lambda_2(X), \dots, \lambda_{p \wedge n}(X)$  denote the singular values of  $X$  in decreasing order. Let  $X^+$  denote the Moore-Penrose pseudoinverse of  $X$ . We refer to random matrices of the form  $\frac{X^\top X}{n}$  as sample covariance matrices. We say that an event  $\Xi$  holds with high probability if the probability that  $\Xi$  happens goes to 1 as  $p$  goes to infinity. We use the big-O notation  $g(n) = O(f(n))$  if there exists a constant  $C$  such that  $g(n) \leq C f(n)$  for large enough  $n$ . Moreover, we use the notation  $g(n) \lesssim f(n)$  if  $g(n) = O(f(n))$ , and the notation  $g(n) \sim f(n)$  if  $g(n) \lesssim f(n)$  and  $f(n) \lesssim g(n)$ . In this paper, we will often write an identity matrix  $\text{Id}_{n \times n}$  as 1 without causing any confusions.

**2. Main Results and Proof Techniques.** In this section, we define our model for the setting of transfer learning, and introduce several transfer learning estimators that will be considered in this paper.

2.1. *Assumptions.* Furthermore, we assume that the entries  $z_{ij}^{(1)}$  and  $z_{ij}^{(2)}$  have finite  $\varphi$ -th moment for some constant  $\varphi > 4$ :

$$(2.1) \quad \mathbb{E}|z_{ij}^{(1)}|^\varphi \leq \tau^{-1}, \quad \mathbb{E}|z_{ij}^{(2)}|^\varphi \leq \tau^{-1}$$

for a small constant  $\tau > 0$ . We assume that  $\Sigma^{(i)}$  has eigendecomposition

$$(2.2) \quad \Sigma^{(i)} = O_i \Lambda_i O_i^\top, \quad \Lambda_i = \text{diag}(\sigma_1^{(i)}, \dots, \sigma_n^{(i)}), \quad i = 1, 2,$$

where  $O_i$  is the eigenmatrix and the eigenvalues satisfy that

$$(2.3) \quad \tau \leq \sigma_p^{(i)} \leq \dots \leq \sigma_2^{(i)} \leq \sigma_1^{(i)} \leq \tau^{-1} \quad i = 1, 2.$$

We assume that  $\varepsilon^{(1)} \in \mathbb{R}^n$  and  $\varepsilon^{(2)} \in \mathbb{R}^n$  are two independent random noise vectors with i.i.d entries of mean zero, variance  $\sigma^2$ , and bounded moment up to any order: for any fixed  $k \in \mathbb{N}$ , there exists a constant  $C_k > 0$  such that

$$(2.4) \quad \mathbb{E}|\varepsilon_i^{(1)}|^k \leq C_k, \quad \mathbb{E}|\varepsilon_i^{(2)}|^k \leq C_k.$$

Finally, we assume that  $\beta^{(1)}$  and  $\beta^{(2)}$  are two arbitrary deterministic or random vectors that are independent of  $X^{(1)}$ ,  $X^{(2)}$ ,  $\varepsilon^{(1)}$  and  $\varepsilon^{(2)}$ .

In this paper, we consider the high-dimensional setting, where the sample ratios satisfy that

$$(2.5) \quad 1 + \tau \leq \rho_1 := \frac{n_1}{p} \leq p^{\tau-1}, \quad 1 + \tau \leq \rho_2 := \frac{n_2}{p} \leq p^{\tau-1}, \quad \tau \leq \frac{\rho_1}{\rho_2} \leq \tau^{-1},$$

for a small constant  $\tau > 0$ . If  $\rho_i > p^{\tau-1}$ ,  $i = 1, 2$ , we are basically in the low-dimensional region, where the law of large numbers and central limit theorem already give good enough results without using the theory developed in this paper. The lower bounds  $\rho_1 > 1 + \tau$  and  $\rho_2 > 1 + \tau$  are to ensure that the sample covariance matrices  $(X^{(1)})^\top X^{(1)}$  and  $(X^{(2)})^\top X^{(2)}$  are non-singular with high probability, so that the ordinary least squares (OLS) estimator is well-defined for the linear regression problem on each task.

We summarize our basic assumptions here for future reference.

ASSUMPTION 2.1. Let  $\tau$  be a small constant.

- (i)  $X^{(1)}$  and  $X^{(2)}$  take the form (1.1), where  $Z^{(1)}$  and  $Z^{(2)}$  are respectively  $n_1 \times p$  and  $n_2 \times p$  random matrices with i.i.d. entries satisfying (1.2) and (2.1),  $\Sigma^{(1)}$  and  $\Sigma^{(2)}$  are deterministic positive definite symmetric matrices satisfying (2.2) and (2.3).
- (ii)  $\varepsilon^{(1)} \in \mathbb{R}^n$  and  $\varepsilon^{(2)} \in \mathbb{R}^n$  are random vectors independent from  $X^{(1)}$  and  $X^{(2)}$ , and with i.i.d entries of mean zero, variance  $\sigma^2$ , and bounded moments as in (2.4).
- (iii)  $\beta^{(1)}$  and  $\beta^{(2)}$  are independent of  $X^{(1)}$ ,  $X^{(2)}$ ,  $\varepsilon^{(1)}$  and  $\varepsilon^{(2)}$ .
- (iv)  $\rho_1$  and  $\rho_2$  satisfy (2.5).

In this paper, we measure the performance of  $\hat{\beta}_2^{\text{HPS}}(\hat{a})$  through the out-of-sample predication loss (test error). Consider a test data point  $(x, y)$  generated from the same model as task 2:  $y = x^\top \beta^{(2)} + \varepsilon$ , where  $x \in \mathbb{R}^p$  and  $\varepsilon \in \mathbb{R}$  are independent of  $X^{(1)}$ ,  $X^{(2)}$ ,  $\varepsilon^{(1)}$  and  $\varepsilon^{(2)}$ , and only  $x$  is observable. We want to use  $x^\top \hat{\beta}_2^{\text{HPS}}(\hat{a})$  to predict  $y$ , and we measure the predication loss using the mean squared error

$$\mathbb{E}_x \left[ \left\| y - x^\top \hat{\beta}_2^{\text{HPS}}(\hat{a}) \right\|^2 \right] = \left\| (\Sigma^{(2)})^{1/2} \left( \hat{\beta}_2^{\text{HPS}}(\hat{a}) - \beta^{(2)} \right) \right\|^2 + \sigma^2.$$

Since  $\sigma^2$  is a constant that does not depend on the model, we ignore it and define the predication loss as

$$(2.6) \quad L(\hat{\beta}_2^{\text{HPS}}(\hat{a})) := \left\| (\Sigma^{(2)})^{1/2} \left( \hat{\beta}_2^{\text{HPS}}(\hat{a}) - \beta^{(2)} \right) \right\|^2.$$

We will compare it to the out-of-sample predication losses of the baseline estimators,  $L(\hat{\beta}_2^{\text{OLS}})$  and  $L(\hat{\beta}^{\text{AVE}}(\lambda))$  for some properly chosen  $\lambda \in [0, 1]$ .

Plugging (??) into (2.6), we get

$$(2.7) \quad L(\hat{\beta}_2^{\text{HPS}}(\hat{a})) = \left\| (\Sigma^{(2)})^{1/2} \hat{\Sigma}(\hat{a})^{-1} (X^{(1)})^\top X^{(1)} (\hat{a} \beta^{(1)} - \hat{a}^2 \beta^{(2)}) \right. \\ \left. + (\Sigma^{(2)})^{1/2} \hat{\Sigma}(\hat{a})^{-1} \left[ (X^{(2)})^\top \varepsilon^{(2)} + \hat{a} (X^{(1)})^\top \varepsilon^{(1)} \right] \right\|^2.$$

Note that if we replace  $\hat{a}$  with a fixed number  $a$  in (2.7), then taking the expectation over  $\varepsilon^{(1)}$  and  $\varepsilon^{(2)}$ , we can get a clean bias-variance decomposition of the predication loss:

$$(2.8) \quad \mathbb{E}_{\varepsilon^{(1)}, \varepsilon^{(2)}} \left[ L(\hat{\beta}_2^{\text{HPS}}(a)) \right] = L_{\text{bias}}(a) + L_{\text{Var}}(a),$$

where

$$(2.9) \quad L_{\text{bias}}(a) := \left\| (\Sigma^{(2)})^{1/2} \hat{\Sigma}(a)^{-1} (X^{(1)})^\top X^{(1)} (a \beta^{(1)} - a^2 \beta^{(2)}) \right\|^2$$

is called the bias term, which depends on the model bias between task 1 and task 2, and

$$(2.10) \quad L_{\text{Var}}(a) := \sigma^2 \text{Tr} \left[ \Sigma^{(2)} \hat{\Sigma}(a)^{-1} \right]$$

is called the variance term, which depends on the noise variance. Using concentration of the noise vectors  $\varepsilon^{(1)}$  and  $\varepsilon^{(2)}$ , we can show that  $L(\hat{\beta}_2^{\text{HPS}}(a))$  is close to (2.8) up to a small error as in the next lemma. In this paper, we say that an event  $\Xi$  holds *with high probability* (w.h.p.) if  $\mathbb{P}(\Xi) \rightarrow 1$  as  $p \rightarrow \infty$ .

**LEMMA 2.2.** *Under Assumption 2.1, for any small constant  $c > 0$  and large constant  $C > 0$ , there exists a high probability event  $\Xi$ , on which the following estimates hold uniformly in  $a \in \mathbb{R}$  and  $\lambda \in [0, 1]$ :*

$$(2.11) \quad L(\hat{\beta}_2^{\text{HPS}}(a)) = \left[ 1 + O(p^{-1/2+c}) \right] \cdot [L_{\text{bias}}(a) + L_{\text{Var}}(a)] \\ + O \left[ p^{-C} \left( \|\beta^{(1)}\|^2 + \|\beta^{(2)}\|^2 \right) \right],$$

$$(2.12) \quad L(\hat{\beta}^{\text{AVE}}(\lambda)) = \left[ 1 + O(p^{-1/2+c}) \right] \cdot \lambda^2 \left\| (\Sigma^{(2)})^{1/2} (\beta^{(1)} - \beta^{(2)}) \right\|^2 \\ + \left[ 1 + O(p^{-1/2+c}) \right] \cdot \sigma^2 \lambda^2 \text{Tr} \left[ \Sigma^{(2)} [(X^{(1)})^\top X^{(1)}]^{-1} \right] \\ + \left[ 1 + O(p^{-1/2+c}) \right] \cdot \sigma^2 (1 - \lambda)^2 \text{Tr} \left[ \Sigma^{(2)} [(X^{(2)})^\top X^{(2)}]^{-1} \right].$$

and

$$(2.13) \quad L(\hat{\beta}_2^{\text{OLS}}) = \left[ 1 + O(p^{-1/2+c}) \right] \cdot \sigma^2 \text{Tr} \left[ \Sigma^{(2)} [(X^{(2)})^\top X^{(2)}]^{-1} \right].$$

Since (2.11) holds uniformly for all  $a \in \mathbb{R}$ , we can also apply it to  $\hat{\beta}_2^{\text{HPS}}(\hat{a})$ , where  $\hat{a}$  is a random variable that may depend on  $\varepsilon^{(1)}$  and  $\varepsilon^{(2)}$ . In practice, the parameter  $a$  is up to one's choice and may not be the global minimizer, so we have stated the result for an completely arbitrary  $a$ . (In fact, the optimization objective  $g(a)$  is generally non-convex, so in some cases one can only find a local minimizer.) For a fixed  $a \in \mathbb{R}$ , the proof of (2.11) is based on the sharp concentration bounds in Lemma A.5 of the supplement [41]. To extend uniformly to all  $a \in \mathbb{R}$ , we will use a standard  $\varepsilon$ -net argument, which leads to a small error  $p^{-C} (\|\beta^{(1)}\|^2 + \|\beta^{(2)}\|^2)$ .

Note that this error is negligible unless  $\beta^{(1)}$  and  $a\beta^{(2)}$  cancel each other almost exactly, and the noise variance  $\sigma$  is very small. The proof of Lemma 2.2 will be given in Appendix B of the supplement [41].

For the single-task predication loss (2.13), we can calculate its asymptotic limit exactly using the following classical result in multivariate statistics.

LEMMA 2.3 (Theorem 2.4 of [11] and Theorem 3.14 of [13]). *Under Assumption 2.1, we have that for any deterministic  $p \times p$  matrix  $\Sigma$ ,*

$$\text{Tr} \left[ \Sigma \frac{1}{(X^{(2)})^\top X^{(2)}} \right] = \frac{1}{n_2 - p} \text{Tr} \left[ \Sigma (\Sigma^{(2)})^{-1} \right] + O \left( \frac{p^c}{\sqrt{n_2 p}} \cdot \frac{p}{n_2} \|A\| \right)$$

with high probability for any small constant  $c > 0$ .

If the entries of  $Z^{(2)}$  are i.i.d. Gaussian, then this result follows from the classical result for the inverse Wishart distribution [1]. For a general non-Gaussian  $Z^{(2)}$ , this result can be obtained using the well-known Stieltjes transform method (cf. Lemma 3.11 of [4]). Here we have presented the results from [11, 13], which give an almost sharp convergence rate. With Lemma 3.7, we obtain that w.h.p.,

$$(2.14) \quad L(\hat{\beta}_2^{\text{OLS}}) = \left[ 1 + O(p^{-1/2+c}) \right] \cdot \frac{p\sigma^2}{n_2 - p},$$

and

$$(2.15) \quad \begin{aligned} L(\hat{\beta}^{\text{AVE}}(\lambda)) &= \left[ 1 + O(p^{-1/2+c}) \right] \cdot \lambda^2 \left\| (\Sigma^{(2)})^{1/2} (\beta^{(1)} - \beta^{(2)}) \right\|^2 \\ &+ \left[ 1 + O(p^{-1/2+c}) \right] \cdot \sigma^2 \left[ \frac{\lambda^2}{n_1 - p} \text{Tr} \left[ \Sigma^{(2)} (\Sigma^{(1)})^{-1} \right] + \frac{(1 - \lambda)^2 p}{n_2 - p} \right]. \end{aligned}$$

On the other hand, much less is known about the predication loss of the HPS estimator. In particular, its exact dependence on the model parameters, including the model bias, noise variance, sample sizes, and population covariance matrices, is not well-understood so far. In Section ??, we give a rigorous analysis of the bias term (2.9) and variance term (2.10) in two different settings: (i) independent  $X^{(1)}$  and  $X^{(2)}$  with different sample sizes and same population covariance matrices  $\Sigma^{(1)} = \Sigma^{(2)}$ ; (ii) independent  $X^{(1)}$  and  $X^{(2)}$  with different sample sizes and different population covariance matrices. In case (i), we provide the exact asymptotics for both the bias and variance terms, together with almost sharp convergence rates. We will use these results to illustrate the effects of the *bias-variance tradeoff* and *varying sample sizes*. In case (ii), we will prove an exact asymptotic variance limit, and employ the result to show the intricate effect of the covariate shift. On the other hand, in case (ii), we will provide an estimate on the bias term, which becomes exact only when  $n_1 \gg p$ . In Section 5, we will consider a simple extension to a multi-task learning setting with more than two tasks and the same covariates for all tasks. We will give the asymptotic limit of the predication loss for the HPS estimator, which provides useful insights into the more rich multi-task learning theory. Due to length constraint, we will explore the multi-task learning setting in greater details in other works.

**2.2. Covariate shift.** In this section, we consider the most general setting, where the feature covariates  $X^{(1)}$  and  $X^{(2)}$  of the two tasks have both different sample sizes and different population covariance matrices. In particular, the fact that population covariance matrices differ across tasks is often called “covariate shift”. In this section, we describe the

exact asymptotic variance limit in the high-dimensional setting, while the bias limit is much more complicated, and we can only give an estimate on it.

Compared to the results in Section 2.3, the spectrum of  $\hat{\Sigma}(a)^{-1}$  now not only depends on the sample sizes of both tasks, but also depends on the “misalignment” between  $\Sigma^{(1)}$  and  $\Sigma^{(2)}$ . To capture this misalignment quantitatively, we introduce the covariate shift matrix

$$M(a) := a(\Sigma^{(1)})^{1/2}(\Sigma^{(2)})^{-1/2}.$$

Let  $\lambda_1(a) \geq \lambda_2(a) \geq \dots \geq \lambda_p(a)$  be the singular values of  $M$  in descending order. By (2.3), these singular values satisfy that

$$(2.16) \quad |a|\tau \leq \lambda_p(a) \leq \dots \leq \lambda_2(a) \leq \lambda_1(a) \leq |a|\tau^{-1}.$$

The main result of this section is the following theorem on the variance limit, which characterizes the exact dependence of  $L_{\text{Var}}(a)$  on the singular values of  $M$ .

**THEOREM 2.4.** *Under Assumption 2.1, for any small constant  $c > 0$ , there exists a high probability event  $\Xi$ , on which the following estimate holds for  $L_{\text{Var}}(a)$  in (2.10):*

$$(2.17) \quad \left| L_{\text{Var}}(a) - \frac{\sigma^2}{n_1 + n_2} \text{Tr} \left[ \frac{1}{a_1 M(a)^\top M(a) + a_2} \right] \right| \leq \frac{(n_1 + n_2)^{2/\varphi+c}}{p^{1/2}(n_1 + n_2)^{1/2}} \cdot \frac{p\sigma^2}{n_1 + n_2},$$

uniformly in all  $a \in \mathbb{R}$ . Here  $(a_1, a_2)$  is the solution of the following system of equations

$$(2.18) \quad a_1 + a_2 = 1 - \frac{p}{n_1 + n_2}, \quad a_1 + \frac{1}{n_1 + n_2} \left( \sum_{i=1}^p \frac{\lambda_i^2 a_1}{\lambda_i^2 a_1 + a_2} \right) = \frac{n_1}{n_1 + n_2}.$$

With (2.16), it is easy to see that

$$\frac{\sigma^2}{n_1 + n_2} \text{Tr} \left[ \frac{1}{a_1 M(a)^\top M(a) + a_2} \right] \sim \frac{p\sigma^2}{n_1 + n_2}.$$

Hence the right-hand side of (2.17) is much smaller than this main term by a factor of  $p^{-1/2}(n_1 + n_2)^{-1/2+2/\varphi+c}$ , which we believe to be sharp up to the  $(n_1 + n_2)^c$  factor. Lemma 3.7 can be also regarded as a special case of Theorem 2.4. To see this, when  $M(a) = 0$ , we solve equation (2.18) to obtain that

$$a_1 = \frac{n_1}{n_1 + n_2}, \quad a_2 = \frac{n_2 - p}{n_1 + n_2},$$

and plug them into (2.17). The proof of Theorem 2.4 is based on some recent developments in random matrix theory [20], and will be given in Appendix F of the supplement [41].

**2.3. The case of isotropic covariances.** In this subsection, we consider the setting where  $X^{(1)}$  and  $X^{(2)}$  are independent and have the same population covariance matrices  $\Sigma^{(1)} = \Sigma^{(2)}$ . However, the two tasks can have different sample sizes  $n_1 \neq n_2$ . In this case, we can obtain the exact asymptotic limits of the bias term (2.9) and the variance term (2.10). We will use these results to illustrate the effects of the bias-variance tradeoff and varying sample sizes on the performance of the HPS estimator.

**THEOREM 2.5.** *Under Assumption 2.1, suppose that  $\Sigma^{(1)} = \Sigma^{(2)}$  and the entries of  $Z^{(1)}$  and  $Z^{(2)}$  are i.i.d. Gaussian random variables. Then for any small constant  $c > 0$  and large constant  $C > 0$ , there exists a high probability event  $\Xi$ , on which the following estimates hold uniformly in all  $a \in \mathbb{R}$ :*

$$(2.19) \quad L_{\text{Var}}(a) = \sigma^2 [\mathcal{L}_1(a) + O(p^c/n_1)],$$



and

$$(2.20) \quad \begin{aligned} L_{\text{bias}}(a) &= \left[ \mathcal{L}_2(a) + O\left(p^{-1/2+c}\right) \right] \cdot \|\beta^{(1)} - a\beta^{(2)}\|^2 \\ &+ O\left[p^{-C} \left(\|\beta^{(1)}\|^2 + \|\beta^{(2)}\|^2\right)\right]. \end{aligned}$$

Here we define the functions

$$\begin{aligned} \mathcal{L}_1(a) &:= \frac{2p}{n_2(1 - \xi_2) + a^2 n_1(1 - \xi_1) + \sqrt{[n_2(1 - \xi_2) + a^2 n_1(1 - \xi_1)]^2 + 4a^2 n_2 n_1 (\xi_1 + \xi_2 - \xi_1 \xi_2)}}, \\ \mathcal{L}_2(a) &:= \frac{1}{a^2} \cdot \frac{1 - 2 \frac{\mathcal{L}_1(a)}{\xi_2[1 + \mathcal{L}_1(a)]} + \kappa(a)}{1 - \xi_2 \kappa(a)}, \end{aligned}$$

where we abbreviate  $\xi_1 := p/n_1$ ,  $\xi_2 := p/n_2$  and

$$\kappa(a) := \frac{\mathcal{L}_1(a)^2}{\xi_2^2[1 + \mathcal{L}_1(a)]^2} \left[ 1 - \frac{a^4 \mathcal{L}_1(a)^2}{\xi_1[1 + a^2 \mathcal{L}_1(a)]^2} \right]^{-1}.$$

We believe the convergence rates  $p^c/n_1$  and  $p^{-1/2+c}$  in (2.19) and (2.20) are both sharp up to the  $p^c$  factor. The proof of Theorem 2.5 will be given in Appendix D in the supplement [41]. For the variance estimate in (2.19), it is not necessary to assume the Gaussian distributions of the  $Z^{(1)}$  and  $Z^{(2)}$  entries. In fact, (2.19) is a special case of Theorem 2.4 below for the more general case with possibly different  $\Sigma^{(1)}$  and  $\Sigma^{(2)}$ . On the other hand, the Gaussian assumption is needed in our current proof of the bias limit (2.20). In the setting of Theorem 2.5, we can write

$$L_{\text{bias}}(a) = \mathbf{v}_a^\top (Z^{(1)})^\top Z^{(1)} \frac{1}{[a^2 (Z^{(1)})^\top Z^{(1)} + (Z^{(2)})^\top Z^{(2)}]^2} (Z^{(1)})^\top Z^{(1)} \mathbf{v}_a,$$

where we abbreviate  $\mathbf{v}(a) := (\Sigma^{(1)})^{1/2} (a\beta^{(1)} - a^2\beta^{(2)})$ . By the rotational invariance of  $(Z^{(1)})^\top Z^{(1)}$  and  $(Z^{(2)})^\top Z^{(2)}$ , we have that

$$(2.21) \quad L_{\text{bias}}(a) \approx \|\mathbf{v}_a\|^2 \frac{1}{p} \text{Tr} \left[ \frac{[(Z^{(1)})^\top Z^{(1)}]^2}{[a^2 (Z^{(1)})^\top Z^{(1)} + (Z^{(2)})^\top Z^{(2)}]^2} \right],$$

up to a small error. Notice that we can write (2.21) into a simpler form

$$L_{\text{bias}}(a) \approx \|\mathbf{v}_a\|^2 \frac{d}{dx} \bigg|_{x=0} \frac{1}{p} \text{Tr} \left[ \frac{1}{a^2 (Z^{(1)})^\top Z^{(1)} + x[(Z^{(1)})^\top Z^{(1)}]^2 + (Z^{(2)})^\top Z^{(2)}} \right].$$

It is well-known that the empirical spectral distributions (ESD) of  $(Z^{(i)})^\top Z^{(i)}$ ,  $i = 1, 2$ , satisfy the famous Marchenko-Pastur (MP) law asymptotically [25]. From the MP law of  $(Z^{(1)})^\top Z^{(1)}$ , we can also derive the asymptotic ESD of  $a^2 (Z^{(1)})^\top Z^{(1)} + x[(Z^{(1)})^\top Z^{(1)}]^2$  for any fixed  $a \in \mathbb{R}$  and  $x > 0$ . Due to the rotational invariance of multivariate Gaussian distributions, the asymptotic ESD of  $a^2 (Z^{(1)})^\top Z^{(1)} + x[(Z^{(1)})^\top Z^{(1)}]^2 + (Z^{(2)})^\top Z^{(2)}$  is given by the free additive convolution (or free addition) of the asymptotic ESD of  $a^2 (Z^{(1)})^\top Z^{(1)} + x[(Z^{(1)})^\top Z^{(1)}]^2$  and the MP law of  $(Z^{(2)})^\top Z^{(2)}$  [28]. In particular, a sharp convergence estimate has been proved in [5, 6] for the free addition of two probability measures. We use that result to obtain a convergence estimate on

$$\frac{1}{p} \text{Tr} \left[ \frac{1}{a^2 (Z^{(1)})^\top Z^{(1)} + x[(Z^{(1)})^\top Z^{(1)}]^2 + (Z^{(2)})^\top Z^{(2)}} \right].$$

Taking derivative with respect to  $x$  at  $x = 0$  gives the exact asymptotic limit of  $L_{\text{bias}}(a)$ . We refer the reader to Appendix D of the supplement [41] for more details.

We believe that the above argument can be extended to the case without the Gaussian assumption. For example, instead of using the results in [5, 6] on free addition, we can use the sharp local laws on polynomials of random matrices in [3]. However, to apply the result in [3], we need to check some difficult technical regularity conditions for our setting, which is not the focus of this work. Hence we do not pursue this direction in this paper.

**2.4. Proof overview.** For the rest of this section, we present an overview of the proof of Theorem 2.4. The central quantity of interest is the inverse of the sum of two sample covariance matrices. We note that the variance equation  $\text{Tr}[\Sigma^{(2)}\hat{\Sigma}^{-1}]$  is equal to  $(n_1 + n_2)^{-1} \text{Tr}[W^{-1}]$ , where  $W$  is

$$(2.22) \quad \frac{\Lambda U^\top (Z^{(1)})^\top Z^{(1)} U \Lambda + V^\top (Z^{(2)})^\top Z^{(2)} V}{n_1 + n_2}.$$

Here  $U \Lambda V^\top$  is defined as the SVD of  $M$ . This formulation is helpful because we know that  $(Z^{(1)})^\top Z^{(1)}$  and  $(Z^{(2)})^\top Z^{(2)}$  are both sample covariance matrices with isotropic population covariance, and  $U, V$  are both orthonormal matrices. For example, if  $Z^{(1)}, Z^{(2)}$  are both Gaussian random matrices, by rotational invariance,  $Z^{(1)}U, Z^{(2)}V$  are still Gaussian random matrices.

Our proof uses the Stieltjes transform or the resolvent method in random matrix theory. We briefly describe the key ideas and refer the interested readers to classical texts such as [4, 37, 16]. For any probability measure  $\mu$  supported on  $[0, \infty)$ , the Stieltjes transform of  $\mu$  is a complex function defined as

$$m_\mu(z) := \int_0^\infty \frac{d\mu(x)}{x - z}, \text{ for any complex } z \in \mathbb{C} \setminus \{0\}.$$

Thus, the Stieltjes transform method reduces the study of a probability measure  $\mu$  to the study of a complex function  $m_\mu(z)$ .

Let  $\mu = p^{-1} \sum_i \delta_{\sigma_i}$  denote the empirical spectral distribution of  $W$ , where the  $\sigma_i$ 's are the eigenvalues of  $W$  and  $\delta_{\sigma_i}$  is the point mass measure at  $\sigma_i$ . Then it is easy to see that the Stieltjes transform of  $\mu$  is equal to

$$m_\mu(z) := \frac{1}{p} \sum_{i=1}^p \frac{1}{\sigma_i - z} = p^{-1} \text{Tr}[(W - z \text{Id})^{-1}].$$

The above matrix  $(W - z \text{Id})^{-1}$  is known as  $W$ 's resolvent or Green's function. We prove the convergence of  $W$ 's resolvent using the so-called "local law" with a sharp convergence rate [11, 16, 20].

We say that  $(W - z \text{Id})^{-1}$  converges to a deterministic  $p \times p$  matrix limit  $R(z)$  if for any sequence of deterministic unit vectors  $v \in \mathbb{R}^p$ ,

$$v^\top [(W - z \text{Id})^{-1} - R(z)] v \rightarrow 0 \text{ when } p \text{ goes to infinity.}$$

To study  $W$ 's resolvent, we observe that  $W$  is equal to  $FF^\top$  for a  $p$  by  $n_1 + n_2$  matrix

$$(2.23) \quad F := (n_1 + n_2)^{-1/2} [\Lambda U^\top (Z^{(1)})^\top, V^\top (Z^{(2)})^\top].$$

Consider the following symmetric block matrix whose dimension is  $p + n_1 + n_2$

$$(2.24) \quad H := \begin{pmatrix} 0 & F \\ F^\top & 0 \end{pmatrix}.$$

For this block matrix, we define its resolvent as

$$G(z) := \left[ H - \begin{pmatrix} z \text{Id}_{p \times p} & 0 \\ 0 & \text{Id}_{(n_1+n_2) \times (n_1+n_2)} \end{pmatrix} \right]^{-1},$$

for any complex value  $z \in \mathbb{C}$ . Using Schur complement formula for the inverse of a block matrix, it is not hard to verify that

$$(2.25) \quad G(z) = \begin{pmatrix} (W - z \text{Id})^{-1} & (W - z \text{Id})^{-1} F \\ F^\top (W - z \text{Id})^{-1} & z(F^\top F - z \text{Id})^{-1} \end{pmatrix}.$$

**Variance asymptotic limit.** In Theorem ??, we will show that for  $z$  in a small neighborhood around 0, when  $p$  goes to infinity,  $G(z)$  converges to the following limit

$$(2.26) \quad \mathfrak{G}(z) := \begin{pmatrix} (a_1(z)\Lambda^2 + (a_2(z) - z) \text{Id}_{p \times p})^{-1} & 0 & 0 \\ 0 & -\frac{n_1+n_2}{n_1} a_1(z) \text{Id}_{n_1 \times n_1} & 0 \\ 0 & 0 & -\frac{n_1+n_2}{n_2} a_2(z) \text{Id}_{n_2 \times n_2} \end{pmatrix},$$

where  $a_1(z)$  and  $a_2(z)$  are the unique solutions to the following self-consistent equations

$$(2.27) \quad \begin{aligned} a_1(z) + a_2(z) &= 1 - \frac{1}{n_1 + n_2} \left( \sum_{i=1}^p \frac{\lambda_i^2 a_1(z) + a_2(z)}{\lambda_i^2 a_1(z) + a_2(z) - z} \right), \\ a_1(z) + \frac{1}{n_1 + n_2} \left( \sum_{i=1}^p \frac{\lambda_i^2 a_1(z)}{\lambda_i^2 a_1(z) + a_2(z) - z} \right) &= \frac{n_1}{n_1 + n_2}. \end{aligned}$$

The existence and uniqueness of solutions to the above system are shown in Lemma F.5. Given this result, we now show that when  $z = 0$ , the matrix limit  $\mathfrak{G}(0)$  implies the variance limit shown in equation (2.17). First, we have that  $a_1 = a_1(0)$  and  $a_2 = a_2(0)$  since the equations in (2.27) reduce to equation (2.18) when  $z = 0$ . Second, since  $W^{-1}$  is the upper-left block matrix of  $G(0)$ , we have that  $W^{-1}$  converges to  $(a_1 \Lambda^2 + a_2 \text{Id})^{-1}$ . Using the fact that  $\text{Tr}[\Sigma^{(2)} \hat{\Sigma}^{-1}] = (n_1 + n_2)^{-1} \text{Tr}[W^{-1}]$ , we get that when  $p$  goes to infinity,

$$\begin{aligned} \text{Tr}[\Sigma^{(2)} \hat{\Sigma}] &\rightarrow \frac{1}{n_1 + n_2} \text{Tr}[(a_1 \Lambda^2 + a_2 \text{Id})^{-1}] = \frac{1}{n_1 + n_2} \text{Tr}[(a_1 M^\top M + a_2 \text{Id})^{-1}] \\ &= \frac{1}{n_1 + n_2} \text{Tr}[\Sigma^{(2)} (a_1 \Sigma^{(1)} + a_2 \Sigma^{(2)})^{-1}], \end{aligned}$$

where we note that  $M^\top M = (\Sigma^{(2)})^{-1/2} \Sigma^{(1)} (\Sigma^{(2)})^{-1/2}$  and its SVD is equal to  $V^\top \Lambda^2 V$ .

**Bias asymptotic limit.** For the bias limit in equation (3.2), we show that it is governed by the derivative of  $(W - z \text{Id})^2$  with respect to  $z$  at  $z = 0$ . First, we can express the empirical bias term in equation (3.2) as

$$(2.28) \quad (n_1 + n_2)^2 \hat{\Sigma}^{-1} \Sigma^{(2)} \hat{\Sigma}^{-1} = \Sigma^{(2)^{-1/2}} V W^{-2} V^\top \Sigma^{(2)^{-1/2}}.$$

Let  $\mathcal{G}(z) := (W - z \text{Id})^{-1}$  denote the resolvent of  $W$ . Our key observation is that  $\frac{d\mathcal{G}(z)}{dz} = \mathcal{G}^2(z)$ . Hence, provided that the limit of  $(W - z \text{Id})^{-1}$  is  $(a_1(z)\Lambda^2 + (a_2(z) - z) \text{Id})^{-1}$  near  $z = 0$ , the limit of  $\frac{d\mathcal{G}(0)}{dz}$  satisfies

$$(2.29) \quad \frac{d\mathcal{G}(0)}{dz} \rightarrow \frac{-\frac{da_1(0)}{dz} \Lambda^2 - (\frac{da_2(0)}{dz} - 1) \text{Id}}{(a_1(0)\Lambda^2 + a_2(0) \text{Id}_p)^2}.$$

To find the derivatives of  $a_1(z)$  and  $a_2(z)$ , we take the derivatives on both sides of the system of equations (2.27). Let  $a_3 = -\frac{da_1(0)}{dz}$  and  $a_4 = -\frac{da_2(0)}{dz}$ . One can verify that  $a_3$  and  $a_4$  satisfy

the self-consistent equations in (3.3) (details omitted). Applying equation (2.29) to equation (2.28), we obtain the bias limit.

As a remark, in order for  $\frac{d\mathcal{G}(z)}{dz}$  to stay close to its limit at  $z = 0$ , we not only need to find the limit of  $\mathcal{G}(0)$ , but also the limit of  $\mathcal{G}(z)$  within a small neighborhood of 0. This is why we consider  $W$ 's resolvent for a general  $z$  (as opposed to the Stieljes transform of its empirical spectral distribution discussed earlier).

**Schur complement and self-consistent equations.** First, we consider the special case where  $Z^{(1)}$  and  $Z^{(2)}$  are both multivariate Gaussian random matrices. By rotational invariance, we have that  $Z^{(1)}U$  and  $Z^{(2)}V$  are still multivariate Gaussian random matrices. Next, we use the Schur complement formula to deal with the resolvent  $G(z)$ . We show that  $G(z)$ 's diagonal entries satisfy a set of self-consistent equations in the limit, leading to equations in (2.27). On the other hand,  $G(z)$ 's off-diagonal entries are approximately zero using standard concentration bounds. Finally, we extend our result to general random matrices under the finite  $\varphi$ -th moment condition. We prove an anisotropic local law using recent developments in random matrix theory [16, 20]. The proof of Theorem 2.4 is shown in Appendix F.

### 3. Theoretical insights.

#### 3.1. Does covariate shift help or hurt performance?

EXAMPLE 3.1. To illustrate the effect of covariate shift, we consider a similar setting as in Example 3.4, such that (3.5) holds. In Proposition 3.5, we have seen that the global minimizer  $\hat{a}$  is close to 1 up to a small error. Hence we take  $a = 1$  in (2.17), and study the asymptotic limit

$$\ell_{\text{Var}}(M) := \frac{\sigma^2}{n_1 + n_2} \text{Tr} \left[ \frac{1}{a_1(M) \cdot M^\top M + a_2(M)} \right],$$

where  $M = (\Sigma^{(1)})^{1/2}(\Sigma^{(2)})^{-1/2}$ , and  $a_1(M)$  and  $a_2(M)$  are defined through (2.18). We compare different choices of  $M$  that are scaled to have the same determinant. More precisely, for a fixed  $\mu > 0$  we define

$$\mathcal{S}_\mu := \left\{ M \left| \prod_{i=1}^p \lambda_i = \mu^p, \tau \leq \lambda_p \leq \lambda_1 \leq \tau^{-1} \right. \right\}.$$

Our first observation is that if  $n_1 \gg n_2$ , i.e. there is enough source data compared to the target data, then  $\ell_{\text{Var}}(M)$  is minimized approximately when  $M$  is a scalar matrix. In fact, from equation (2.18), we obtain the following estimates on  $a_1(M)$  and  $a_2(M)$  for any  $M \in \mathcal{S}_\mu$ :

$$(3.1) \quad a_1(M) = \frac{n_1 + O(p)}{n_1 + n_2}, \quad a_2(M) = \frac{n_2 + O(p)}{n_1 + n_2}.$$

Inserting (3.1) into  $\ell_{\text{Var}}(M)$ , we obtain that

$$\ell_{\text{Var}}(M) = \left[ 1 + O\left(\frac{n_2}{n_1}\right) \right] \cdot \frac{\sigma^2}{n_1} \text{Tr} \left( \frac{1}{M^\top M} \right).$$

By AM-GM inequality, we observe that

$$\text{Tr} \left( \frac{1}{M^\top M} \right) = \sum_{i=1}^p \frac{1}{\lambda_i^2}$$

is minimized when  $\lambda_1 = \dots = \lambda_p = \mu$  under the restriction  $\prod_{i=1}^p \lambda_i = \mu^p$ . Hence in this case,  $M = \mu \text{Id}_{p \times p}$  is approximately the optimal choice.

However, we now use an example to show that the above observation fails when  $n_1$  is comparable to  $n_2$ . We take  $\mu = 1$ , and consider the subset of covariate shift matrices satisfying  $M = M^{-1}$ . In other words, half of the singular values of  $M$  satisfy that  $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_{p/2} \geq 1$ , while the other half eigenvalues are  $\lambda_{p/2}^{-1} \geq \dots \geq \lambda_2^{-1} \geq \lambda_1^{-1}$ . When  $\lambda_1/\lambda_{p/2} = 1$ , we have  $M = \text{Id}_{p \times p}$  and there is no covariate shift. We claim the following dichotomy.

- (i) If  $n_1 \geq n_2$ , then the variance limit is smallest when there is no covariate shift.
- (ii) If  $n_1 < n_2$ , then the variance limit is largest when there is no covariate shift.

We explain why the above dichotomy happens. We can write the variance limit as

$$\ell_{\text{Var}}(M) = \frac{\sigma^2}{n_1 + n_2} \sum_{i=1}^{p/2} \left( \frac{1}{\lambda_i^2 a_1 + a_2} + \frac{1}{\lambda_i^{-2} a_1 + a_2} \right).$$

When  $M = \text{Id}_{p \times p}$ , by the first equation of (2.18), we have

$$\ell_{\text{Var}}(\text{Id}_{p \times p}) = \frac{\sigma^2}{n_1 + n_2} \sum_{i=1}^{p/2} \frac{2}{1 - \gamma},$$

where we abbreviate  $\gamma := p/(n_1 + n_2)$ . Then using  $a_1 + a_2 = 1 - \gamma$ , through a direct calculation we find that

$$\ell_{\text{Var}}(M) - \ell_{\text{Var}}(\text{Id}_{p \times p}) = \frac{\sigma^2}{n_1 + n_2 - p} \sum_{i=1}^{p/2} \frac{(\lambda_i^2 - 1)^2 a_1(M) [a_1(M) - a_2(M)]}{[a_1(M) + \lambda_i^2 a_2(M)][\lambda_i^2 a_1(M) + a_2(M)]}.$$

We claim that  $a_1(M) > a_2(M)$  if and only if  $n_1 > n_2$ , which then explains the dichotomy. In fact, if  $a_1 > a_2$ , then the first equation in (2.18) gives that  $a_1 > (1 - \gamma)/2$ , and the second equation in (2.18) gives that

$$\frac{n_1}{n_1 + n_2} > a_1 + \frac{1}{n_1 + n_2} \sum_{i=1}^{p/2} \left( \frac{\lambda_i^2}{\lambda_i^2 + 1} + \frac{\lambda_i^{-2}}{\lambda_i^{-2} + 1} \right) = \frac{1 - \gamma}{2} + \frac{\gamma}{2} = \frac{1}{2}.$$

This implies  $n_1 > n_2$ . The other direction follows from a similar argument.

For the bias limit, we have the following proposition.

**PROPOSITION 3.2.** *Under Assumption 2.1, for any small constant  $c > 0$  and large constant  $C > 0$ , there exists a high probability event  $\Xi$ , on which the following estimate holds for  $L_{\text{bias}}(a)$  in (2.9):*

$$\begin{aligned} & \left| L_{\text{bias}}(a) - (\beta^{(1)} - a\beta^{(2)})^\top (\Sigma^{(1)})^{1/2} \Pi(a) (\Sigma^{(1)})^{1/2} (\beta^{(1)} - a\beta^{(2)}) \right| \\ & \leq \left[ \left( 1 + \sqrt{\frac{p}{n_1}} \right)^4 - 1 + O\left(n_1^{-1/2+2/\varphi+c}\right) \right] \frac{n_1^2 \lambda_1^2 \|(\Sigma^{(1)})^{1/2} (\beta^{(1)} - a\beta^{(2)})\|^2}{[(\sqrt{n_1} - \sqrt{p})^2 \lambda_p^2 + (\sqrt{n_2} - \sqrt{p})^2]^2} \\ (3.2) \quad & + p^{-C} \left[ \|\beta^{(1)}\|^2 + \|\beta^{(2)}\|^2 \right], \end{aligned}$$

uniformly in all  $a \in \mathbb{R}$ . Here  $\lambda_1$  and  $\lambda_p$  are respectively the largest and smallest singular values of  $M(a)$ ,  $\Pi(a)$  is a  $p \times p$  matrix defined as

$$\Pi(a) := \frac{n_1^2}{(n_1 + n_2)^2} M(a) \frac{a_3 M(a)^\top M(a) + (a_4 + 1)}{[a_1 M(a)^\top M(a) + a_2]^2} M(a)^\top,$$

and  $(a_3, a_4)$  is the solution of the following system of equations

$$(3.3) \quad \begin{aligned} a_3 + a_4 &= \frac{1}{n_1 + n_2} \sum_{i=1}^p \frac{1}{\lambda_i^2 a_1 + a_2}, \\ a_3 + \frac{1}{n_1 + n_2} \sum_{i=1}^p \frac{\lambda_i^2 (a_2 a_3 - a_1 a_4)}{(\lambda_i^2 a_1 + a_2)^2} &= \frac{1}{n_1 + n_2} \sum_{i=1}^p \frac{\lambda_i^2 a_1}{(\lambda_i^2 a_1 + a_2)^2}, \end{aligned}$$

where we recall that  $(a_1, a_2)$  is the solution of (2.18).

Note that the first error term on the right-hand side of (3.2) is typically smaller than the main term  $(\beta^{(1)} - a\beta^{(2)})^\top (\Sigma^{(1)})^{1/2} \Pi(a) (\Sigma^{(1)})^{1/2} (\beta^{(1)} - a\beta^{(2)})$  by a factor of  $O(\sqrt{p/n_1} + n_1^{-1/2+2/\varphi+c})$ . Hence (3.2) only gives an exact asymptotic limit in the regime  $n_1 \gg p$ . Moreover, by equations (2.18) and (3.3) we have

$$a_1 = \frac{n_1}{n_1 + n_2} + O\left(\frac{p}{n_1 + n_2}\right), \quad a_3 = \frac{n_3}{n_1 + n_2} + O\left(\frac{p}{n_1 + n_2}\right),$$

and

$$a_3 = O\left(\frac{p}{n_1 + n_2}\right), \quad a_4 = O\left(\frac{p}{n_1 + n_2}\right).$$

Using these estimates, it is easy to check that

$$(3.4) \quad \begin{aligned} &(\beta^{(1)} - a\beta^{(2)})^\top (\Sigma^{(1)})^{1/2} \Pi(a) (\Sigma^{(1)})^{1/2} (\beta^{(1)} - a\beta^{(2)}) \\ &= \left\| (\Sigma^{(2)})^{1/2} \frac{1}{a^2 \Sigma^{(1)} + \Sigma^{(2)}} a \Sigma^{(1)} (\beta^{(1)} - a\beta^{(2)}) \right\|^2 + O\left(\frac{p \|\beta^{(1)} - a\beta^{(2)}\|^2}{n_1 + n_2}\right). \end{aligned}$$

Hence (3.2) is consistent with the result obtained by replacing  $(X^{(1)})^\top X^{(1)}$  and  $(X^{(2)})^\top X^{(2)}$  with  $n_1 \Sigma^{(1)}$  and  $n_2 \Sigma^{(2)}$ , respectively, in  $L_{\text{bias}}(a)$  using the law of large numbers in the regime  $n_1 \gg p$ . However, simulations show that our estimate (3.2) is more precise than the first term on the right-hand side of (3.4).

**REMARK 3.3.** The main error in Proposition 3.2 comes from approximating  $(Z^{(1)})^\top Z^{(1)}$  by  $n_1 \text{Id}_{n_1 \times n_2}$  using Corollary A.7 in the supplement [41]. In order to improve this estimate and obtain an exact asymptotic result, one needs to study the singular value distribution of the random matrix  $\mathcal{X} + a^2$  for any fixed  $a \in \mathbb{R}$ , where  $\mathcal{X} := [(X^{(1)})^\top X^{(1)}]^{-1} (X^{(2)})^\top X^{(2)}$ . We remark that the eigenvalues of  $\mathcal{X}$  have been studied in the name of Fisher matrices [44]. However, since  $\mathcal{X}$  is not symmetric, its singular values are different from its eigenvalues. To the best of our knowledge, the asymptotic singular value behavior of  $\mathcal{X}$  is still an open problem in random matrix theory, and the study of the singular values of  $\mathcal{X} + a^2$  will be even harder. We leave this problem to future study.

We also remark for the general case with covariate shift, the method in Section 2.3 for the bias term also fails, because we cannot reduce the problem into the free addition of two random matrices that are asymptotically freely independent.

[FY: add simulations to check our results] <<HZ notes: there will be a separate section next to describe the examples>>

To describe quantitatively the bias-variance tradeoff phenomenon and the effect of varying sample sizes on the predication loss, we consider a *random-effect model*, which has been studied for single-task linear regression and ridge regression (see e.g. [14, 15]).

EXAMPLE 3.4. Suppose each  $\beta^{(i)}$  consists of two random components, one that is shared among the two tasks and one that is task-specific. More precisely, we let

$$\beta^{(i)} = \beta_0 + \tilde{\beta}^{(i)}, \quad i = 1, 2,$$

where  $\beta_0$  denotes the shared component, and  $\tilde{\beta}^{(i)}$  denotes the  $i$ -th task-specific component whose entries are i.i.d. Gaussian random variables of mean zero and variance  $p^{-1}d^2$ . First, we show that if  $\|\beta_0\|^2 \gg d^2$ , then the global minimizer  $\hat{a}$  of the function  $g(a)$  in (??) is close to 1. The proof of Proposition 3.5 will be given in Appendix E.

PROPOSITION 3.5. Suppose Assumption 2.1 and the above setting of random effect model hold. Suppose that for a constant  $c_0 > 0$ ,

$$(3.5) \quad \|\beta_0\|^2 \geq p^{c_0} d^2 + p^{-1/2+c_0} \sigma^2.$$

Then we have that for any small constant  $c > 0$  and large constant  $C > 0$ ,

$$(3.6) \quad \hat{a} = 1 + O\left(\frac{d^2}{\|\beta_0\|^2} + p^{-1/4+c} \frac{d + \sigma}{\|\beta_0\|} + p^{-C}\right) \quad w.h.p.$$

We emphasize that unlike Theorem 2.5, for Proposition 3.5 we do not assume  $\Sigma^{(1)} = \Sigma^{(2)}$  and the Gaussian distributions of the entries of  $Z^{(1)}$  and  $Z^{(2)}$ . Combining Lemma 2.2, Theorem 2.5 and Proposition 3.5, and using that  $\|\beta^{(1)} - \beta^{(2)}\|^2 = (2 + o(1))d^2$  with high probability, the predication loss  $L(\hat{\beta}_2^{\text{HPS}}(\hat{a}))$  is approximately equal to

$$\ell(n_1, n_2) = \sigma^2 \mathcal{L}_1(1) + 2d^2 \mathcal{L}_2(1) = \frac{p\sigma^2}{n_1 + n_2 - p} + 2d^2 \frac{n_1^2(n_1 + n_2 - p) + pn_1n_2}{(n_1 + n_2)^2(n_1 + n_2 - p)},$$

with high probability, where in the second step we obtain  $\mathcal{L}_1(1)$  and  $\mathcal{L}_2(1)$  through direct calculations. Now we compare  $\ell(n_1, n_2)$  with (2.14). First, we notice that the variance term  $\sigma^2 \mathcal{L}_1(1)$  is smaller than  $L(\hat{\beta}_2^{\text{OLS}})$ , while the bias term always increases (because the bias in single-task linear regression is zero). This gives a *bias-variance tradeoff* for the predication loss of the HPS estimator. Second, calculating the derivative with respect to  $n_1$ , it is not hard to see that the variance term always decreases as  $n_1$  increases, while the bias term always increases with  $n_1$ . Hence how the performance of the HPS estimator changes with respect to  $n_1$  also depends on an intricate bias-variance tradeoff.

Now fix an  $n_2$ , we study the bias-variance tradeoff with respect to  $n_1$  using the following function of  $\rho := \rho_1 + \rho_2$ , which is  $L(\hat{\beta}_2^{\text{OLS}}) - \ell(n_1, n_2)$  divided by  $2d^2$ :

$$h(\rho) := \frac{p}{n_2 - p} \cdot \frac{\sigma^2}{2d^2} - \frac{\ell(\rho_1 p, \rho_2 p)}{2d^2} = \frac{\rho - \rho_2}{(\rho - 1)(\rho_2 - 1)} \cdot \frac{\sigma^2}{2d^2} - \frac{(\rho - \rho_2)^2(\rho - 1) + (\rho - \rho_2)\rho_2}{\rho^2(\rho - 1)}.$$

This function characterizes  $L(\hat{\beta}_2^{\text{OLS}}) - L(\hat{\beta}_2^{\text{HPS}}(\hat{a}))$ , and hence gives the quantitative information transfer from the source task to the target task. First, we have positive (resp. negative) transfer if and only if  $h(\rho) > 0$  (resp.  $h(\rho) < 0$ ). Moreover, the sign of  $h(\rho)$  is determined by the sign of the second order polynomial

$$(3.7) \quad \left(\frac{1}{\rho_2 - 1} \cdot \frac{\sigma^2}{2d^2} - 1\right) \rho^2 + (\rho_2 + 1)\rho - 2\rho_2.$$

We observe the following dichotomy.

- (i) If  $\frac{1}{\rho_2 - 1} \cdot \frac{\sigma^2}{2d^2} - 1 > 0$ , then the polynomial (3.7) is positive for all  $\rho \in (\rho_2 + 1, \infty)$ , so that the transfer is always positive.
- (ii) If  $\frac{1}{\rho_2 - 1} \cdot \frac{\sigma^2}{2d^2} - 1 < 0$ , then we have the following cases.

- If  $(\rho_2 + 1)^2 < 8\rho_2 \left(1 - \frac{1}{\rho_2 - 1} \cdot \frac{\sigma^2}{2d^2}\right)$ , the polynomial (3.7) is negative for all  $\rho$ , so that the transfer is always negative.
- If  $(\rho_2 + 1)^2 > 8\rho_2 \left(1 - \frac{1}{\rho_2 - 1} \cdot \frac{\sigma^2}{2d^2}\right)$ , the polynomial (3.7) has two positive roots, where one of them is always smaller than  $\rho_2 + 1$ . Hence if the larger root, say  $\rho_c$ , is smaller than  $\rho_2 + 1$ , then the transfer is always negative for  $\rho \in (\rho_2 + 1, \infty)$ ; otherwise, there is a transition from positive transfer to negative transfer as  $\rho$  crosses  $\rho_c$ .

Second, we calculate the derivative of  $h(\rho)$ , and find that its sign is determined by the sign of the third order polynomial

$$(3.8) \quad \frac{1}{\rho_2} \cdot \frac{\sigma^2}{2d^2} \rho^3 - 2(\rho - \rho_2)(\rho - 1)(\rho - 2) - (\rho_2 - 1)\rho.$$

Then we observe the following dichotomy.

- If  $\frac{1}{\rho_2} \cdot \frac{\sigma^2}{2d^2} > 2$ , the polynomial (3.8) is always positive for all  $\rho \in (\rho_2 + 1, \infty)$ , so that the information transfer always increases as  $n_1$  increases.
- If  $\frac{1}{\rho_2} \cdot \frac{\sigma^2}{2d^2} < 2$ , the polynomial (3.8) is positive initially around  $\rho = \rho_2 + 1$ , and then becomes negative when  $\rho$  crosses its unique root, say  $\rho_c$ , in  $(\rho_2 + 1, \infty)$ . Hence the information transfer achieves the global maximum at  $\rho = \rho_c$ .

*3.1.0.1. How does hard parameter sharing scale with sample size  $n$ ?* Obviously, the concentration error decreases with  $n$ . First, we consider the variance of  $\hat{\beta}_i^{\text{HPS}}$ , which is  $\sigma^2 \|a_i^*\|^2 \text{Tr} [\Sigma(X^\top X)^{-1}]$ ? It turns out that this quantity converges to a fixed limit in the high-dimensional setting, which is formally stated in the following assumption.

**ASSUMPTION 3.6.** Let  $\tau > 0$  be a small enough constant. In the high-dimensional setting, the sample size  $n$  grows to infinity proportionally with the feature dimension  $p$ , i.e.  $n/p \rightarrow \rho \in (\tau, 1/\tau)$  as  $p$  goes to infinity.

Under the above assumption, we can use the following result to simplify the variance of  $\hat{\beta}_i^{\text{HPS}}$ .

**FACT 3.7** (cf. Theorem 2.4 in [11]). With high probability over the randomness of  $X$ , we have that

$$\text{Tr} [\Sigma(X^\top X)^{-1}] = \frac{p}{n - p} \pm O(n^{-c_\varphi}).$$

*Remark.* The above result has a long history in random matrix theory. For a multivariate Gaussian random matrix, this result follows from the classical result for the mean of inverse Wishart distribution [1]. For a non-Gaussian random matrix, this result can be obtained using the well-known Stieltjes transform method (cf. Lemma 3.11 of [4]). Applying Fact 3.7 to Theorem 5.1, we obtain that hard parameter sharing's variance is

$$\sigma^2 \|a_i^*\|^2 \text{Tr} [\Sigma(X^\top X)^{-1}] = \sigma^2 \|a_i^*\|^2 \frac{p}{n - p} \pm O(p^{-c_\varphi}).$$

To illustrate the bias-variance tradeoff quantitatively, we consider an extension of the random-effect model in Example 3.4 to the multi-task setting.

**EXAMPLE 3.8.** Suppose that  $\beta^{(i)} = \beta_0 + \tilde{\beta}^{(i)}$  for  $i = 1, 2, \dots, t$ , where  $\beta_0$  denotes the shared component, and  $\tilde{\beta}^{(i)}$  denotes the  $i$ -th task-specific component whose entries are i.i.d.



Gaussian random variables of mean zero and variance  $p^{-1}d^2$ . In this random-effect model, using the concentration of Gaussian random vectors (e.g. Lemma A.5 in the supplement [41]), the  $(i, j)$ -th entry of  $B^{\star\top}\Sigma B^{\star}$  is equal to

$$(3.9) \quad \beta_i^{\top}\Sigma\beta_j = \beta_0^{\top}\Sigma\beta_0 + \delta_{ij}\frac{d^2}{p}\text{Tr}\Sigma + O\left(p^{-1/2+c}\|\beta_0\|^2 + p^{-1/2+c}d^2\right),$$

with high probability for any constant  $c > 0$ . We omit the details to show the error bound using Lemma A.5. With (3.9), it is easy to calculate that with high probability, the eigenvalues of  $B^{\star\top}\Sigma B^{\star}$  are given by

$$\lambda_1 = \left[1 + O(p^{-1/2+c})\right] \cdot \left(t\beta_0^{\top}\Sigma\beta_0 + \frac{d^2}{p}\text{Tr}\Sigma\right),$$

and

$$\lambda_i = \left[1 + O(p^{-1/2+c})\right] \cdot \frac{d^2}{p}\text{Tr}\Sigma, \quad i = 2, \dots, t.$$

Thus for the best rank- $r$  approximation  $A^{\star}A^{\star\top}$  of  $B^{\star\top}\Sigma B^{\star}$ , we have

$$\left\|\Sigma^{1/2}B^{\star}(A^{\star}A^{\star\top} - \text{Id}_{t \times t})\right\|_F^2 = [1 + O(p^{-1/2+c})] \cdot (t-r)\frac{d^2}{p}\text{Tr}\Sigma$$

with high probability. Then using (5.8), we obtain that

$$\frac{1}{t}\sum_{i=1}^t L_i(\hat{\beta}_i^{\text{HPS}}) = \left(1 - \frac{r}{t}\right)\frac{d^2}{p}\text{Tr}\Sigma + \frac{r}{t} \cdot \frac{p\sigma^2}{n-p} + o(\|\beta_0\|^2 + d^2 + \sigma^2), \quad \text{w.h.p.}$$

Comparing the above equation with (2.14) (and ignoring the small error), we have the following observations.

- (i) **Positive vs. negative transfer.** The averaged HPS prediction loss is smaller than the single-task OLS prediction loss if and only if  $\frac{d^2}{p}\text{Tr}\Sigma < \frac{p\sigma^2}{n-p}$ , that is, the “task-specific variance” is smaller than the “noise variance” up to some constant factor.
- (ii) **The optimal rank  $r$ .** If  $\frac{d^2}{p}\text{Tr}\Sigma < \frac{\sigma^2 p}{n-p}$ , then the smallest averaged HPS prediction loss is achieved when  $r = 1$ . Hence increasing the width  $r$  of the shared feature representation layer does not help.
- (iii) **Sample efficiency.** Suppose  $\frac{d^2}{p}\text{Tr}\Sigma < \frac{\sigma^2 p}{n-p}$  and we choose the optimal rank  $r = 1$ . Following [FY: add citation], we define the data efficiency ratio of HPS as the proportion of labelled data needed to achieve comparable performance to single-task linear regression. More precisely, for some  $x \in (0, 1)$ , if we only use  $xn$  many data, then the averaged HPS prediction loss is

$$\frac{1}{t}\sum_{i=1}^t L_i(\hat{\beta}_i^{\text{HPS}}, x) = \left(1 - \frac{1}{t}\right)\frac{d^2}{p}\text{Tr}\Sigma + \frac{1}{t} \cdot \frac{p\sigma^2}{xn-p} + o(d^2 + \sigma^2), \quad \text{with high probability.}$$

Comparing it to the single-task OLS prediction loss  $t^{-1}\sum_{i=1}^t L_i(\hat{\beta}_i^{\text{OLS}})$ , we find that HPS requires at most (recall that  $\rho = n/p$ )

$$x = \frac{1}{\rho} + \frac{1 - \rho^{-1}}{t - (t-1)(\rho-1)\frac{d^2}{\sigma^2} \cdot \frac{1}{p}\text{Tr}\Sigma}$$

proportion of the samples to achieve the same performance. This is the data efficiency ratio for the above random-effect model.

We demonstrate the accuracy of our results in simulations. While our theory is asymptotic (with error terms that are negligible when  $p$  is sufficiently large), we observe that they are incredibly accurate in a moderate dimension of  $p = 200$ .

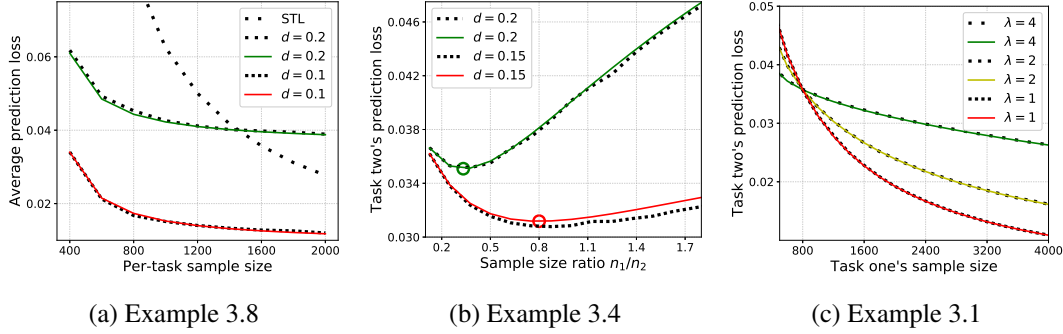


Fig 2: Our estimated losses (solid line) match the empirical losses (dotted line) accurately under various settings in dimension  $p = 200$ . **Left.** Validating Example 3.8 for ten tasks: the noise variance  $\sigma^2$  is  $1/4$ . **Middle.** Validating Example 3.4 for two tasks: we discover an interesting phenomena by fixing task two’s sample size and increasing task one’s sample size. Moreover, our result accurately predicts the critical point (marked in circle) of the loss curve. **Right.** We show how different levels of covariate shift affect hard parameter sharing when there is no bias. Having covariate shift increases task two’s prediction loss when task two’s sample size is smaller than task one. Otherwise, having covariate shift (surprisingly) decreases task two’s prediction loss.

*3.1.0.2. Sample efficiency.* First, we validate the result of Example 3.8. Figure 2a shows the average prediction loss over ten tasks as we increase the number of samples per-task from 400 to 2000. In all the parameter settings, our results estimate the empirical losses accurately. We also observe a trend that the average prediction loss increases as we increase distance  $d$  from 0.1 to 0.2. Our work explains the differences between these two settings since  $d^2 = 0.1^2$  is always smaller than  $\frac{\sigma^2 p}{n-p}$ , but  $d^2 = 0.2^2$  is not. Indeed, we observe a crossover point between hard parameter sharing and STL. Finally, for  $d = 0.2$ , looking horizontally, we find that HPS requires fewer samples per-task than STL to achieve the same loss level.

*3.1.0.3. Sample size ratio.* Second, we validate the result of Example 3.4. Figure 2b shows task two’s prediction loss as we increase the sample ratio  $n_1/n_2$  from  $1/10$  to  $7/10$ . We consider a regime where task two consists of 80,000 samples, and task one’s sample size varies from 8,000 to 56,000. The task-specific variance (which scales with model distance) is  $d = 0.2$ , the noise variance is  $\sigma^2 = 4^2$ , and the shared signal variance is 1. We observe that as we increase the sample ratio, task two’s prediction loss decreases initially but later will increase when the sample ratio is above a certain level. On the other hand, when  $d = 0.15$ , task two’s prediction loss decreases faster. Intuitively, this is because bias increases less for smaller  $d^2$ .

*3.1.0.4. Covariate shift.* Finally, we validate the result of Example 3.1. Figure 2c shows task two’s prediction loss as we increase task one’s sample size. Recall that  $\lambda$  measures the severity of covariate shifts—a larger  $\lambda$  means a larger covariate shift. We indeed observe the dichotomy in Example 3.1 at  $n_1 = 800$ . The sample size  $n_2$  is 800 and the noise variance  $\sigma^2$  is  $1/4$ .

**4. Algorithmic implications.** One estimator that is sometimes employed in the literature is simply an average of the OLS estimators for two tasks [7]

$$(4.1) \quad \hat{\beta}^{\text{AVE}}(\lambda) = \lambda \cdot \hat{\beta}_1^{\text{OLS}} + (1 - \lambda) \cdot \hat{\beta}_2^{\text{OLS}},$$

**Algorithm 1** An incremental training schedule for efficient multi-task learning with two tasks**Input:** Two tasks  $(X_1, Y_1)$  and  $(X_2, Y_2)$ .**Parameter:** A shared module  $B$ , output layers  $W_1, W_2$  as in the hard parameter sharing architecture.**Require:** # batches  $S$ , epochs  $T$ , task 2's validation accuracy  $\hat{g}(B; W_2)$ , a threshold  $\tau \in (0, 1)$ .**Output:** The trained modules  $B, W_2$  optimized for task 2.

```

1: Divide  $(X_1, Y_1)$  randomly into  $S$  batches:  $(x^{(1)}, y^{(1)}), \dots, (x^{(S)}, y^{(S)})$ .
2: for  $i = 1, \dots, S$  do
3:   for  $j = 1, \dots, T$  do
4:     Update  $B, W_1, W_2$  using the training data  $\{x^{(k)}, y^{(k)}\}_{k=1}^i$  and  $(X_2, Y_2)$ .
5:   end for
6:   Let  $a_i = \hat{g}(B; W_2)$  be the validation accuracy.
7:   if  $a_i < a_{i-1}$  or  $a_i > \tau$  then
8:     break
9:   end if
10: end for

```

where  $\lambda \in [0, 1]$  is an averaging parameter subject to choice in practice, and we recall that the OLS estimators are given by

$$\hat{\beta}_i^{\text{OLS}} = [(X^{(i)})^\top X^{(i)}]^{-1} (X^{(i)})^\top Y^{(i)}, \quad i = 1, 2.$$

The estimator in (4.1) is conventionally called an *averaging estimator*. In particular, when  $\lambda = 0$  and 1, we get the OLS estimators for tasks 2 and 1, respectively.

**4.0.0.1. Further Studies on Text Classification Tasks.** Our results and simulations are all in the high-dimensional linear regression setting. How well do they extend to other scenarios? In this section, we conduct further studies on six text classification datasets. Our datasets include a movie review sentiment dataset (MR) [31], a sentence subjectivity dataset (SUBJ) [30], a customer reviews dataset (CR) [19], a question type dataset (TREC) [24], an opinion polarity dataset (MPQA) [39], and the Stanford sentiment treebank (SST) dataset [35]. Our model consists of a word embedding layer with GloVe embeddings [32] followed by a long-short term memory (LSTM) or a multi-layer perceptron (MLP) layer [22].<sup>1</sup>

**4.0.0.2. Sample size ratio..** First, we show that our observation in Figure 2b also occurs in the text classification tasks. In Figure 3a, we observe that for multiple example task pairs, increasing task one's sample size improves task two's prediction accuracy initially, but hurts eventually. On the  $y$ -axis, we plot task two's test accuracy using HPS, subtracted by its STL test accuracy. We fix task two's sample size at 1000 and increase task one's sample size from 100 to 3000.

These examples and the one in Figure 2b suggest a natural progressive training schedule, where we add samples progressively until performance drops. Concretely, here is one implementation of this idea.

- We divide the training data into  $S$  batches. We divide the training procedure into  $S$  stages. During every stage, we progressively add one more data batch.
- During every stage, we train for  $T$  epochs using only the  $S$  batches. If the validation accuracy drops compared to the previous round's result or reach a desired threshold  $\tau$ , we terminate.

If we apply this procedure to the settings of Figure 3a and 2b, it will terminate once reaching the optimal sample ratio. The advantage of this procedure is that it reduces the computational

<sup>1</sup>For MLP, we apply an average pooling layer over word embeddings. For LSTM, we add a shared feature representation layer on top of word embeddings.

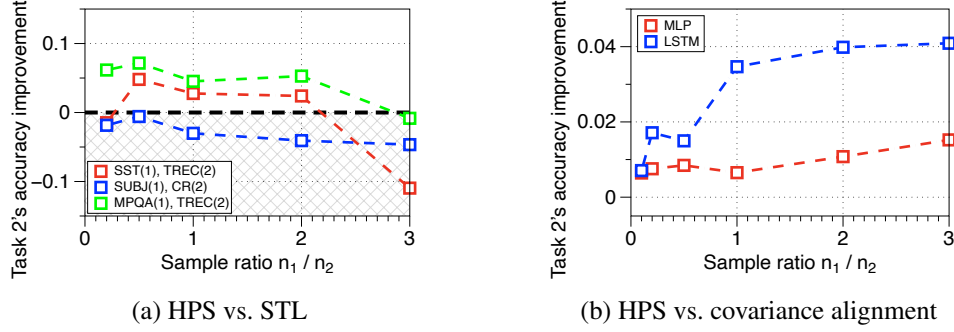


Fig 3: Comparing hard parameter sharing (HPS) to single-task learning (STL) and a covariance alignment approach proposed by [40]: In Figure 3a, we observe that for multiple task pairs, increasing task one’s sample size improves task two’s prediction accuracy initially, but hurts eventually – a phenomenon similar to Figure 2b. In Figure 3b, we observe that as task one’s sample size increases, covariance alignment improves more over HPS.

cost compared to standard round-robin training schedules. For example, if the procedure terminates at 30% of all batches, then SGD only passes over 30% of its data, whereas standard round-robin training passes over 100% of task one’s data.

We evaluate the progressive training procedure on the six text classification datasets. First, we conduct multi-task training over all 15 two-task pairs from the six datasets. We focus on task two’s test accuracy and set  $\tau$  as task two’s test accuracy obtained via the standard round-robin training schedule. We include all of task two’s data and progressively add task one’s data using the procedure described above. Since the prediction accuracy has been controlled the same, we compare the computational cost. We find that when averaged over all 15 two-task pairs, this procedure requires only 45% of the computational cost to reach the desired accuracy  $\tau$  for task two. Second, we conduct multi-task training on all six datasets jointly. We extend our procedure to all six datasets. We include the data from all tasks except SST. For SST, we progressively add data similar to the above procedure. We set  $\tau$  to be the average test accuracy of all six tasks obtained using standard round-robin training. We find that adding samples progressively from SST requires less than 35% of the computational cost to reach the same average test accuracy  $\tau$ .

**4.0.0.3. Covariate shift.** Recall from Example 3.1 that having covariate shifts worsens the variance (hence the loss) of hard parameter sharing when the sample ratio increases. This highlights the need for correcting covariate shifts when the sample size ratio rises. To this end, we study a covariance alignment procedure proposed in [40], designed to correct covariate shifts. The idea is to add an alignment module between the input and the shared module  $B$ . This module is then trained together with  $B$  and the output layers. We refer to [40] for more details about the procedure and the implementation.

We conduct multi-task training on all 15 task pairs from the six datasets. In Figure 3b, we measure the performance gains from performing covariance alignment vs. HPS. To get a robust comparison, we average the improvements over the 15 task pairs. The result shows that as the sample size ratio increases, performing covariance alignment provides more significant gains over HPS. We fix task two’s sample size at 1,000, and increase task one’s sample size from 1,000 to 3,000.

**5. Transferring from multiple source tasks.** Hard parameter sharing is a commonly used architecture in multi-task learning. However, there have been few theoretical results

on the performance of the HPS estimators in high-dimensional multi-task learning. In this section, we extend our results on the predication loss of the HPS estimator to a multi-task linear regression, where all tasks have the same covariates. We make this extension for the following reasons. First, its restriction to the two-task case provides a rare example where the output layers  $A_1$  and  $A_2$  can be characterized exactly. Second, the proof of the multi-task case is no harder than the two-task case, but it can provide much clearer geometric intuition as we will discuss below. Third, the corresponding multi-task setting is prevalent in applications of multi-task learning to image classification, where there are multiple prediction labels/tasks for every image [33, 17]. Finally, it provides useful insights into a more general theory of multi-task learning, which we will explore in greater details in future works.

**Multi-task setting.** Suppose we have  $t$  datasets whose sample sizes are all equal to  $n$  and whose feature covariates are all equal to  $X \in \mathbb{R}^{n \times p}$ . The label vector of the  $i$ -th task follows a linear model

$$Y^{(i)} = X\beta^{(i)} + \varepsilon^{(i)}, \quad i = 1, 2, \dots, t.$$

We assume that  $X = Z\Sigma^{1/2}$  is a random matrix satisfying the same assumption as  $X^{(2)}$  in Assumption 2.1, that is,  $Z$  is an  $n \times p$  random matrix with i.i.d. entries satisfying (1.2) and (2.1),  $\Sigma$  is a deterministic positive definite symmetric matrix satisfying (2.2) and (2.3), and  $\rho := n/p$  satisfies (2.5).  $\varepsilon^{(i)} \in \mathbb{R}^n$ ,  $i = 1, 2, \dots, t$ , are independent random vectors with i.i.d. entries of mean zero, variance  $\sigma^2$ , and bounded moments as in (2.4). Finally,  $X$ ,  $\varepsilon^{(i)}$  and  $\beta^{(i)}$ ,  $i = 1, 2, \dots, t$ , are all independent from each other.

To define the HPS parameter for the above setting, we study the following minimization problem

$$(5.1) \quad f(A, B) = \sum_{j=1}^t \left\| XBA_j - Y^{(j)} \right\|^2,$$

where  $B \in \mathbb{R}^{p \times r}$  is a rank- $r$  shared feature representation layer, and  $A := [A_1, A_2, \dots, A_t] \in \mathbb{R}^{r \times t}$  with  $A_i \in \mathbb{R}^r$  being a separate output layer for task  $i$ . We will focus on cases with  $r < t$ , because otherwise the global minimum of  $f(A, B)$  reduces to single-task learning (cf. Proposition 1 of [40]).

For the optimization objective in (5.1), using the local optimality condition over  $B$ , that is,  $\frac{\partial f}{\partial B} = 0$ , we obtain  $\hat{B}$  as a function of  $A$ :

$$(5.2) \quad \hat{B}(A) = (X^\top X)^{-1} X^\top Y A^\top (A A^\top)^+,$$

where  $Y := [Y^{(1)}, Y^{(2)}, \dots, Y^{(t)}]$  and  $(A A^\top)^+$  denotes the pseudoinverse of  $A A^\top$ . Plugging  $\hat{B}(A)$  into equation (5.1), we obtain the following objective that only depends on  $A$  (in matrix notation):

$$(5.3) \quad g(A) = \left\| X(X^\top X)^{-1} X^\top Y A^\top (A A^\top)^+ A - Y \right\|_F^2.$$

Let  $\hat{A}$  be the global minimizer of  $g(A)$ . Then  $(\hat{A}, \hat{B}(\hat{A}))$  is the global minimizer of  $f(A, B)$ . We define the HPS estimator for task  $i$  as  $\hat{\beta}_i^{\text{HPS}} := \hat{B}(\hat{A})\hat{A}_i$ , and its (out-of-sample) prediction loss as

$$(5.4) \quad L_i(\hat{\beta}_i^{\text{HPS}}) = \left\| \Sigma^{1/2} \left( \hat{\beta}_i^{\text{HPS}} - \beta^{(i)} \right) \right\|^2.$$

Our main result of this section, Theorem 5.1, shows that hard parameter sharing essentially approximates all tasks through a rank- $r$  subspace. To formalize this geometric intuition, as in the two-task case, we introduce the matrix  $B^* := [\beta^{(1)}, \beta^{(2)}, \dots, \beta^{(t)}] \in \mathbb{R}^{p \times t}$  formed by

the linear model parameters of all the  $t$  tasks. Let  $A^*A^{*\top}$  denote the best rank- $r$  subspace approximation of  $B^{*\top}\Sigma B^*$  (which can be regarded as the covariance of the task labels):

$$(5.5) \quad A^* := \arg \min_{U \in \mathbb{R}^{t \times r}: U^\top U = \text{Id}_{r \times r}} \langle UU^\top, B^{*\top}\Sigma B^* \rangle,$$

where  $\langle \cdot, \cdot \rangle$  denotes the Frobenius inner product between two matrices. To ensure that  $A^*$  is unique, we assume that the  $r$ -th largest eigenvalue of  $B^{*\top}\Sigma B^*$  is strictly larger than the  $(r+1)$ -th largest eigenvalue. Otherwise,  $A^*$  is not well-defined and Theorem 5.1 will give a null result. Let  $a_i^* := A^*A^{*\top}e_i \in \mathbb{R}^r$  denote the  $i$ -th column of  $A^*A^{*\top}$ , where  $e_i$  is the standard basis unit vector along  $i$ -th direction. Then we have the following result.

**THEOREM 5.1.** *Suppose the above multi-task setting holds. Let  $c > 0$  be an arbitrary (small) constant. Then for any task  $i = 1, \dots, t$ , we have that with high probability,*

$$(5.6) \quad \left\| \hat{A}^\top (\hat{A}\hat{A}^\top)^+ \hat{A} - A^*A^{*\top} \right\|_F \leq \left[ \frac{n^{-1/2+2/\varphi+c} \|B^{*\top}\Sigma B^*\| + n^{-1/2+c}\sigma^2}{\lambda_r - \lambda_{r+1}} \right]^{1/2},$$

where  $\lambda_r$  and  $\lambda_{r+1}$  are respectively the  $r$ -th and  $(r+1)$ -th largest eigenvalues of  $B^{*\top}\Sigma B^*$ . Moreover, the prediction loss of the HPS estimator  $\hat{\beta}_i^{\text{HPS}}$  satisfies that with high probability,

$$(5.7) \quad \left| L_i(\hat{\beta}_i^{\text{HPS}}) - L_i(B^*a_i^*) - \frac{p\sigma^2}{n-p} \|a_i^*\|^2 \right| \leq \left[ \frac{n^{-1/2+2/\varphi+c} \|B^{*\top}\Sigma B^*\| + n^{-1/2+c}\sigma^2}{\lambda_r - \lambda_{r+1}} \right]^{1/2} \left( \|B^{*\top}\Sigma B^*\| + \sigma^2 \right).$$

Finally, we have a better bound for the averaged prediction loss: with high probability,

$$(5.8) \quad \left| \frac{1}{t} \sum_{i=1}^t L_i(\hat{\beta}_i^{\text{HPS}}) - \frac{1}{t} \left\| \Sigma^{1/2} B^* (A^*A^{*\top} - \text{Id}_{t \times t}) \right\|_F^2 - \frac{p\sigma^2}{n-p} \cdot \frac{r}{t} \right| \leq n^{-1/2+2/\varphi+c} \|B^{*\top}\Sigma B^*\| + n^{-1/2+c}\sigma^2.$$

Recall that  $\varphi$  is a constant larger than 4, hence  $n^{-1/2+2/\varphi+c}$  is a negligible factor asymptotically as long as  $c$  is smaller than  $1/2 - 2/\varphi$ . Moreover, the factor  $(\lambda_r - \lambda_{r+1})^{-1}$  is natural, because the best rank- $r$  subspace approximation of  $B^{*\top}\Sigma B^*$  is not stable when  $\lambda_r$  and  $\lambda_{r+1}$  are close to each other. The bound (5.6) verifies our intuition that hard parameter sharing approximates the matrix  $B^{*\top}\Sigma B^*$  through a best rank- $r$  subspace. The estimate (5.7) gives the exact asymptotic limit of  $L_i(\hat{\beta}_i^{\text{HPS}}(\hat{a}))$ , which shows that the prediction loss of  $\hat{\beta}_i^{\text{HPS}}$  decomposes into a bias term  $L_i(B^*a_i^*)$  that measures the prediction loss of  $B^*a_i^*$ , plus a variance term that scales with  $\|a_i^*\|^2$ . Since  $\|a_i^*\|^2 \leq 1$ , compared with the single-task prediction loss (2.14), the variance term always decreases for the multi-task HPS estimator. On the other hand, the bias term always increases (because the bias in single-task linear regression is zero). Hence as in the transfer learning setting, whether the HPS estimator is better than the OLS estimator depends on an intricate bias-variance tradeoff. We can observe a similar bias-variance tradeoff for the averaged prediction loss in (5.8) using the fact that  $r < t$ . Note that the estimate (5.8) can be applied even when the best rank- $r$  subspace approximation of  $B^{*\top}\Sigma B^*$  is not unique. For all the estimates in Theorem 5.1, we believe that their convergence rates are asymptotically tight when  $n$  goes to infinity.

The proof of Theorem 5.1 will be given in Appendix C of the supplement [41]. Moreover, by setting  $t = 2$  in Theorem 5.1, we can obtain the prediction loss for the HPS estimator

for the transfer learning setting where the two tasks have the same covariates  $X^{(1)} = X^{(2)}$ . For the reader's convenience, we give the precise statement in Corollary 5.2. We define  $A^* \in \mathbb{R}^2$  as the normalized eigenvector corresponding to the larger eigenvalue of the  $2 \times 2$  matrix  $B^{*\top} \Sigma B^*$ , where recall that  $B^* := [\beta^{(1)}, \beta^{(2)}] \in \mathbb{R}^{p \times 2}$  by definition. Without loss of generality, we assume that the two eigenvalues of  $B^{*\top} \Sigma B^*$  are not degenerate, so that  $A^*$  is uniquely defined. In the following corollary, the estimate (5.9) shows that the minimizer  $\hat{a}$  is approximately equal to  $A^*(1)/A^*(2)$ , while (5.10) gives the exact asymptotic limit of  $L_2(\hat{\beta}_2^{\text{HPS}}(\hat{a}))$ , together with an explicit convergence rate that we believe to be sharp.

**COROLLARY 5.2.** *Under Assumption 2.1, suppose that  $X^{(1)} = X^{(2)}$  and  $n_1 = n_2 \equiv n$ . Let  $c > 0$  be an arbitrary (small) constant. Then we have that with high probability,*

$$(5.9) \quad \left\| u_{\hat{a}} u_{\hat{a}}^\top - A^* A^{*\top} \right\|_F \leq \left[ \frac{n^{-1/2+2/\varphi+c} \|B^{*\top} \Sigma B^*\| + n^{-1/2+c} \sigma^2}{\lambda_1 - \lambda_2} \right]^{1/2},$$

where  $u_{\hat{a}}$  is the unit vector defined as  $u_{\hat{a}} := \frac{1}{\hat{a}^2+1} \begin{pmatrix} \hat{a} \\ 1 \end{pmatrix}$ , and  $\lambda_1$  and  $\lambda_2$  are respectively the larger and smaller eigenvalues of  $B^{*\top} \Sigma B^*$ . Moreover, the prediction loss of the HPS estimator satisfies that with high probability,

$$(5.10) \quad \begin{aligned} & \left| L_2(\hat{\beta}_2^{\text{HPS}}(\hat{a})) - \left\| (\Sigma^{(2)})^{1/2} \left( A^*(2) \cdot B^* A^* - \beta^{(2)} \right) \right\|^2 - |A^*(2)|^2 \frac{p\sigma^2}{n-p} \right| \\ & \leq \left[ \frac{n^{-1/2+2/\varphi+c} \|B^{*\top} \Sigma B^*\| + n^{-1/2+c} \sigma^2}{\lambda_1 - \lambda_2} \right]^{1/2} \left( \|\Sigma^{1/2} B^*\|^2 + \sigma^2 \right), \end{aligned}$$

where  $A^*(2)$  denotes the second entry of  $A^*$ .

**6. Conclusions.** This work studied generalization properties of a widely used hard parameter sharing approach for multi-task learning. We provided sharp bias-variance tradeoffs of HPS in high-dimensional linear regression. Using these results, we analyzed how varying sample sizes and covariate shifts impact HPS, and rigorously explained several empirical phenomena such as negative transfer and covariate shift related to these dataset properties. We validated our theory and conducted further studies on text classification tasks. We describe several open questions for future work. First, our result in Corollary 2.5 involves an error term that scales down with  $n_1$ . Tightening this error bound requires showing the limit of  $\|(Z^{(1)\top} Z^{(1)} + Z^{(2)\top} Z^{(2)})^{-1} Z^{(1)\top} Z^{(1)}\|_F^2$  for two isotropic sample covariance matrices. This requires studying the asymptotic singular values distribution of the non-symmetric matrix  $(Z^{(1)\top} Z^{(1)})^{-1} Z^{(2)\top} Z^{(2)} + \text{Id}$ , which is still an open problem in random matrix theory. The eigenvalue distribution of this matrix, which has been obtained in [44], might be helpful towards resolving this problem. Second, it would be interesting to extend our results to classification problems. Several recent work have made remarkable progress for logistic regression in the high-dimensional setting, e.g. [36]. An interesting question is to study logistic regression in a multiple-sample setting.

## SUPPLEMENTARY MATERIAL

**Supplement to “High-dimensional Asymptotics of Transferring from Different Domains in Linear Regression”.** In the Internet Appendix [41], we provide the proofs of the technical results in Sections 2-2.2, including Lemma 2.2, Theorem 5.1, Theorem 2.5, Proposition 3.5, Theorem 2.4 and Proposition 3.2.

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