
Revisiting the Bias-Variance Tradeoff of Multi-Task Learning in High Dimensions

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Abstract

Multi-task learning is a powerful approach in many applications such as image and text classification. Yet, there is little rigorous understanding of when multi-task learning outperforms single-task learning. In this work, we provide a rigorous study to answer the question in the high-dimensional linear regression setting. We show that a bias-variance tradeoff of multi-task learning determines the effect of information transfer and develop new concentration bounds to analyze the tradeoff. Our key observation is that three properties of task data, namely *task similarity*, *sample size*, and *covariate shift* can affect transfer in the high-dimensional linear regression setting. We relate each property to the bias and variance of multi-task learning and explain three negative effects with decreased task similarity, increased source sample size, and covariate shift under increased source sample size. We validate the three effects on text classification tasks. Inspired by our theory, we show two practical connections of interest. First, single-task results can help understand when multi-task learning gives gains. Second, incrementally adding training data can mitigate negative transfer and improve multi-task training efficiency.

1 Introduction

Multi-task learning is a powerful approach to improve performance for many tasks in computer vision [1, 2], natural language processing [3, 4], and other areas [5]. In many settings, multiple source tasks are available to help predict a particular target task. The performance of multi-task learning depends on the relationship between the source and target tasks [6]. When the sources are relatively different from the target, multi-task learning (MTL) has often been observed to perform worse than single-task learning (STL) [7, 8], which is referred to as *negative transfer* [9]. While many empirical approaches have been proposed to mitigate negative transfer [5], a precise understanding of when negative transfer occurs remains elusive in the literature [10].

Understanding negative transfer requires developing generalization bounds that scale tightly with properties of each task data, such as its sample size. This presents a technical challenge in the multi-task setting because of the difference among task features, even for two tasks. For Rademacher complexity or VC-based techniques, the generalization error scales down as the sample sizes of all tasks increase, when applied to the multi-task setting [11, 12, 13, 14, 15]. Without a tight lower bound for multi-task learning, comparing its performance to single-task learning results in vacuous bounds. From a practical standpoint, developing a better understanding of multi-task learning in terms of properties of task data can provide guidance for downstream applications [16].

In this work, we study the bias and variance of multi-task learning in the high-dimensional linear regression setting [17, 18]. Our key observation is that three properties of task data, including *task similarity*, *sample size*, and *covariate shift*, can affect whether multi-task learning outperforms single-task learning (which we refer to as *positive transfer*). As an example, we vary each property in Figure 1 for two linear regression tasks and measure the improvement of multi-task learning over single-task learning for a particular task. We observe that the effect of transfer can be positive or negative as we vary each property. These phenomena cannot be explained using previous techniques [15]. The high-dimensional linear regression setting allows us to measure the three properties precisely. We

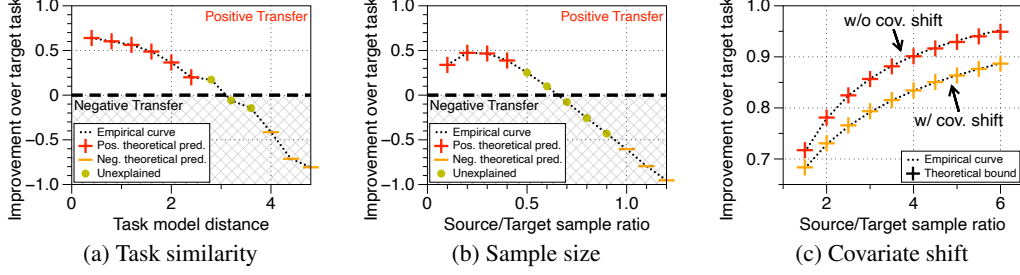


Figure 1: We observe a transition from positive to negative transfer as (a) *task model distance* increases and (b) *source/target sample ratio* increases. For the special case of having the same task model, we observe in (c) that as *source/target sample ratio* increases, having *covariate shift* worsens the performance of MTL. The y -axis measures the loss of STL minus MTL.

41 define each property for the case of two tasks and our definition applies to general settings. We refer
 42 to the first task as the source task and the second as the target task.

- 43 • **Task similarity:** Assume that both tasks follow a linear model with parameters $\beta_1, \beta_2 \in \mathbb{R}^p$,
 44 respectively. We measure the distance between them by $\|\beta_1 - \beta_2\|$.
- 45 • **Sample size:** Let $n_1 = \rho_1 \cdot p, n_2 = \rho_2 \cdot p$ be the sample size of each task, where $\rho_1, \rho_2 > 1$ are
 46 both fixed values that do not grow with p . We measure the source/target sample ratio by ρ_1/ρ_2 .
- 47 • **Covariate shift:** Assume that the task features are random vectors with positive semidefinite co-
 48 variance matrix $\Sigma_1, \Sigma_2 \in \mathbb{R}^{p \times p}$, respectively. We measure covariate shift with matrix $\Sigma_1^{1/2} \Sigma_2^{-1/2}$.

49 We consider a multi-task estimator obtained using a shared linear layer for all tasks and a separate
 50 output layer for each task [15]. This two-layer model is inspired by a commonly used idea of hard
 51 parameter sharing in multi-task learning [10, 19]. We consider the bias and variance of the multi-task
 52 estimator for predicting a target task and compare its performance to single-task learning.

53 **Main results.** First, we develop tight bounds for the bias and variance of the multi-task estimator
 54 for two tasks by applying recent development in random matrix theory [20, 21, 22]. We observe
 55 that the variance of the multi-task estimator is *always smaller* than single-task learning, because of
 56 added source task samples. On the other hand, the bias of the multi-task estimator is *always larger*
 57 than single-task learning, because of model distances. Hence, the tradeoff between bias and variance
 58 determines whether the transfer is positive or negative. We provide a sharp analysis of the *variance*
 59 that scales with sample size and covariate shift. We extend the analysis to the bias, which in *addition*
 60 scales with task similarity. Combining both, we analyze the bias-variance tradeoff for two tasks in
 61 Theorem 3.2 and extend the analysis to many tasks with the same features in Theorem 3.6.

62 Second, we explain the phenomena in Figure 1 in isotropic and covariate shifted settings.

- 63 • We provide conditions to predict the effect of transfer as a parameter of model distance $\|\beta_1 - \beta_2\|$
 64 (Section 3.2). As model distance increases, the bias becomes larger, resulting in negative transfer.
- 65 • We provide conditions to predict transfer as a parameter of sample ratio ρ_1/ρ_2 (Section 3.3).
 66 Adding source task samples helps initially by reducing variance, but hurts eventually due to bias.
- 67 • For a special case of $\beta_1 = \beta_2$, we show that MTL performs best when the singular values of
 68 $\Sigma_1^{1/2} \Sigma_2^{-1/2}$ are all equal (Section 3.4). Otherwise, the variance reduces less with covariate shift.

69 Along the way, we analyze the benefit of MTL for reducing labeled data to achieve comparable
 70 performance to STL, which has been empirically observed in Taskonomy by Zamir et al. [2].

71 Our study also leads to several algorithmic consequences with practical interest. First, we show
 72 that single-task learning results can help predict positive or negative transfer for multi-task learning.
 73 We validate this observation on ChestX-ray14 [1] and sentiment analysis datasets [23]. Second, we
 74 propose a new multi-task training schedule by incrementally adding task data batches to the training
 75 procedure. This is inspired by our observation in Figure 1b where adding more source task data helps
 76 initially, but hurts eventually. Using our incremental training schedule, we reduce the computational
 77 cost by 65% compared to baseline multi-task training over six sentiment analysis datasets while
 78 keeping the accuracy the same. Third, we provide a fine-grained insight on a covariance alignment
 79 procedure proposed in [15]. We show that the alignment procedure provides more significant
 80 improvement when the source/target sample ratio is large. Finally, we validate our three theoretical
 81 findings on sentiment analysis tasks.

2 Problem Formulation for Multi-Task Learning

We begin by defining our problem setup including the multi-task estimator we study. Then, we describe the bias-variance tradeoff of the multi-task estimator and connect the bias and variance of the estimator to *task similarity*, *sample size*, and *covariate shift*.

Problem setup. Suppose we have t datasets, where t is a fixed value that does not grow with the feature dimension p . In the high-dimensional linear regression setting (e.g. [17, 18]), the features of the k -th task, denoted by $X_k \in \mathbb{R}^{n_k \times p}$, consist of n_k feature vectors given by x_1, x_2, \dots, x_{n_k} . And each feature $x_i = \Sigma^{1/2} z_i$, where $z_i \in \mathbb{R}^p$ consists of i.i.d. entries with mean zero and unit variance. The sample size n_k equals $\rho_k \cdot p$ for a fixed value ρ_k . The labels $Y_k = X_k \beta_k + \varepsilon_k$, where β_k denotes the linear model parameters and ε_k denotes i.i.d. noise with mean zero and variance σ^2 .

We focus on the commonly used hard parameter sharing model for multi-task learning [10]. When specialized to the linear regression setting, the model consists of a linear layer $B \in \mathbb{R}^{p \times r}$ that is shared by all tasks and t output layers W_1, \dots, W_t that are in \mathbb{R}^r . The width of B , denoted by r , plays an important role in regularization. As observed in Proposition 1 of [15], if $r \geq t$, there is no regularization effect. Hence, we assume that $r < t$ in our study. For example, when there are only two tasks, $r = 1$ and B reduces to a vector whereas W_1, W_2 become scalars. We study the following procedure inspired by how hard parameter sharing models are trained in practice (e.g. [19]).

- Separate each dataset (X_i, Y_i) randomly into a training set (X_i^{tr}, Y_i^{tr}) and a validation set (X_i^{val}, Y_i^{val}) . The size of each set is described below.
- Learn the shared layer B : minimize the training loss over B and W_1, \dots, W_t , leading to a closed form equation for \hat{B} that depends on W_1, \dots, W_t .

$$f(B; W_1, \dots, W_t) = \sum_{k=1}^t \|X_k^{tr} B W_k - Y_k^{tr}\|^2. \quad (2.1)$$

- Tune the output layers W_i : set $B = \hat{B}$ and minimize the validation loss over W_1, \dots, W_t .

$$g(W_1, \dots, W_t) = \sum_{k=1}^t \|X_k^{val} \hat{B} W_k - Y_k^{val}\|^2. \quad (2.2)$$

We make several remarks. In general, the objective $f(\cdot)$ is non-convex in B and the W_k 's. Therefore, we first minimize B in equation (2.1) and then minimize W_k given B in equation (2.2). For our purpose, a validation set of size $\rho_i \cdot p^{0.99}$ that is much larger than the number of output layer parameters $r \cdot t$ suffices. The size of the training set is then $\rho_i(p - p^{0.99})$. The advantage of tuning the output layers on the validation set is to reduce the effect of noise from \hat{B} .

Problem statement. We focus on predicting a particular task, say the t -th task, without loss of generality. Let $\hat{\beta}_t^{\text{MTL}}$ denote the multi-task estimator obtained from the procedure above. Our goal is to compare the prediction loss of $\hat{\beta}_t^{\text{MTL}}$, defined by

$$L(\hat{\beta}_t^{\text{MTL}}) = \mathbb{E}_{\{\varepsilon_i\}_{i=1}^t} \mathbb{E}_{x \sim \Sigma^{1/2} z} \left[(x^\top \hat{\beta} - x^\top \beta_t)^2 \right] = \mathbb{E}_{\{\varepsilon_i\}_i^t} \left\| \Sigma_2^{1/2} (\hat{\beta}_t^{\text{MTL}} - \beta_t) \right\|^2,$$

to the prediction loss $L(\hat{\beta}_t^{\text{STL}})$ of the single-task estimator $\hat{\beta}_t^{\text{STL}} = (X_t^\top X_t)^{-1} X_t^\top Y_t$. We say there is negative transfer if $L(\hat{\beta}_t^{\text{MTL}}) > L(\hat{\beta}_t^{\text{STL}})$ and positive transfer otherwise.

As an example, for the setting of two tasks, we can decompose $L(\hat{\beta}_t^{\text{MTL}}) - L(\hat{\beta}_t^{\text{STL}})$ into a bias term and a variance term as follows (derived in Appendix A).

$$L(\hat{\beta}_t^{\text{MTL}}) - L(\hat{\beta}_t^{\text{STL}}) = \hat{v}^2 \left\| \Sigma_2^{1/2} (\hat{v}^2 X_1^\top X_1 + X_2^\top X_2)^{-1} X_1^\top X_1 (\beta_1 - \hat{v} \beta_2) \right\|^2 \quad (2.3)$$

$$+ \sigma^2 \left(\text{Tr} \left[(\hat{v}^2 X_1^\top X_1 + X_2^\top X_2)^{-1} \Sigma_2 \right] - \text{Tr} \left[(X_2^\top X_2)^{-1} \Sigma_2 \right] \right). \quad (2.4)$$

In the above, $\hat{v} = W_1/W_2$ where W_1, W_2 are obtained from solving equation (2.2) (recalling that W_1, W_2 are scalars for two tasks). The role of \hat{v} is to scale the shared subspace B to fit each task.

Equation (2.3) corresponds to the bias of $\hat{\beta}_t^{\text{MTL}}$. Hence, the bias term introduces a negative effect that depends on the *similarity* between β_1 and β_2 . Equation (2.4) corresponds to the variance of $\hat{\beta}_t^{\text{MTL}}$ minus the variance of $\hat{\beta}_t^{\text{STL}}$, which is always negative. Intuitively, the more *samples* we have, the smaller the variance is. Meanwhile, *covariate shift* also affects how small the variance can be.

3 Comparing Multi-Task Learning to Single-Task Learning

We provide tight bounds on the bias and variance of the multi-task estimator for two tasks. We show theoretical implications for understanding the performance of multi-task learning. (a) *Task similarity*: we explain the phenomenon of negative transfer precisely as tasks become more different. (b) *Sample size*: we further explain a curious phenomenon where increasing the source sample size helps initially, but hurts eventually. (c) *Covariate shift*: as the source sample size increases, we show that the covariate shift worsens the performance of the multi-task estimator. Finally, we extend our results from two tasks to many tasks with the same features.

3.1 Analyzing the Bias-Variance Tradeoff using Random Matrix Theory

A well-known result in the high-dimensional linear regression setting states that $\text{Tr}[(X_2^\top X_2)^{-1} \Sigma_2]$ is concentrated around $1/(\rho_2 - 1)$ (e.g. Chapter 6 of [24]), which scales with the sample size of the target task. Our main technical contribution is to extend this result to two tasks. We show how the variance of the multi-task estimator scales with sample size and covariate shift in the following result. **Lemma 3.1** (Variance bound). *In the setting of two tasks, let $n_1 = \rho_1 \cdot p$ and $n_2 = \rho_2 \cdot p$ be the sample size of the two tasks. Let $\lambda_1, \dots, \lambda_p$ be the singular values of the covariate shift matrix $\Sigma_1^{1/2} \Sigma_2^{-1/2}$ in decreasing order. With high probability, the variance of the multi-task estimator $\hat{\beta}_t^{\text{MTL}}$ equals*

$$\frac{\sigma^2}{n_1 + n_2} \cdot \text{Tr} \left[(\hat{v}^2 a_1 \Sigma_2^{-1/2} \Sigma_1 \Sigma_2^{-1/2} + a_2 \text{Id})^{-1} \right] + O \left(p^{-1/2+o(1)} \right),$$

where a_1, a_2 are solutions of the following equations:

$$a_1 + a_2 = 1 - \frac{1}{\rho_1 + \rho_2}, \quad a_1 + \frac{1}{\rho_1 + \rho_2} \cdot \frac{1}{p} \sum_{i=1}^p \frac{\hat{v}^2 \lambda_i^2 a_1}{\hat{v}^2 \lambda_i^2 a_1 + a_2} = \frac{\rho_1}{\rho_1 + \rho_2}.$$

Lemma 3.1 allows us to get a tight bound on equation (2.4), that only depends on *sample size*, *covariate shift* and the scalar \hat{v} . As a remark, the concentration error $O(p^{-1/2+o(1)})$ of our result is nearly optimal. For the bias term of equation (2.3), a similar result that scales with task model distance in addition to sample size and covariate shift holds (cf. Lemma B.3 in Appendix B). Combining the two lemmas, we provide a sharp analysis of the bias-variance tradeoff of the multi-task estimator. For a matrix X , let $\lambda_{\min}(X)$ denote its smallest singular value and $\|X\|$ denote its spectral norm.

Theorem 3.2 (Two tasks). *For the setting of two tasks, let $\delta > 0$ be a fixed error margin, $\rho_2 > 1$ and $\rho_1 \gtrsim \delta^{-2} \cdot \lambda_{\min}(\Sigma_1^{1/2} \Sigma_2^{-1/2})^{-4} \|\Sigma_1\| \max(\|\beta_1\|^2, \|\beta_2\|^2)$. There exist two deterministic functions Δ_{bias} and Δ_{var} that only depend on $\{\hat{v}, \Sigma_1, \Sigma_2, \rho_1, \rho_2, \beta_1, \beta_2\}$ such that*

- If $\Delta_{\text{bias}} - \Delta_{\text{var}} < -\delta$, then w.h.p. over the randomness of X_1, X_2 , we have $L(\hat{\beta}_t^{\text{MTL}}) < L(\hat{\beta}_t^{\text{STL}})$.
- If $\Delta_{\text{bias}} - \Delta_{\text{var}} > \delta$, then w.h.p. over the randomness of X_1, X_2 , we have $L(\hat{\beta}_t^{\text{MTL}}) > L(\hat{\beta}_t^{\text{STL}})$.

Theorem 3.2 applies to settings where large amounts of source task data are available but the target sample size is small. For such settings, we obtain a sharp transition from positive transfer to negative transfer determined by $\Delta_{\text{bias}} - \Delta_{\text{var}}$. While the general form of these functions can be complex (as are previous generalization bounds for MTL), they admit interpretable forms for simplified settings. The proof of Theorem 3.2 is presented in Appendix B and the proof of Lemma 3.1 is in Appendix E.

3.2 Task Similarity

It is well-known since the seminal work of Caruana [6] that how well multi-task learning performs depends on task relatedness. We formalize this connection in the following simplified setting, where we can perform explicit calculations. We show that as we increase the distance between β_1 and β_2 , there is a transition from positive transfer to negative transfer in MTL.

The isotropic model. Consider two tasks with isotropic covariances $\Sigma_1 = \Sigma_2 = \text{Id}$. Each task has sample size $n_1 = \rho_1 \cdot p$ and $n_2 = \rho_2 \cdot p$. Assume that for task two, β_2 has i.i.d. entries with mean zero and variance κ^2 . For the source task, β_1 equals β_2 plus i.i.d. entries with mean 0 and variance d^2 . The labels are $Y_i = X_i \beta_i + \varepsilon_i$, where ε_i consists of i.i.d. entries with mean zero and variance σ^2 . For our purpose, it is enough to think of the order of d being $1/\sqrt{p}$ and pd^2/σ^2 being constant.

We introduce the following notations.

$$\Psi(\beta_1, \beta_2) = \mathbb{E} [\|\beta_1 - \beta_2\|^2] / \sigma^2, \quad \Phi(\rho_1, \rho_2) = \frac{(\rho_1 + \rho_2 - 1)^2}{\rho_1(\rho_1 + \rho_2)(\rho_2 - 1)}.$$

168

169 **Proposition 3.3** (Task model distance). *In the isotropic model, suppose that ρ_1 and $\rho_2 > 1$. Then*

- 170 • If $\Psi(\beta_1, \beta_2) < \frac{1}{\nu} \cdot \Phi(\rho_1, \rho_2)$, then w.h.p. over the randomness of X_1, X_2 , $L(\hat{\beta}_t^{MTL}) < L(\hat{\beta}_t^{STL})$.
 171 • If $\Psi(\beta_1, \beta_2) > \nu \cdot \Phi(\rho_1, \rho_2)$, then w.h.p. over the randomness of X_1, X_2 , $L(\hat{\beta}_t^{MTL}) > L(\hat{\beta}_t^{STL})$.

172 Here $\nu = (1 + o(1)) \cdot (1 - 1/\sqrt{\rho_1})^{-4}$. Concretely, if $\rho_1 > 40$, then $\nu \in (1, 2)$.

173 Proposition 3.3 simplifies Theorem 3.2 in the isotropic model, allowing for a more explicit statement
 174 of the bias-variance tradeoff. Concretely, $\Psi(\beta_1, \beta)$ and $\Phi(\rho_1, \rho_2)$ corresponds to Δ_{bias} and Δ_{var} ,
 175 respectively. Roughly speaking, the transition threshold scales as $\frac{pd^2}{\sigma^2} - \frac{1}{\rho_1} - \frac{1}{\rho_2}$. We apply Proposition
 176 3.3 to the parameter setting of Figure 1a (the details are left to Appendix F.1). We can see that our
 177 result is able to predict positive or negative transfer accurately and matches the empirical curve.
 178 There are several unexplained observations near the transition threshold 0, which are caused by the
 179 concentration error ν . The proof of Proposition 3.3 can be found in Appendix C.1. A key part of the
 180 analysis shows that $\hat{\nu} \approx 1$ in the isotropic model, thus simplifying the result of Theorem 3.2.

181 **Algorithmic consequence.** We can in fact extend the result to the cases where the noise variances
 182 are different. In this case, we will see that MTL is particularly effective. Concretely, suppose the
 183 noise variance σ_1^2 of task 1 differs from the noise variance σ_2^2 of task 2. If σ_1^2 is too large, the source
 184 task provides a negative transfer to the target. If σ_1^2 is small, the source task is more helpful. We leave
 185 the result to Proposition C.3 in Appendix C.1. Inspired by the observation, we propose a single-task
 186 based metric to help understand MTL results using STL results.

- 187 • For each task, we train a single-task model. Let z_s and z_t be the prediction accuracy of each task,
 188 respectively. Let $\tau \in (0, 1)$ be a fixed threshold.
 189 • If $z_s - z_t > \tau$, then we predict that there will be positive transfer when combining the two tasks
 190 using MTL. If $z_s - z_t < -\tau$, then we predict negative transfer.

191

3.3 Sample Size

192 In classical Rademacher or VC based theory of multi-task learning, the generalization bounds are
 193 usually presented for settings where the sample sizes are equal for all tasks [11, 13, 14]. On the other
 194 hand, uneven sample sizes between different tasks (or even dominating tasks) have been empirically
 195 observed as a cause of negative transfer [25]. For such settings, we have also observed that adding
 196 more labeled data from one task does not always help. In the isotropic model, we consider what
 197 happens if we vary the source task sample size. Our theory accurately predicts a curious phenomenon,
 198 where increasing the sample size of the source task results in negative transfer!

199 **Proposition 3.4** (Source/target sample ratio). *In the isotropic model, suppose that $\rho_1 > 40$ and
 200 $\rho_2 > 110$ are fixed constants, and $\Psi(\beta_1, \beta_2) > 2/(\rho_2 - 1)$. Then we have that*

- 201 • If $\frac{n_1}{n_2} = \frac{\rho_1}{\rho_2} < \frac{1}{\nu} \cdot \frac{1-2\rho_2^{-1}}{\Psi(\beta_1, \beta_2)(\rho_2-1)-\nu^{-1}}$, then w.h.p. $L(\hat{\beta}_t^{MTL}) < L(\hat{\beta}_t^{STL})$.
 202 • If $\frac{n_1}{n_2} = \frac{\rho_1}{\rho_2} > \nu \cdot \frac{1-2\rho_2^{-1}}{\Psi(\beta_1, \beta_2)(\rho_2-1.5)-\nu}$, then w.h.p. $L(\hat{\beta}_t^{MTL}) > L(\hat{\beta}_t^{STL})$.

203 Proposition 3.4 describes the bias-variance tradeoff in terms of the sample ratio ρ_1/ρ_2 . We apply
 204 the result to the setting of Figure 1b (described in Appendix F.1). There are several unexplained
 205 observations near $y = 0$ caused by ν . The proof of Proposition 3.4 can be found in Appendix C.2.

206 **Connection to Taskonomy.** We use our tools to explain a key result of Taskonomy by Zamir et al.
 207 [2], which shows that MTL can reduce the amount of labeled data needed to achieve comparable
 208 performance to STL. For $i = 1, 2$, let $\hat{\beta}_i^{MTL}(x)$ denote the estimator trained using $x \cdot n_i$ datapoints
 209 from every task. The data efficiency ratio is defined as

$$\arg \min_{x \in (0,1)} L_1(\hat{\beta}_1^{MTL}(x)) + L_2(\hat{\beta}_2^{MTL}(x)) \leq L_1(\hat{\beta}_1^{STL}) + L_2(\hat{\beta}_2^{STL}).$$

210 For example, the data efficiency ratio is 1 if there is negative transfer. Using our tools, we show that
 211 in the isotropic model, the data efficiency ratio is roughly

$$\frac{1}{\rho_1 + \rho_2} + \frac{2}{(\rho_1 + \rho_2)(\rho_1^{-1} + \rho_2^{-1} - \Theta(\Psi(\beta_1, \beta_2)))}.$$

212 Compared with Proposition 3.3, we see that when $\Psi(\beta_1, \beta_2)$ is smaller than $\rho_1^{-1} + \rho_2^{-1}$ (up to a
 213 constant multiple), the transfer is positive. Moreover, the data efficiency ratio quantifies how effective
 214 the positive transfer is using MTL. The result can be found in Proposition C.4 in Appendix C.2.

Algorithmic consequence. An interesting consequence of Proposition 3.4 is that $L(\hat{\beta}_t^{MTL})$ is not monotone in ρ_1 . In particular, Figure 1b (and our analysis) shows that $L(\hat{\beta}_t^{MTL})$ behaves as a quadratic function over ρ_1 . More generally, depending on how large $\Psi(\beta_1, \beta_2)$ is, $L(\hat{\beta}_t^{MTL})$ may also be monotonically increasing or decreasing. Based on this insight, we propose an incremental optimization schedule to improve MTL training efficiency.

- We divide the source task data into S batches. For S rounds, we incrementally add the source task data by adding one batch at a time.
- After training T epochs, if the validation accuracy becomes worse than the previous round's result, we terminate. Algorithm 1 in Appendix F describes the procedure in detail.

3.4 Covariate Shift

So far we have considered the isotropic model where $\Sigma_1 = \Sigma_2$. This setting is relevant for settings where different tasks share the same input features such as multi-class image classification. In general, the covariance matrices of the two tasks may be different such as in text classification. In this part, we consider what happens when $\Sigma_1 \neq \Sigma_2$. We show that when n_1/n_2 is large, MTL with covariate shift can be suboptimal compared to MTL without covariate shift.

Example. We measure covariate shift by $M = \Sigma_1^{1/2} \Sigma_2^{-1/2}$. Assume that $\Psi(\beta_1, \beta_2) = 0$ for simplicity. We compare two cases: (i) when $M = \text{Id}$; (ii) when M has $p/2$ singular values that are equal to λ and $p/2$ singular values that are equal to $1/\lambda$. Hence, λ measures the severity of the covariate shift. Figure 1c shows a simulation of this setting by varying λ . We observe that as source/target sample ratio increases, the performance gap between the two cases increases.

We compare different choices of M that belong to the following bounded set. Let λ_i be the i -th singular value of M . Let $\mu_{\min} < \mu < \mu_{\max}$ be fixed values that do not grow with p .

$$\mathcal{S}_\mu := \left\{ M \left| \prod_{i=1}^p \lambda_i \leq \mu^p, \mu_{\min} \leq \lambda_i \leq \mu_{\max}, \text{ for all } 1 \leq i \leq p \right. \right\},$$

Proposition 3.5 (Covariate shift). *Assume that $\Psi(\beta_1, \beta_2) = 0$ and $\rho_1, \rho_2 > 1$. Let $g(M)$ denote the prediction loss of $\hat{\beta}_t^{MTL}$ when $M = \Sigma_1^{1/2} \Sigma_2^{-1/2} \in \mathcal{S}_\mu$. We have that*

$$g(\mu \text{Id}) \leq (1 + O(\rho_2/\rho_1)) \min_{M \in \mathcal{S}_\mu} g(M).$$

This proposition shows that when source/target sample ratio is large, then having no covariate shift is optimal. The proof of Proposition 3.5 is left to Appendix C.3.

Algorithmic consequence. Our observation highlights the need to correct covariate shift when n_1/n_2 is large. Hence for such settings, we expect procedures that aim at correcting covariate shift to provide more significant gains. We consider a covariance alignment procedure proposed in [15], which is designed for the purpose of correcting covariate shift. The idea is to add an alignment module between the input and the shared module B . This new module is then trained together with B and the output layers. We validate our insight on this procedure in the experiments.

3.5 Extensions

Next, we describe our result for more than two tasks with same features, i.e. $X_i = X$ for any i . This setting is prevalent in applications of multi-task learning to image classification, where there are multiple prediction labels/tasks for every image [1, 26].

Theorem 3.6 (Many tasks). *For the setting of t tasks where $X_i = X$, for all $1 \leq i \leq t$, let $B^* := [\beta_1, \beta_2, \dots, \beta_t]$ and $U_r \in \mathbb{R}^{t \times r}$ denote the linear model parameters. Let $U_r U_r^\top$ denote the best rank- r subspace approximation of $(B^*)^\top \Sigma B^*$. Assume that $\lambda_{\min}(B^*^\top \Sigma B^*) \gtrsim \sigma^2$. Let v_i denote the i -th row vector of U_r . There exists a value $\delta = o(\|B^*\|^2 + \sigma^2)$ such that*

- If $(1 - \|v_t\|^2) \frac{\sigma^2}{\rho-1} - \|\Sigma(B^* U_r v_t - \beta_t)\|^2 > \delta$, then w.h.p $L(\hat{\beta}_t^{MTL}) < L(\hat{\beta}_t^{STL})$.
- If $(1 - \|v_t\|^2) \frac{\sigma^2}{\rho-1} - \|\Sigma(B^* U_r v_t - \beta_t)\|^2 < -\delta$, then w.h.p. $L(\hat{\beta}_t^{MTL}) > L(\hat{\beta}_t^{STL})$.

Theorem 3.6 provides a sharp analysis of the bias-variance tradeoff beyond two tasks. Specifically, $(1 - \|v_t\|^2) \sigma^2 / (\rho - 1)$ shows the amount of reduced variance and $\|\Sigma(B^* U_r v_t - \beta_t)\|^2$ shows the bias of the multi-task estimator. The proof of 3.6 can be found in Appendix D.

4 Experiments

We validate our algorithmic insights and then our theory. In Section 4.2, we first show that single-task learning results can help predict positive or negative transfer. Second, our proposed incremental training schedule improves the training efficiency of standard multi-task training on sentiment analysis tasks. In Section 4.3, we validate our theoretical results. We further show that when the sample ratio is large, performing the alignment procedure of [15] provides more improvement for MTL.

4.1 Experimental Setup

We consider a text classification task and an image classification task as follows.

Sentiment Analysis. We consider six tasks: movie review sentiment (MR) [27], sentence subjectivity (SUBJ) [28], customer reviews (CR) [29], question type (TREC) [30], opinion polarity (MPQA) [31], and the Stanford sentiment treebank (SST) tasks [32]. We use an embedding layer with GloVe embeddings [33] followed by an LSTM, MLP or CNN layer proposed by [34].

ChestX-ray14. This dataset contains 112,120 frontal-view X-ray images [1]. There are 14 diseases (tasks) for every image that we would like to predict. We use densenet121 as the shared module [35].

For all models, we use a shared module for all tasks and assign a separate output layer on top of the shared module for each task. The baseline training schedule for MTL is the round-robin training schedule. We measure the test accuracy of predicting a target task. We measure computational cost by summing over all epochs the number of samples used in every epoch.

4.2 Experimental Results

Predicting transfer effect via STL results. We show that the single-task based metric proposed in Section 3.2 can predict positive or negative transfer in MTL. A common challenge in the study of MTL is that the results can be hard to understand. It is difficult to predict when MTL performs well without running extensive trials. Our insight is that we can use STL results to help understand MTL results. Table 1 shows the result on both the sentiment analysis and the ChestX-ray14 tasks. We find that using a threshold of $\tau = 0.1$, the STL results correctly predict positive or negative transfer with 75.6% precision and 38.8% recall among 30 times 5 (random seeds) task pairs! We observe similar results for 91 task pairs from the ChestX-ray14 dataset.

Mitigating negative transfer via incremental training. First, we show that our proposed incremental training schedule (Algorithm 1) can help mitigate negative transfer for predicting a particular target task. Over all 15 pairs from the sentiment analysis tasks, we find that Algorithm 1 requires only 45% of the computational cost to achieve similar performance on the target task, compared to the MTL baseline. Our insight is that since adding more samples from the source task does not always help, we can improve efficiency by adding source samples *incrementally* during training.

Our next result shows the incremental training schedule applies to multiple tasks as well. In Table 2, we find that over all six sentiment analysis tasks, incremental training requires less than 35% of the computational cost compared to baseline MTL training, while achieving the same accuracy averaged over all six tasks. As a further validation, excluding TREC, we observe similar comparative results.

4.3 Validating the Theoretical Results

We first validate our theoretical results in Section 3.2 and 3.3. In Figure 2a, we compare the performance training with a semantically similar task versus a dissimilar task with a target task. We select each task pair based on our domain knowledge. We observe that adding a similar task helps the target task whereas adding a dissimilar task hurts. In Figure 2b, we validate that adding more source samples does not always improve performance on the target task. Finally, we validate the algorithmic

Threshold	Sentiment analysis		ChestX-ray14	
	Precision	Recall	Precision	Recall
0.0	0.596	1.000	0.593	1.000
0.1	0.756	0.388	0.738	0.462
0.2	0.919	0.065	0.875	0.044

Table 1: Single-task learning results can help predict positive or negative transfer in multi-task learning.

Models	Sentiment analysis	
	all tasks	w/o TREC
MLP	31%	29%
LSTM	35%	34%
CNN	30%	28%

Table 2: Efficiency of incremental training compared to baseline MTL.

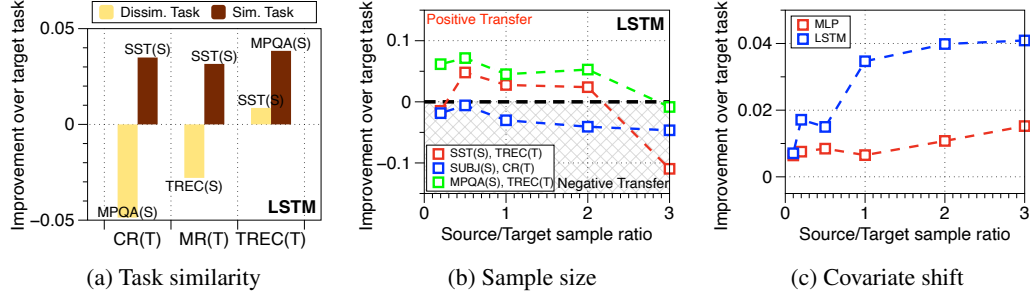


Figure 2: Validating the three results of Section 3 on sentiment analysis tasks. (a) Adding a semantically similar source task in MTL performs better than adding a dissimilar task. (b) As source/target sample ratio increases, we observe a transition from positive to negative transfer. (c) As source/target sample ratio increases, aligning task covariances [15] improves more over the baseline. Note: (S) denotes the source task and (T) denotes the target task.

consequence of Section 3.4. In Figure 2c, we measure the performance gains from performing the alignment procedure proposed in [15] minus baseline MTL. We average the results over all 15 task pairs. The result shows that as the source samples increases, the alignment procedure shows a bigger improvement over MTL. The rest of experimental procedures are left to Appendix F.2.

5 Related Work

We refer the interested readers to several excellent surveys on multi-task learning for a comprehensive survey [9, 10, 5, 36]. Below, we describe several lines of work that are most related to this work.

Theoretical works. Some of the earliest works on multi-task learning are Baxter [11], Ben-David and Schuller [37]. Mauer [13] studies generalization bounds for linear separation settings of MTL. Ben-David et al. [38] provides uniform convergence bounds that combines source and target errors optimally. The benefit of learning multi-task representations has been studied for learning certain half-spaces [14] and sparse regression [39, 40]. Our work is closely related to Wu et al. [15]. While Wu et al. provide generalization bounds to show that adding more labeled helps learn the target task more accurately, their techniques cannot be used to explain when MTL outperforms STL.

Methodological works. Ando and Zhang [12] introduces an alternating minimization framework for learning multiple tasks. Argyriou et al. [41] present a convex algorithm which learns common sparse representations across a pool of related tasks. Evgeniou et al. [42] develop a framework for multi-task learning in the context of kernel methods. The multi-task learning model that we have focused on uses the idea of hard parameter sharing [43, 44, 10]. We believe that our theoretical framework can apply to other approaches to multi-task learning.

Random matrix theory. The random matrix theory tool and related proof of our work fall into a paradigm of the so-called local law of random matrices [20]. For a sample covariance matrix $X^\top X$ with $\Sigma = \text{Id}$, such a local law was proved in [21]. It was later extended to sample covariance matrices with non-identity Σ [22], and separable covariance matrices [45]. On the other hand, one may derive the asymptotic result in Theorem 3.1 with error $o(1)$ using the free addition of two independent random matrices in free probability theory [46]. To the best of my knowledge, we do not find an *explicit result* for the sum of two sample covariance matrices with general covariates in the literature.

6 Conclusions and Open Problems

In this work, we analyzed the bias and variance of multi-task learning versus single-task learning. We provided tight concentration bounds for the bias and the variance. Based on these bounds, we analyzed the impact of three properties, including task similarity, sample size, and covariate shift on the bias and variance, to derive conditions for transfer. We validated our theoretical results. Based on the theory, we proposed to train multi-task models by incrementally adding labeled data and showed encouraging results inspired by our theory. We describe several open questions for future work. First, our bound on the bias term (cf. Lemma B.3) involves an error term that scales down with ρ_1 . Tightening this error bound might cover the unexplained observations in Figure 1. Second, it would be interesting to extend our results to non-linear settings. We remark that this likely requires addressing significant technical challenges to deal with non-linearity.

Broader Impacts

In this work, we provide a theoretical framework to help understand when multi-task learning performs well. We approach this question by studying the bias-variance tradeoff of multi-task learning. We provide new technical tools to analyze the bias and variance of multi-task learning.

Our theoretical framework has the potential to impact many other neighboring areas in the ML community. (i) Our concentration bounds can apply to different settings such as soft parameter sharing [10], kernel methods [42], and convex formulation of multi-task learning [47]. (ii) Our analysis of the bias-variance tradeoff can extend to transfer learning and domain adaptation [48]. (iii) Our insights on positive and negative transfer can be useful in multimodal learning, where the data sources are usually heterogeneous. (iv) Our fine-grained study on sample sizes have the potential to provide new insight in meta learning, where limited labeled samples presents a significant challenge. Finally, since multi-task learning connects to a wide range of areas [36] such as semi-supervised learning, representation learning, and reinforcement learning [25]. We believe that the tools we have developed and the framework we have provided can inspire followup works in these areas.

Our proposed algorithmic consequences also have the potential to help both researchers and practitioners to better develop their use cases of multi-task learning. For one example, many medical applications use multi-task learning to train large-scale image classification models by combining multiple datasets [1, 26]. Unlike the applications of multi-task learning in text classification where we can collect large amounts of labeled data [3], in medical applications it is typically difficult and expensive to acquire labeled data. For such settings, our proposed training scheduler might improve the model training efficiency by using less labeled data. For another example, practitioners in industry often need to improve prediction performance by training many related tasks. But the results are not always positive and practitioners have a hard time figuring out why. Our proposed metric can provide guidance for selecting which tasks should be trained together in a multi-task model.

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Organizations. The appendix is organized as follows. In Section A, we describe an extended background and a further reivew of related work. In Section B, we present the analysis of the bias-variance tradeoff for the case of two tasks. In Section C, we illustrate the above analysis in simplified settings including the isotropic model and covariate shifted settings without model distance. In Section D, we extend our analysis to many tasks with the same features. In Section E, we prove the bias and variance bounds used in the analysis. Finally in Section F, we fill in the missing details of our experiments.

A Extended Background and Related Work

We restate our linear regression setting, in particular the moment assumption required by our random matrix model. We then derive a closed-form solution of the multi-task estimator that is defined in Section 2. Finally, we describe further related work that is covered in the main text.

First, we give the basic assumption for our main objects—the random matrices X_i , $i = 1, 2$.

Assumption A.1 (Moment assumptions). *We will consider $n \times p$ random matrices of the form $X = Z\Sigma^{1/2}$, where Σ is a $p \times p$ deterministic positive definite symmetric matrix, and $Z = (z_{ij})$ is an $n \times p$ random matrix with real i.i.d. entries with mean zero and variance one. Note that the rows of X are i.i.d. centered random vectors with covariance matrix Σ . For simplicity, we assume that all the moments of z_{ij} exists, that is, for any fixed $k \in \mathbb{N}$, there exists a constant $C_k > 0$ such that*

$$\mathbb{E}|z_{ij}|^k \leq C_k, \quad 1 \leq i \leq n, \quad 1 \leq j \leq p. \quad (\text{A.1})$$

We assume that $n = \rho p$ for some fixed constant $\rho > 1$. Without loss of generality, after a rescaling we can assume that the norm of Σ is bounded by a constant $C > 0$. Moreover, we assume that Σ is well-conditioned: $\kappa(\Sigma) \leq C$, where $\kappa(\cdot)$ denotes the condition number.

Here we have assumed (A.1) solely for simplicity of representation. If the entries of Z only have finite a -th moment for some $a > 4$, then all the results below still hold except that we need to replace $O(p^{-\frac{1}{2}+\varepsilon})$ with $O(p^{-\frac{1}{2}+\frac{2}{a}+\varepsilon})$ in some error bounds. We will not get deeper into this issue in this section, but refer the reader to Corollary E.8 in Section E.1.

Then we make the following assumptions on the data models.

Assumption A.2 (Linear regression model). *For some fixed $t \in \mathbb{N}$, let $Y_i = X_i\beta_i + \varepsilon_i$, $1 \leq i \leq t$, be independent data models, where X_i , β_i and ε_i are also independent of each other. Suppose that $X_i = Z_i\Sigma_i^{1/2} \in \mathbb{R}^{n_i \times p}$ satisfy Assumption A.1 with $\rho_i := n_i/p > 1$ being fixed constants. $\varepsilon_i \in \mathbb{R}^{n_i}$ are random vectors with i.i.d. entries with mean zero, variance σ_i^2 and all moments as in (A.1).*

Throughout the appendix, we shall say an event Ξ holds with high probability (w.h.p.) if for any fixed $D > 0$, $\mathbb{P}(\Xi) \geq 1 - p^{-D}$ for large enough p . Moreover, we shall use $o(1)$ to mean a small positive quantity that converges to 0 as $p \rightarrow \infty$.

Next, we derive a closed-form solution of the multi-task learning estimator for the case of two tasks. From [15], we know that we need to explicitly restrict the output dimension r of B so that there is transfer between the two tasks. Hence for the case of two tasks, we consider the setting where $r = 1$. For simplicity of notations, we shall denote (X_i^{tr}, Y_i^{tr}) and (X_i^{val}, Y_i^{val}) as (X_i, Y_i) and $(\tilde{X}_i, \tilde{Y}_i)$, respectively. Then equation (2.1) simplifies to

$$f(B; w_1, w_2) = \|X_1 B w_1 - Y_1\|^2 + \|X_2 B w_2 - Y_2\|^2, \quad (\text{A.2})$$

where $B \in \mathbb{R}^p$ and w_1, w_2 are both real numbers. To solve the above problem, suppose that w_1, w_2 are fixed, by local optimality, we find the optimal B as

$$\begin{aligned} \hat{B}(w_1, w_2) &= (w_1^2 X_1^\top X_1 + w_2^2 X_2^\top X_2)^{-1} (w_1 X_1^\top Y_1 + w_2 X_2^\top Y_2) \\ &= \frac{1}{w_2} \left(\frac{w_1^2}{w_2^2} X_1^\top X_1 + X_2^\top X_2 \right)^{-1} \left(\frac{w_1}{w_2} X_1^\top Y_1 + X_2^\top Y_2 \right) \\ &= \frac{1}{w_2} \left[\beta_2 + \left(\frac{w_1^2}{w_2^2} X_1^\top X_1 + X_2^\top X_2 \right)^{-1} \left(X_1^\top X_1 \left(\frac{w_1}{w_2} \beta_1 - \frac{w_1^2}{w_2^2} \beta_2 \right) + \left(\frac{w_1}{w_2} X_1^\top \varepsilon_1 + X_2^\top \varepsilon_2 \right) \right) \right]. \end{aligned} \quad (\text{A.3})$$

As a remark, when $w_1 = w_2 = 1$, we obtain linear regression. If β_1 is a scaling of β_2 , then w_1, w_2 can be scaled accordingly to fix both tasks more accurately than linear regression.

579 Next we consider N_i independent samples of the training set $\{(\tilde{x}_k^{(i)}, \tilde{y}_k^{(i)}) : 1 \leq k \leq N_i\}$ from task- i ,
 580 $i = 1, 2$. With these sample, we form the random matrices $\tilde{X}_i \in \mathbb{R}^{N_i \times p}$ and $\tilde{Y}_i \in \mathbb{R}^{N_i}$, $i = 1, 2$,
 581 whose row vectors are given by $\tilde{x}_k^{(i)}$ and $\tilde{y}_k^{(i)}$. We assume that N_1 and N_2 satisfy $N_1/N_2 = n_1/n_2$
 582 and $N_i \geq n_i^{1-\varepsilon_0}$ for some constant $\varepsilon_0 > 0$. Then we write the validation loss in (2.2) as

$$g(w_1, w_2) = \left\| \tilde{X}_1 \hat{B} w_1 - \tilde{Y}_1 \right\|^2 + \left\| \tilde{X}_2 \hat{B} w_2 - \tilde{Y}_2 \right\|^2. \quad (\text{A.4})$$

583 Inserting (A.3) into (A.4), one can see that the optimal solution of g only depends on the ratio
 584 $v := w_1/w_2$. Hence we overload the notation by writing $g(v)$ in the following discussion. The
 585 expectation of $g(v)$ can be written as follows.

$$\begin{aligned} \text{val}(v) &:= \mathbb{E}_{\varepsilon_1, \varepsilon_2} \left[\sum_{i=1}^2 \left\| \Sigma_i^{1/2} (\hat{B} w_i - \beta_i) \right\|^2 \right] \\ &= N_1 \cdot \left\| \Sigma_1^{1/2} (v^2 X_1^\top X_1 + X_2^\top X_2)^{-1} X_2^\top X_2 (\beta_1 - v \beta_2) \right\|^2 \\ &\quad + N_2 \cdot v^2 \left\| \Sigma_2^{1/2} (v^2 X_1^\top X_1 + X_2^\top X_2)^{-1} X_1^\top X_1 (\beta_1 - v \beta_2) \right\|^2 \\ &\quad + N_1 \cdot v^2 \text{Tr} \left[\Sigma_1 (v^2 X_1^\top X_1 + X_2^\top X_2)^{-2} (\sigma_1^2 \cdot v^2 X_1^\top X_1 + \sigma_2^2 \cdot X_2^\top X_2) \right] \\ &\quad + N_2 \cdot \text{Tr} \left[\Sigma_2 (v^2 X_1^\top X_1 + X_2^\top X_2)^{-2} (\sigma_1^2 \cdot v^2 X_1^\top X_1 + \sigma_2^2 \cdot X_2^\top X_2) \right]. \end{aligned}$$

586 **Claim A.3.** *In the setting described above, we have that*

$$g(v) = [\text{val}(v) + (N_1 \sigma_1^2 + N_2 \sigma_2^2)] \cdot \left(1 + O(p^{-(1-\varepsilon_0)/2+\varepsilon}) \right). \quad (\text{A.5})$$

Proof. We use the fact that our random vectors have i.i.d. entries. Recall that $Y_i = X_i \beta_i + \varepsilon_i$ and $\tilde{Y}_i = \tilde{X}_i \beta_i + \tilde{\varepsilon}_i$, $i = 1, 2$, all satisfy Assumption A.2. Then we rewrite (A.4) as

$$g(v) = \sum_{i=1}^2 \left\| \tilde{X}_i \tilde{\beta}_i - \tilde{\varepsilon}_i \right\|^2, \quad \tilde{\beta} := \hat{B} w_i - \beta_i.$$

587 Since $\tilde{X}_i \tilde{\beta}$ and $\tilde{\varepsilon}_i$ are independent random vectors with i.i.d. centered entries, we can use the
 588 concentration result, Lemma E.14, to get that for any constant $\varepsilon > 0$,

$$\begin{aligned} \left| \left\| \tilde{X}_i \tilde{\beta}_i - \tilde{\varepsilon}_i \right\|^2 - \mathbb{E}_{\tilde{X}_i, \tilde{\varepsilon}_i} \left[\left\| \tilde{X}_i \tilde{\beta}_i - \tilde{\varepsilon}_i \right\|^2 \right] \right| &= \left| \left\| \tilde{X}_i \tilde{\beta}_i - \tilde{\varepsilon}_i \right\|^2 - N_i (\tilde{\beta}_i^\top \Sigma_i \tilde{\beta}_i + \sigma_i^2) \right| \\ &\leq N_i^{1/2+\varepsilon} (\tilde{\beta}_i^\top \Sigma_i \tilde{\beta}_i + \sigma_i^2), \end{aligned}$$

with high probability. Thus we obtain that

$$g(v) = \left[\sum_{i=1}^2 N_i \left\| \Sigma_i^{1/2} (\hat{B} w_i - \beta_i) \right\|^2 + (N_1 \sigma_1^2 + N_2 \sigma_2^2) \right] \cdot \left(1 + O(p^{-(1-\varepsilon_0)/2+\varepsilon}) \right),$$

where we also used $N_i \geq p^{-1+\varepsilon_0}$. Inserting (A.3) into the above expression and using again the concentration result, Lemma E.14, we get that

$$\sum_{i=1}^2 N_i \left\| \Sigma_i^{1/2} (\hat{B} w_i - \beta_i) \right\|^2 = \text{val}(v) \cdot \left(1 + O(p^{-1/2+\varepsilon}) \right)$$

589 with high probability. Thus we conclude the proof. \square

590 Hence to minimize $g(v)$, it suffices to minimize $\text{val}(v)$ over v . Let $\hat{v} = \hat{w}_1/\hat{w}_2$ be the global
 591 minimizer of $g(v)$. Now we can define the multi-task learning estimator for the target task as

$$\hat{\beta}_2^{\text{MTL}} = \hat{w}_2 \hat{B}(\hat{w}_1, \hat{w}_2).$$

592 The prediction loss of using $\hat{\beta}_2^{\text{MTL}}$ for the target task is

$$L(\hat{\beta}_2^{\text{MTL}}) = \hat{v}^2 \left\| \Sigma_2^{1/2} (\hat{v}^2 X_1^\top X_1 + X_2^\top X_2)^{-1} X_1^\top X_1 (\beta_1 - \hat{v} \beta_2) \right\|^2 \\ + \text{Tr} \left[\Sigma_2 (\hat{v}^2 X_1^\top X_1 + X_2^\top X_2)^{-2} (\sigma_1^2 \cdot \hat{v}^2 X_1^\top X_1 + \sigma_2^2 \cdot X_2^\top X_2) \right], \quad (\text{A.6})$$

593 which only depends on \hat{v} , the sample covariance matrices, and β_1, β_2 .

594 **Extended related work.** Our setting is closely related to domain adaptation [49, 50, 51, 52, 53, 54, 55, 56, 57]. The important distinction is that we focus on predicting the target task using a
595 hard parameter sharing model. For such models, their output dimension plays an important role
596 of regularization [44]. Linear models in multi-task learning have been studied in various settings,
597 including representation learning [58], online learning [59, 60], and sparse regression [40].

599 B Proof for the Case of Two Tasks

600 We now state several helper lemmas to get estimates on $L(\hat{\beta}_t^{\text{STL}})$ and $L(\hat{\beta}_t^{\text{MTL}})$ for $t = 2$. The first
601 lemma, which is a folklore result in random matrix theory, helps to determine the asymptotic limit
602 of $L(\hat{\beta}_t^{\text{STL}})$ as $p \rightarrow \infty$. When the entries of X are multivariate Gaussian, this lemma recovers the
603 classical result for the mean of inverse Wishart distribution [61]. For general non-Gaussian random
604 matrices, it can be obtained using Stieltjes transform method; see e.g., Lemma 3.11 of [62]. Here we
605 shall state a result obtained from Theorem 2.4 in [21], which gives an almost sharp error bound.

606 **Lemma B.1.** *Suppose X satisfies assumption A.1. Let A be any $p \times p$ matrix that is independent of*
607 *X . We have that for any constant $\varepsilon > 0$,*

$$\text{Tr} [(X^\top X)^{-1} A] = \frac{1}{\rho - 1} \frac{1}{p} \text{Tr} (\Sigma^{-1} A) + O \left(\|A\| p^{-1/2+\varepsilon} \right) \quad (\text{B.1})$$

608 *with high probability.*

609 We shall refer to random matrices of the form $X^\top X$ as sample covariance matrices following the
610 standard notations in high-dimensional statistics. The second lemma extends Lemma B.1 for a single
611 sample covariance matrix to the sum of two independent sample covariance matrices. It is the main
612 random matrix theoretical input of this paper.

613 **Lemma B.2** (Variance bound: Lemma 3.1 restated). *Suppose $X_1 = Z_1 \Sigma_1^{1/2} \in \mathbb{R}^{n_1 \times p}$ and $X_2 =$*
614 *$Z_2 \Sigma_2^{1/2} \in \mathbb{R}^{n_2 \times p}$ satisfy Assumption A.1 with $\rho_1 := n_1/p > 1$ and $\rho_2 := n_2/p > 1$ being fixed*
615 *constants. Denote by $M = \Sigma_1^{1/2} \Sigma_2^{-1/2}$ and let $\lambda_1, \lambda_2, \dots, \lambda_p$ be the singular values of M in*
616 *descending order. Let A be any $p \times p$ matrix that is independent of X_1 and X_2 . We have that for any*
617 *constant $\varepsilon > 0$,*

$$\text{Tr} [(X_1^\top X_1 + X_2^\top X_2)^{-1} A] = \frac{1}{\rho_1 + \rho_2} \frac{1}{p} \text{Tr} [(a_1 \Sigma_1 + a_2 \Sigma_2)^{-1} A] + O \left(\|A\| p^{-1/2+\varepsilon} \right) \quad (\text{B.2})$$

618 *with high probability, where (a_1, a_2) is the solution to the following deterministic equations:*

$$a_1 + a_2 = 1 - \frac{1}{\rho_1 + \rho_2}, \quad a_1 + \frac{1}{\rho_1 + \rho_2} \cdot \frac{1}{p} \sum_{i=1}^p \frac{\lambda_i^2 a_1}{\lambda_i^2 a_1 + a_2} = \frac{\rho_1}{\rho_1 + \rho_2}. \quad (\text{B.3})$$

619 Finally, the last lemma describes the asymptotic limit of $(X_1^\top X_1 + X_2^\top X_2)^{-1} \Sigma_2 (X_1^\top X_1 + X_2^\top X_2)^{-1}$,
620 which will be needed when we estimate the first term on the right-hand side of (A.6).

621 **Lemma B.3** (Bias bound). *In the setting of Lemma B.2, let $\beta \in \mathbb{R}^p$ be any vector that is independent*
622 *of X_1 and X_2 . We have that for any constant $\varepsilon > 0$,*

$$(n_1 + n_2)^2 \left\| \Sigma_2^{1/2} (X_1^\top X_1 + X_2^\top X_2)^{-1} \beta \right\|^2 \\ = \beta^\top \Sigma_2^{-1/2} \frac{(1 + a_3) \text{Id} + a_4 M^\top M}{(a_1 M^\top M + a_2)^2} \Sigma_2^{-1/2} \beta + O(p^{-1/2+\varepsilon} \|\beta\|^2), \quad (\text{B.4})$$

623 *with high probability, where a_3 and a_4 satisfy the following system of linear equations:*

$$(\rho_2 a_2^{-2} - b_0) \cdot a_3 - b_1 \cdot a_4 = b_0, \quad (\rho_1 a_1^{-2} - b_2) \cdot a_4 - b_1 \cdot a_3 = b_1. \quad (\text{B.5})$$

Here b_0 , b_1 and b_2 are defined as

$$b_k := \frac{1}{p} \sum_{i=1}^p \frac{\lambda_i^{2k}}{(a_2 + \lambda_i^2 a_1)^2}, \quad k = 0, 1, 2.$$

Proof overview. The proofs of Lemma B.2 and Lemma B.3 are based on the Stieltjes transform method (or the resolvent method) in random matrix theory [62, 63, 20]. Roughly speaking, we study the resolvent $R(z) := [\Sigma_2^{-1/2}(X_1^\top X_1 + X_2^\top X_2)\Sigma_2^{-1/2} - z]^{-1}$ for $z \in \mathbb{C}$ around $z = 0$. Using the methods in [22, 45], we find the asymptotic limit, say $R_\infty(z)$, of $R(z)$ for any z as $p \rightarrow \infty$ with an almost optimal convergence rate. In particular, when $z = 0$, $\text{Tr}[\Sigma_2^{-1/2} A \Sigma_2^{-1/2} R_\infty(0)]$ gives the limit in (B.2). On the other hand, we can write

$$\left\| \Sigma_2^{1/2} (X_1^\top X_1 + X_2^\top X_2)^{-1} \beta \right\|^2 = \beta^\top \Sigma_2^{-1/2} R'(0) \Sigma_2^{-1/2} \beta.$$

Hence its limit can be calculated through $R'_\infty(z)$, which gives the expression in (B.4). The details can be found in Appendix E.

We remark that one can probably derive the same asymptotic result using free probability theory (see e.g. [46]), but our results (B.2) and (B.4) also give an almost sharp error bound $O(p^{-1/2+\epsilon})$.

For the rest of this section, we shall state and prove the formal version of Theorem 3.2. First, we introduce several quantities that will be used in our statement, and they are also related to the quantities in Lemma B.2 and Lemma B.3. Given the optimal ratio \hat{v} , let (\hat{a}_1, \hat{a}_2) be the solution to the following system of deterministic equations,

$$\hat{a}_1 + \hat{a}_2 = 1 - \frac{1}{\rho_1 + \rho_2}, \quad \hat{a}_1 + \frac{1}{\rho_1 + \rho_2} \cdot \frac{1}{p} \sum_{i=1}^p \frac{\hat{v}^2 \lambda_i^2 \hat{a}_1}{\hat{v}^2 \lambda_i^2 \hat{a}_1 + \hat{a}_2} = \frac{\rho_1}{\rho_1 + \rho_2}. \quad (\text{B.6})$$

After obtaining (\hat{a}_1, \hat{a}_2) , we can solve the following linear equations to get (\hat{a}_3, \hat{a}_4) :

$$(\rho_2 \hat{a}_2^{-2} - \hat{b}_0) \cdot \hat{a}_3 - \hat{b}_1 \cdot \hat{a}_4 = \hat{b}_0, \quad (\rho_1 \hat{a}_1^{-2} - \hat{b}_2) \cdot \hat{a}_4 - \hat{b}_1 \cdot \hat{a}_3 = \hat{b}_1. \quad (\text{B.7})$$

where we denoted

$$\hat{b}_k := \frac{1}{p} \sum_{i=1}^p \frac{\hat{v}^{2k} \lambda_i^{2k}}{(\hat{a}_2 + \hat{v}^2 \lambda_i^2 \hat{a}_1)^2}, \quad k = 0, 1, 2.$$

Then we introduce the following matrix

$$\Pi \equiv \Pi(\hat{v}) = \frac{\rho_1^2}{(\rho_1 + \rho_2)^2} \cdot \hat{v}^2 M \frac{(1 + \hat{a}_3) \text{Id} + \hat{a}_4 \hat{v}^2 M^\top M}{(\hat{a}_1 \hat{v}^2 M^\top M + \hat{a}_2)^2} M^\top. \quad (\text{B.8})$$

We introduce two factors that will appear often in our statements and discussions:

$$\alpha_-(\rho_1) := \left(1 - \rho_1^{-1/2}\right)^2, \quad \alpha_+(\rho_1) := \left(1 + \rho_1^{-1/2}\right)^2.$$

In fact, $\alpha_-(\rho_1)$ and $\alpha_+(\rho_1)$ correspond to the largest and smallest singular values of $Z_1/\sqrt{n_1}$, respectively, as given by the famous Marčenko-Pastur law [64]. In particular, as ρ_1 increases, both α_- and α_+ will converge to 1 and $Z_1/\sqrt{n_1}$ will be more close to an isometry. Finally, we introduce the error term

$$\delta \equiv \delta(\hat{v}) := \frac{\alpha_+(\rho_1) - 1}{\alpha_-^2(\rho_1) \hat{v}^2 \lambda_{\min}^2(M)} \cdot \|\Sigma_1^{1/2}(\beta_1 - \hat{v}\beta_2)\|^2. \quad (\text{B.9})$$

Note that this factor converges to 0 as ρ_1 increases.

Now we are ready to state our main result for two tasks with both covariate and model shift. It shows that the information transfer is determined by two deterministic quantities Δ_{bias} and Δ_{var} , which give the change of model shift bias and the change of variance, respectively.

Theorem B.4 (Theorem 3.2 restated). *Consider two data models $Y_i = X_i \beta_i + \varepsilon_i$, $i = 1, 2$, that satisfy Assumption A.2 with $\sigma_1^2 = \sigma_2^2 = \sigma^2$. Then with high probability, we have*

$$L(\hat{\beta}_t^{\text{MTL}}) \leq L(\hat{\beta}_t^{\text{STL}}) \quad \text{when: } \Delta_{\text{var}} - \Delta_{\text{bias}} \geq \delta(\hat{v}) \quad (\text{B.10})$$

$$L(\hat{\beta}_t^{\text{MTL}}) \geq L(\hat{\beta}_t^{\text{STL}}) \quad \text{when: } \Delta_{\text{var}} - \Delta_{\text{bias}} \leq -\delta(\hat{v}), \quad (\text{B.11})$$

644 where

$$\Delta_{\text{var}} := \sigma^2 \left(\frac{1}{\rho_2 - 1} - \frac{1}{\rho_1 + \rho_2} \cdot \frac{1}{p} \text{Tr} [(\hat{a}_1 \hat{v}^2 M^\top M + \hat{a}_2 \text{Id})^{-1}] \right) \quad (\text{B.12})$$

$$\Delta_{\text{bias}} := (\beta_1 - \hat{v}\beta_2)^\top \Sigma_1^{1/2} \Pi(\hat{v}) \Sigma_1^{1/2} (\beta_1 - \hat{v}\beta_2). \quad (\text{B.13})$$

645 The proof of Theorem B.4 is based on Lemma B.2, Lemma B.3, and the following bound on the
646 singular values of Z_1 : for any fixed $\varepsilon > 0$, we have

$$\alpha_-(\rho_1) - O(p^{-1/2+e}) \preceq n_1^{-1} Z_1^\top Z_1 \preceq \alpha_+(\rho_1) + O(p^{-1/2+e}) \quad \text{w.h.p.} \quad (\text{B.14})$$

647 In fact, $n_1^{-1} Z_1^\top Z_1$ is a standard sample covariance matrix, and it is well-known that its eigenvalues
648 are inside the support of the Marchenko-Pastur law $[\alpha_-(\rho_1) - o(1), \alpha_+(\rho_1) + o(1)]$ with probability
649 $1 - o(1)$ [65]. The estimate (B.14) provides tight bounds for the concentration error. The result is
650 formally stated in Lemma E.4 below.

The main error δ of Theorem B.4 comes from approximating $n_1^{-1} Z_1^\top Z_1$ by Id using (B.14); see the
estimate (B.18) below. In order to improve this estimate and obtain an exact asymptotic result, one
needs to study the singular value distribution of the following random matrix:

$$(X_1^\top X_1)^{-1} X_2^\top X_2 + \hat{v}^2.$$

651 In fact, the eigenvalues of $\mathcal{X} := (X_1^\top X_1)^{-1} X_2^\top X_2$ have been studied in the name of Fisher matrices;
652 see e.g. [66]. However, since \mathcal{X} is not symmetric, it is known that the singular values of \mathcal{X} are
653 different from its eigenvalues. To the best of our knowledge, the asymptotic singular value behavior
654 of \mathcal{X} is still unknown in random matrix theory literature, and the study of the singular values of
655 $\mathcal{X} + \hat{v}^2$ will be even harder. We leave this problem to future study.

656 *Proof of Theorem B.4.* Note that

$$\begin{aligned} L(\hat{\beta}_t^{\text{STL}}) - L(\hat{\beta}_t^{\text{MTL}}) &= \sigma^2 \left(\text{Tr} [(X_2^\top X_2)^{-1} \Sigma_2] - \text{Tr} [(\hat{v}^2 X_1^\top X_1 + X_2^\top X_2)^{-1} \Sigma_2] \right) \\ &\quad - \hat{v}^2 \left\| \Sigma_2^{1/2} (\hat{v}^2 X_1^\top X_1 + X_2^\top X_2)^{-1} X_1^\top X_1 (\beta_1 - \hat{v}\beta_2) \right\|^2 =: \delta_{\text{var}}(\hat{v}) - \delta_{\text{bias}}(\hat{v}). \end{aligned}$$

657 We introduce the notation $\hat{M} \equiv \hat{M}(v) = v \Sigma_1^{1/2} \Sigma_2^{-1/2}$ for $v \in \mathbb{R}$. Then the proof is divided into the
658 following four steps.

- 659 (i) We first consider $\hat{M}(v)$ for a fixed $v \in \mathbb{R}$. Then we use Lemma B.1 and Lemma B.2 to
660 calculate the variance reduction $\delta_{\text{var}}(v)$, which will lead to the Δ_{var} term.
- 661 (ii) Using the approximate isometry property of Z_1 in (B.14), we will bound the bias term
662 $\delta_{\text{bias}}(v)$ through

$$\tilde{\delta}_{\text{bias}}(v) := v^2 n_1^2 \left\| \Sigma_2^{1/2} (v^2 X_1^\top X_1 + X_2^\top X_2)^{-1} \Sigma_1 (\beta_1 - v\beta_2) \right\|^2. \quad (\text{B.15})$$

- 663 (iii) We use Lemma B.3 to calculate (B.15), which will lead to the Δ_{bias} term.
- 664 (iv) Finally we use a standard ε -net argument to extend the above results to $\hat{M}(\hat{v})$ for a possibly
665 random \hat{v} which depends on Y_1 and Y_2 .

Step I: Variance reduction. Consider $\hat{M}(v)$ for any fixed $v \in \mathbb{R}$. Using Lemma B.2, we can
obtain that for any constant $\varepsilon > 0$,

$$\sigma^2 \cdot \text{Tr} [(X_2^\top X_2)^{-1} \Sigma_2] = \frac{\sigma^2}{\rho_2 - 1} \left(1 + O(p^{-1/2+e}) \right),$$

and

$$\sigma^2 \cdot \text{Tr} [(v^2 X_1^\top X_1 + X_2^\top X_2)^{-1} \Sigma_2] = \frac{\sigma^2}{\rho_1 + \rho_2} \cdot \frac{1}{p} \text{Tr} [(\hat{a}_1 \hat{M}^\top \hat{M} + \hat{a}_2 \text{Id})^{-1}] \left(1 + O(p^{-1/2+e}) \right),$$

666 with high probability, where \hat{a}_1 and \hat{a}_2 satisfy (B.6) with \hat{v} replaced by v . Combining them, we get

$$\delta_{\text{var}}(v) = \Delta_{\text{var}}(v) + O(\sigma^2 p^{-1/2+e}) \quad \text{w.h.p.}, \quad (\text{B.16})$$

667 where $\Delta_{\text{var}}(v)$ is defined as in (B.12) but with \hat{v} replaced by v .

668 **Step II: Bounding the bias term.** Next we use (B.14) to approximate $\delta_{\text{bias}}(v)$ with $\tilde{\delta}_{\text{bias}}(v)$.

669 **Claim B.5.** In the setting of Theorem B.4, we denote by $K = (v^2 X_1^\top X_1 + X_2^\top X_1)^{-1}$, and

$$\delta_{\text{err}}(v) := n_1^2 v^2 \left\| \Sigma_1^{1/2} K \Sigma_2 K \Sigma_1^{1/2} \right\| \cdot \left\| \Sigma_1^{1/2} (\beta_1 - v \beta_2) \right\|^2.$$

670 Then we have w.h.p.

$$\left| \delta_{\text{bias}}(v) - \tilde{\delta}_{\text{bias}}(v) \right| \leq \left(\alpha_+^2(\rho_1) - 1 + O(p^{-1/2+\varepsilon}) \right) \delta_{\text{err}}.$$

671 *Proof.* Denote by $\mathcal{E} = Z_1^\top Z_1 - n_1 \text{Id}$. Then we can write

$$\begin{aligned} \delta_{\text{bias}}(v) - \tilde{\delta}_{\text{bias}}(v) &= 2v^2 n_1 (\beta_1 - v \beta_2)^\top \Sigma_1^{1/2} \mathcal{E} \left(\Sigma_1^{1/2} K \Sigma_2 K \Sigma_1^{1/2} \right) \Sigma_1^{1/2} (\beta_1 - v \beta_2) \\ &\quad + v^2 \left\| \Sigma_2^{1/2} K \Sigma_1^{1/2} \mathcal{E} \Sigma_1^{1/2} (\beta_1 - v \beta_2) \right\|^2. \end{aligned} \quad (\text{B.17})$$

Using (B.14), we can bound

$$\|\mathcal{E}\| \leq \left(\alpha_+(\rho_1) - 1 + O(p^{-1/2+\varepsilon}) \right) n_1, \quad \text{w.h.p.}$$

672 Thus we can estimate that

$$\begin{aligned} |\delta_{\text{bias}}(v) - \tilde{\delta}_{\text{bias}}(v)| &\leq v^2 (2n_1 \|\mathcal{E}\| + \|\mathcal{E}\|^2) \left\| \Sigma_1^{1/2} K \Sigma_2 K \Sigma_1^{1/2} \right\| \left\| \Sigma_1^{1/2} (\beta_1 - v \beta_2) \right\|^2 \\ &= v^2 \left[(n_1 + \|\mathcal{E}\|)^2 - n_1^2 \right] \left\| \Sigma_1^{1/2} K \Sigma_2 K \Sigma_1^{1/2} \right\| \left\| \Sigma_1^{1/2} (\beta_1 - v \beta_2) \right\|^2 \\ &\leq v^2 n_1^2 \left[\alpha_+^2(\rho_1) + O(p^{-1/2+\varepsilon}) - 1 \right] \left\| \Sigma_1^{1/2} K \Sigma_2 K \Sigma_1^{1/2} \right\| \left\| \Sigma_1^{1/2} (\beta_1 - v \beta_2) \right\|^2, \end{aligned}$$

673 which concludes the proof by the definition of δ_ε . \square

674 Note by (B.14), we have with high probability,

$$\begin{aligned} v^2 n_1^2 \Sigma_1^{1/2} K \Sigma_2 K \Sigma_1^{1/2} &= n_1^2 \hat{M} (\hat{M}^\top Z_1^\top Z_1 \hat{M} + Z_2^\top Z_2)^{-2} \hat{M}^\top \\ &\leq n_1^2 \hat{M} \left[n_1 \alpha_-(\rho_1) \hat{M}^\top \hat{M} + n_2 \alpha_-(\rho_2) + O(p^{1/2+\varepsilon}) \right]^{-2} \hat{M}^\top \\ &\leq \left[\alpha_-^2(\rho_1) \hat{M} \hat{M}^\top + 2 \frac{\rho_2}{\rho_1} \alpha_-(\rho_1) \alpha_-(\rho_2) + 2 \left(\frac{\rho_2}{\rho_1} \right)^2 \alpha_-^2(\rho_2) (\hat{M} \hat{M}^\top)^{-1} \right]^{-1} + O(p^{-1/2+\varepsilon}) \\ &\leq [\alpha_-^2(\rho_1) \lambda_{\min}^2(\hat{M})]^{-1} \cdot (1 - c) \end{aligned}$$

675 for some small enough constant $c > 0$. Together with Claim B.5, we get with high probability,

$$\left| \delta_{\text{bias}}(v) - \tilde{\delta}_{\text{bias}}(v) \right| \leq (1 - c) \delta(v) \quad (\text{B.18})$$

676 for some small constant $c > 0$, where we recall $\delta(v)$ defined in (B.9).

677 **Step III: The limit of $\tilde{\delta}_{\text{bias}}(v)$.** Using Lemma B.3 with Σ_1 and M replaced by $v^2 \Sigma_1$ and \hat{M} , we
678 obtain that

$$\begin{aligned} \tilde{\delta}_{\text{bias}}(v) &= \frac{\rho_1^2}{(\rho_1 + \rho_2)^2} \cdot v^2 (\beta_1 - v \beta_2)^\top \Sigma_1 \Sigma_2^{-1/2} \frac{(1 + \hat{a}_3) \text{Id} + \hat{a}_4 \hat{M}^\top \hat{M}}{(\hat{a}_1 \hat{M}^\top \hat{M} + \hat{a}_2)^2} \Sigma_2^{-1/2} \Sigma_1 (\beta_1 - v \beta_2) + O(p^{-1/2+\varepsilon}) \\ &= (\beta_1 - v \beta_2)^\top \Sigma_1^{1/2} \Pi \Sigma_1^{1/2} (\beta_1 - v \beta_2) + O(p^{-1/2+\varepsilon}) =: \Delta_{\text{bias}}(v) + O(p^{-1/2+\varepsilon}), \end{aligned}$$

679 with high probability. Together with and (B.16) and (B.18), we obtain that w.h.p.,

$$\begin{cases} \delta_{\text{var}}(v) > \delta_{\text{bias}}(v), & \text{if } \Delta_{\text{var}}(v) - \Delta_{\text{bias}}(v) \geq \delta(v), \\ \delta_{\text{var}}(v) < \delta_{\text{bias}}(v), & \text{if } \Delta_{\text{var}}(v) - \Delta_{\text{bias}}(v) \leq -\delta(v). \end{cases} \quad (\text{B.19})$$

Step IV: An ε -net argument. Finally, it remains to extend the above result (B.19) to $v = \hat{v}$, which is random and depends on X_1 and X_2 . We first show that for any fixed constant $C_0 > 0$, there exists a high probability event Ξ on which (B.19) holds uniformly for all $v \in [-C_0, C_0]$. In fact, we consider v belonging to a discrete set

$$V := \{v_k = kp^{-1} : -(C_0p + 1) \leq k \leq C_0p + 1\}.$$

Then using the arguments for the first three steps and a simple union bound, we get that (B.19) holds simultaneously for all $v \in V$ with high probability. On the other hand, by (B.14) the event

$$\Xi_1 := \left\{ \alpha_-(\rho_1)/2 \preceq \frac{Z_1^T Z_1}{n_1} \preceq 2\alpha_+(\rho_1), \alpha_-(\rho_2)/2 \preceq \frac{Z_2^T Z_2}{n_2} \preceq 2\alpha_+(\rho_2) \right\}$$

holds with high probability. Now it is easy to check that on Ξ_1 , for all $v_k \leq v \leq v_{k+1}$ we have the following estimates:

$$\begin{aligned} |\delta_{\text{var}}(v) - \delta_{\text{var}}(v_k)| &\lesssim p^{-1} \delta_{\text{var}}(v_k), \quad |\delta_{\text{bias}}(v) - \delta_{\text{bias}}(v_k)| \lesssim p^{-1} \delta_{\text{bias}}(v_k), \quad |\delta(v) - \delta(v_k)| \lesssim p^{-1} \delta(v_k), \\ |\Delta_{\text{bias}}(v) - \Delta_{\text{bias}}(v_k)| &\lesssim p^{-1} \Delta_{\text{bias}}(v_k), \quad |\Delta_{\text{var}}(v) - \Delta_{\text{var}}(v_k)| \lesssim p^{-1} \Delta_{\text{var}}(v_k). \end{aligned}$$

Then a simple application of triangle inequality gives that the event

$$\Xi_2 = \{(\text{B.19}) \text{ holds simultaneously for all } -C_0 \leq v \leq C_0\}$$

holds with high probability. On the other hand, on Ξ_1 one can see that for any small constant $\varepsilon > 0$, there exists a large enough constant $C_0 > 0$ depending on ε such that

$$\begin{aligned} |\delta_{\text{var}}(v) - \delta_{\text{var}}(C_0)| &\leq \varepsilon \delta_{\text{var}}(C_0), \quad |\delta_{\text{bias}}(v) - \delta_{\text{bias}}(C_0)| \leq \varepsilon \delta_{\text{bias}}(C_0), \quad |\delta(v) - \delta(C_0)| \leq \varepsilon \delta(C_0), \\ |\Delta_{\text{bias}}(v) - \Delta_{\text{bias}}(C_0)| &\leq \varepsilon \Delta_{\text{bias}}(C_0), \quad |\Delta_{\text{var}}(v) - \Delta_{\text{var}}(C_0)| \leq \varepsilon \Delta_{\text{var}}(C_0), \end{aligned}$$

for all $v \geq C_0$. Similar estimates hold for $v \leq -C_0$ if we replace C_0 with $-C_0$ in the above estimates. Together with the estimate at $\pm C_0$, we get that (B.19) holds simultaneously for all $v \in \mathbb{R}$ on the high probability event $\Xi_1 \cap \Xi_2$. This concludes the proof since v must be one of the real values. \square

For the isotropic model in Section 3.2, we actually have an easier and sharper bound than Theorem B.4 as follows.

Lemma B.6 (The isotropic model). *In the setting of Theorem B.4, assume that $\Sigma_1 = \text{Id}$, β_2 is a random vector with i.i.d. entries with mean 0, variance κ^2 and all moments, and β_1 is a random vector such that $(\beta_1 - v\beta_2)$ is a random vector with i.i.d. entries with mean 0, variance d^2 and all moments. Denote $\Delta_{\text{bias}}^* := ((1 - v)^2 \kappa^2 + d^2) \text{Tr}[\Pi(\hat{v})]$. Then we have with high probability,*

$$\begin{aligned} L(\hat{\beta}_t^{\text{MTL}}) &\leq L(\hat{\beta}_t^{\text{STL}}) \quad \text{when: } \Delta_{\text{var}} \geq (\alpha_+^2(\rho_1) + o(1)) \cdot \Delta_{\text{bias}}^*, \\ L(\hat{\beta}_t^{\text{MTL}}) &\geq L(\hat{\beta}_t^{\text{STL}}) \quad \text{when: } \Delta_{\text{var}} \leq (\alpha_-^2(\rho_1) - o(1)) \cdot \Delta_{\text{bias}}^*. \end{aligned}$$

Proof. The proof of Lemma B.6 is similar to that for Theorem B.4, except that we can replace (B.18) with a tighter bound. We only describe the main difference.

For any fixed $v \in \mathbb{R}$, $\beta_1 - v\beta_2$ is a random vector with i.i.d. entries with mean 0 and variance $(1 - v)^2 \kappa^2 + d^2$. Then using the concentration result, Lemma E.14, we get that for any constant $\varepsilon > 0$,

$$\begin{aligned} &|\delta_{\text{bias}}(v) - [(1 - v)^2 \kappa^2 + d^2] \text{Tr}(\mathcal{K}^\top \mathcal{K})| \\ &= |(\beta_1 - v\beta_2)^\top \mathcal{K}^\top \mathcal{K} (\beta_1 - v\beta_2) - [(1 - v)^2 \kappa^2 + d^2] \text{Tr}(\mathcal{K}^\top \mathcal{K})| \\ &\leq p^\varepsilon [(1 - v)^2 \kappa^2 + d^2] \left\{ \text{Tr}[(\mathcal{K}^\top \mathcal{K})^2] \right\}^{1/2} \lesssim p^{1/2+\varepsilon} [(1 - v)^2 \kappa^2 + d^2], \end{aligned} \quad (\text{B.20})$$

where we denoted $\mathcal{K} := v\Sigma_2^{1/2}(v^2 X_1^\top X_1 + X_2^\top X_2)^{-1} X_1^\top X_1$, and in the last step we used $\|\mathcal{K}\| = O(1)$ by (B.14). Now for $\text{Tr}(\mathcal{K}^\top \mathcal{K})$, we rewrite it as

$$v^2 \text{Tr}[(v^2 X_1^\top X_1 + X_2^\top X_2)^{-1} \Sigma_2 (v^2 X_1^\top X_1 + X_2^\top X_2)^{-1} (X_1^\top X_1)^2].$$

Bounding $(X_1^\top X_1)^2 = (Z_1^\top Z_1)^2$ using (B.14) again, we obtain that

$$\delta_{\text{bias}}^*(v) \cdot (\alpha_-^2(\rho_1) - O(p^{-1/2+\varepsilon})) \leq [(1 - v)^2 \kappa^2 + d^2] \text{Tr}(\mathcal{K}^\top \mathcal{K}) \leq \delta_{\text{bias}}^*(v) \cdot (\alpha_+^2(\rho_1) + O(p^{-1/2+\varepsilon})), \quad (\text{B.21})$$

where

$$\delta_{\text{bias}}^*(v) := n_1^2 v^2 [(1-v)^2 \kappa^2 + d^2] \text{Tr} [(v^2 X_1^\top X_1 + X_2^\top X_2)^{-1} \Sigma_2 (v^2 X_1^\top X_1 + X_2^\top X_2)^{-1}].$$

701 Note that $\delta_{\text{bias}}^*(v) \sim p$, hence combining (B.20) and (B.21) we get

$$\delta_{\text{bias}}^*(v) \cdot (\alpha_-^2(\rho_1) - O(p^{-1/2+\varepsilon})) \leq \delta_{\text{bias}}(v) \leq \delta_{\text{bias}}^*(v) \cdot (\alpha_+^2(\rho_1) + O(p^{-1/2+\varepsilon})). \quad (\text{B.22})$$

702 Now we can replace the estimate (B.18) with this stronger estimate, and repeat all the other parts
703 of the proof of Theorem B.4 to conclude Lemma B.6. In particular, one can calculate $\delta_{\text{bias}}^*(v)$ using
704 Lemma B.3 and get the $\Delta_{\text{bias}}^*(v)$ term. We omit the details. \square

705 C Proofs for Isotropic and Covariate Shifted Settings

706 We show that for the isotropic model, the optimum of \hat{v} is very close to 1. This allows us to simplify
707 the expression of $L(\hat{\beta}_2^{\text{MTL}})$ significantly. More precisely, we have the following lemma. Later on, we
708 combine the following lemma with Lemma B.6 together to analyze the bias-variance tradeoff.

709 **Lemma C.1.** *In the isotropic model, for some constant $c_0 > 0$, suppose that*

$$\frac{pd^2}{\sigma^2} \leq O(1), \quad p^{-1+c_0} \leq \frac{\kappa^2}{\sigma^2} \leq p^{-\varepsilon_0-c_0}. \quad (\text{C.1})$$

710 Then we have

$$\begin{aligned} L(\hat{\beta}_2^{\text{MTL}}) &= (1 + O(n^{-\varepsilon})) \cdot d^2 \text{Tr} [(X_1^\top X_1 + X_2^\top X_2)^{-2} (X_1^\top X_1)^2] \\ &\quad + (1 + O(n^{-\varepsilon})) \cdot \sigma^2 \text{Tr} [(X_1^\top X_1 + X_2^\top X_2)^{-1}] \end{aligned} \quad (\text{C.2})$$

711 w.h.p. for some constant $\varepsilon > 0$.

712 *Proof.* Using Lemma E.14, we obtain that $\text{val}(v) = N_2 \cdot h(v) (1 + O(p^{-1/2+\varepsilon}))$. We define the
713 function

$$\begin{aligned} h(v) &= \frac{\rho_1}{\rho_2} \left[d^2 + (v-1)^2 \kappa^2 \right] \cdot \text{Tr} [(v^2 X_1^\top X_1 + X_2^\top X_2)^{-2} (X_2^\top X_2)^2] \\ &\quad + v^2 \left[d^2 + (v-1)^2 \kappa^2 \right] \cdot \text{Tr} [(v^2 X_1^\top X_1 + X_2^\top X_2)^{-2} (X_1^\top X_1)^2] \\ &\quad + \left(\frac{\rho_1}{\rho_2} v^2 + 1 \right) \sigma^2 \cdot \text{Tr} [(v^2 X_1^\top X_1 + X_2^\top X_2)^{-1}]. \end{aligned}$$

714 Hence the validation loss in (A.5) reduces to

$$g(v) = [N_2 \cdot h(v) + (N_1 \sigma_1^2 + N_2 \sigma_2^2)] \cdot \left(1 + O(p^{-(1-\varepsilon_0)/2+\varepsilon}) \right) \quad (\text{C.3})$$

715 with high probability for any constant $\varepsilon > 0$.

716 Let \hat{w} the minimizer of $h(v)$. The proof consists of two steps.

- 717 • First, we show that \hat{w} is close to 1.
- 718 • Second, with (C.3) we show that \hat{v} is close to \hat{w} . Then we plug \hat{v} into $L(\hat{\beta}_2^{\text{MTL}})$ to get (C.2).

719 For the first step, we will prove the following result.

720 **Claim C.2.** *There exists a constant $C > 0$ such that*

$$|\hat{w} - 1| \leq C \left(\frac{d^2}{\kappa^2} + \frac{\sigma^2}{p\kappa^2} \right) \quad \text{w.h.p.} \quad (\text{C.4})$$

721 *Proof.* To be consistent with the notation \hat{w} , we shall change the name of the argument to w in the
722 proof. First it is easy to observe that $h(w) < h(-w)$ for $w > 0$. Hence it suffices to assume that
723 $w \geq 0$. We first consider the case $w \geq 1$. We write

$$\begin{aligned} h(w) &= \frac{\rho_1}{\rho_2} \left[\frac{d^2}{w^4} + \frac{(w-1)^2}{w^4} \kappa^2 \right] \cdot \text{Tr} [(X_1^\top X_1 + w^{-2} X_2^\top X_2)^{-2} (X_2^\top X_2)^2] \\ &\quad + \left[\frac{d^2}{w^2} + \frac{(w-1)^2}{w^2} \kappa^2 \right] \cdot \text{Tr} [(X_1^\top X_1 + w^{-2} X_2^\top X_2)^{-2} (X_1^\top X_1)^2] \\ &\quad + \frac{\rho_1}{\rho_2} \sigma^2 \cdot \text{Tr} [(X_1^\top X_1 + w^{-2} X_2^\top X_2)^{-1}] + \sigma^2 \cdot \text{Tr} [(w^2 X_1^\top X_1 + X_2^\top X_2)^{-1}]. \end{aligned}$$

Notice that

$$\text{Tr} [(X_1^\top X_1 + w^{-2} X_2^\top X_2)^{-2} (X_i^\top X_i)^2], \quad i = 1, 2, \quad \text{and} \quad \text{Tr} [(X_1^\top X_1 + w^{-2} X_2^\top X_2)^{-1}]$$

are increasing functions in w . Hence taking derivative of $h(w)$ with respect to w , we obtain that

$$\begin{aligned} h'(w) &\geq \frac{\rho_1}{\rho_2} \left[\frac{2(w-1)(2-w)}{w^5} \kappa^2 - \frac{4d^2}{w^5} \right] \text{Tr} [(X_1^\top X_1 + w^{-2} X_2^\top X_2)^{-2} (X_2^\top X_2)^2] \\ &\quad + \left[\frac{2(w-1)}{w^3} \kappa^2 - \frac{2d^2}{w^3} \right] \cdot \text{Tr} [(X_1^\top X_1 + w^{-2} X_2^\top X_2)^{-2} (X_1^\top X_1)^2] \\ &\quad - 2 \frac{\sigma^2}{w^3} \cdot \text{Tr} [(X_1^\top X_1 + w^{-2} X_2^\top X_2)^{-2} X_1^\top X_1] = \text{Tr} [(X_1^\top X_1 + w^{-2} X_2^\top X_2)^{-2} \mathcal{A}], \end{aligned}$$

where the matrix \mathcal{A} is

$$\mathcal{A} := \frac{\rho_1}{\rho_2} \left[\frac{2(w-1)(2-w)}{w^5} \kappa^2 - \frac{4d^2}{w^5} \right] (X_2^\top X_2)^2 + \left[\frac{2(w-1)}{w^3} \kappa^2 - \frac{2d^2}{w^3} \right] (X_1^\top X_1)^2 - 2 \frac{\sigma^2}{w^3} X_1^\top X_1.$$

Using the estimate (B.14), we get that \mathcal{A} is lower bounded as

$$\begin{aligned} \mathcal{A} &\succeq - \frac{4d^2}{w^5} n_1 n_2 (\alpha_+(\rho_2) + o(1))^2 + \left[\frac{2(w-1)}{w^3} \kappa^2 - \frac{2d^2}{w^3} \right] n_1^2 (\alpha_-(\rho_1) - o(1))^2 \\ &\quad - 2 \frac{\sigma^2}{w^3} n_1 (\alpha_+(\rho_1) + o(1)) \succ 0, \end{aligned}$$

as long as

$$w > w_1 := 1 + \frac{d^2}{\kappa^2} + \frac{\sigma^2}{n_1 \kappa^2} \frac{\alpha_+(\rho_1) + o(1)}{\alpha_-^2(\rho_1)} + \frac{2d^2}{\kappa^2} \frac{\rho_2 (\alpha_+^2(\rho_2) + o(1))}{\rho_1 \alpha_-^2(\rho_1)}.$$

Hence $h'(w) > 0$ on (w_1, ∞) , i.e. $h(w)$ is strictly increasing for $w > w_1$. This gives $\hat{w} \leq w_1$.

Then we consider the case $w \leq 1$, and the proof is similar as above. Taking derivative of $h(w)$, we obtain that

$$\begin{aligned} h'(w) &\leq \frac{\rho_1}{\rho_2} [2(w-1)\kappa^2] \cdot \text{Tr} [(w^2 X_1^\top X_1 + X_2^\top X_2)^{-2} (X_2^\top X_2)^2] \\ &\quad + [2wd^2 + 2w(w-1)(2w-1)\kappa^2] \cdot \text{Tr} [(w^2 X_1^\top X_1 + X_2^\top X_2)^{-2} (X_1^\top X_1)^2] \\ &\quad + \frac{\rho_1}{\rho_2} (2w\sigma^2) \cdot \text{Tr} [(w^2 X_1^\top X_1 + X_2^\top X_2)^{-2} X_2^\top X_2] \\ &= \frac{\rho_1}{\rho_2} \text{Tr} [(w^2 X_1^\top X_1 + X_2^\top X_2)^{-1} \mathcal{B}], \end{aligned} \tag{C.5}$$

where the matrix \mathcal{B} is

$$\mathcal{B} = 2(w-1)\kappa^2 (X_2^\top X_2)^2 + \frac{\rho_2}{\rho_1} [2wd^2 + 2w(w-1)(2w-1)\kappa^2] (X_1^\top X_1)^2 + 2w\sigma^2 X_2^\top X_2.$$

Using the estimate (B.14), we get that \mathcal{B} is upper bounded as

$$\mathcal{B} \preceq -2(1-w)\kappa^2 n_2^2 (\alpha_-(\rho_2) - o(1))^2 + 2wd^2 n_1 n_2 (\alpha_+(\rho_1) + o(1))^2 + 2w\sigma^2 n_2 (\alpha_+(\rho_2) + o(1)) \prec 0,$$

as long as

$$w < w_2 := 1 - \frac{d^2}{\kappa^2} \frac{\rho_1 (\alpha_+(\rho_1) + o(1))^2}{\rho_2 \alpha_-^2(\rho_2)} - \frac{\sigma^2}{n_2 \kappa^2} \frac{\alpha_+(\rho_2) + o(1)}{\alpha_-^2(\rho_2)}.$$

Hence $h'(w) < 0$ on $[0, w_2)$, i.e. $h(w)$ is strictly decreasing for $w < w_2$. This gives $\hat{w} \geq w_2$.

In sum, we obtain that $w_2 \leq w \leq w_1$. Note that under our assumptions, we have

$$\max(|w_1 - 1|, |w_2 - 1|) = O\left(\frac{d^2}{\kappa^2} + \frac{\sigma^2}{p\kappa^2}\right),$$

which concludes the proof. \square

733 Next we prove the following estimate on the optimizer \hat{v} : with high probability,

$$|\hat{v} - 1| = O(\mathcal{E}), \quad \mathcal{E} := \frac{d^2}{\kappa^2} + \frac{\sigma^2}{p\kappa^2} + p^{-1/2+\varepsilon_0/2+2\varepsilon}. \quad (\text{C.6})$$

In fact, from the proof of Claim C.2 above, one can check that if $C\mathcal{E} \leq |w - 1| \leq 2C\mathcal{E}$ for a large enough constant $C > 1$, then $|h'(w)| \gtrsim pd^2$. Moreover, under (C.1) we have

$$h(w) = O(pd^2), \quad \text{for } |w - 1| \leq 2C\mathcal{E}.$$

Thus we obtain that for $|w - 1| \geq 2C\mathcal{E}$,

$$|h(w) - h(\hat{w})| \geq |h(w) - \min(h(w_1), h(w_2))| \gtrsim pd^2\mathcal{E} \gtrsim \mathcal{E} \cdot h(\hat{w}),$$

734 which leads to $g(w) > g(\hat{w})$ w.h.p. by (C.3). Thus w cannot be a minimizer of $g(v)$, and we must
735 have $|\hat{v} - 1| \leq 2C\mathcal{E}$.

736 Inserting (C.6) into (A.6) and applying Lemma E.14 to $(\beta_1 - \hat{v}\beta_s)$ again, we get w.h.p.,

$$\begin{aligned} L(\hat{\beta}_2^{\text{MTL}}) &= (1 + O(\mathcal{E})) \cdot [d^2 + O(\mathcal{E}^2\kappa^2)] \text{Tr}[(X_1^\top X_1 + X_2^\top X_2)^{-2}(X_1^\top X_1)^2] \\ &\quad + (1 + O(\mathcal{E})) \cdot \sigma^2 \text{Tr}[(X_1^\top X_1 + X_2^\top X_2)^{-1}]. \end{aligned} \quad (\text{C.7})$$

In order to study the phenomenon of bias-variance trade-off, we need the bias term with d^2 and the variance term with σ^2 to be of the same order. With estimate (B.14), we see that

$$\text{Tr}[(X_1^\top X_1 + X_2^\top X_2)^{-2}(X_1^\top X_1)^2] \sim p, \quad \text{Tr}[(X_1^\top X_1 + X_2^\top X_2)^{-1}] \sim \frac{p}{n_1 + n_2}.$$

737 Hence we need to choose that $pd^2 \sim \sigma^2$. On the other hand, we want the error term $\mathcal{E}^2\kappa^2$ to be much
738 smaller than d^2 , which leads to the condition $p^{-1+\varepsilon_0+4\varepsilon}\kappa^2 \ll d^2 \ll \kappa^2$. The above considerations
739 lead to the choices of parameters in (C.1). Moreover, under (C.1) we can simplify (C.7) to (C.2). \square

740 C.1 Missing Proofs regarding Task Similarity

741 With (C.2) and Lemma B.6, we can prove Proposition 3.3, which gives a transition threshold with
742 respect to the ratio between the model bias and the noise level. With slight abuse of notations, we
743 shall write \hat{a}_i and \hat{b}_k as a_i and b_k throughout the proof.

744 *Proof of Proposition 3.3.* In the setting of Proposition 3.3, we have $M = \Sigma_1^{1/2}\Sigma_2^{-1/2} = \text{Id}$. Then
745 solving equations (B.3) and (B.5) with $\lambda_i = 1$, we get that

$$a_1 = \frac{\rho_1(\rho_1 + \rho_2 - 1)}{(\rho_1 + \rho_2)^2}, \quad a_2 = \frac{\rho_2(\rho_1 + \rho_2 - 1)}{(\rho_1 + \rho_2)^2}, \quad (\text{C.8})$$

$$a_3 = \frac{\rho_2}{(\rho_1 + \rho_2)(\rho_1 + \rho_2 - 1)}, \quad a_4 = \frac{\rho_1}{(\rho_1 + \rho_2)(\rho_1 + \rho_2 - 1)}. \quad (\text{C.9})$$

746 Using Lemma B.1 and Lemma B.2, we can track the reduction of variance from $\hat{\beta}_2^{\text{MTL}}$ to $\hat{\beta}_2^{\text{STL}}$ as

$$\begin{aligned} \delta_{\text{var}} &:= \sigma^2 \text{Tr}[(X_2^\top X_2)^{-1}] - (1 + O(n^{-\varepsilon})) \cdot \sigma^2 \text{Tr}[(X_1^\top X_1 + X_2^\top X_2)^{-1}] \\ &= \Delta_{\text{var}} \cdot (1 + O(n^{-\varepsilon})) \end{aligned} \quad (\text{C.10})$$

747 with high probability, where

$$\Delta_{\text{var}} := \sigma^2 \left(\frac{1}{\rho_2 - 1} - \frac{1}{\rho_1 + \rho_2} \cdot \frac{1}{a_1 + a_2} \right) = \sigma^2 \cdot \frac{\rho_1}{(\rho_2 - 1)(\rho_1 + \rho_2 - 1)}.$$

Next for the model shift bias

$$\delta_{\text{bias}} := (1 + O(n^{-\varepsilon})) \cdot d^2 \text{Tr}[(X_1^\top X_1 + X_2^\top X_2)^{-2}(X_1^\top X_1)^2],$$

748 we can get from Lemma B.6 (or rather its proof) that

$$\alpha_-^2(\rho_1) - o(1) \leq \frac{\delta_{\text{bias}}}{\Delta_{\text{bias}}} \leq \alpha_+^2(\rho_1) + o(1), \quad (\text{C.11})$$

where

$$\Delta_{\text{bias}} := pd^2 \cdot \frac{\rho_1^2}{(\rho_1 + \rho_2)^2} \frac{1 + a_3 + a_4}{(a_1 + a_2)^2} = pd^2 \cdot \frac{\rho_1^2(\rho_1 + \rho_2)}{(\rho_1 + \rho_2 - 1)^3}.$$

749 Note that

$$L(\hat{\beta}_2^{\text{STL}}) - L(\hat{\beta}_2^{\text{MTL}}) = \delta_{\text{var}} - \delta_{\text{bias}}. \quad (\text{C.12})$$

750 Then we can track its sign using (C.10) and (C.11).

751 **Positive transfer.** With (C.10) and (C.11), we conclude that if

$$pd^2 \cdot \frac{\rho_1^2(\rho_1 + \rho_2)}{(\rho_1 + \rho_2 - 1)^3} \cdot (\alpha_+^2(\rho_1) + o(1)) < \sigma^2 \cdot \frac{\rho_1}{(\rho_2 - 1)(\rho_1 + \rho_2 - 1)}, \quad (\text{C.13})$$

752 we have that $\delta_{\text{var}} > \delta_{\text{bias}}$, which implies $L(\hat{\beta}_2^{\text{MTL}}) < L(\hat{\beta}_2^{\text{STL}})$. We can simplify (C.13) to

$$\frac{pd^2}{\sigma^2} < \Phi(\rho_1, \rho_2) \cdot (\alpha_+^2(\rho_1) + o(1))^{-1}, \quad (\text{C.14})$$

753 Since $\Psi(\beta_1, \beta_2) = pd^2/\sigma^2$ and $\nu \geq \alpha_+^2(\rho_1) + o(1)$, it gives the first statement of Proposition 3.3.

754 **Negative transfer.** On the other hand, if

$$pd^2 \cdot \frac{\rho_1^2(\rho_1 + \rho_2)}{(\rho_1 + \rho_2 - 1)^3} \cdot (\alpha_-^2(\rho_1) - o(1)) > \sigma^2 \cdot \frac{\rho_1}{(\rho_2 - 1)(\rho_1 + \rho_2 - 1)}, \quad (\text{C.15})$$

755 we have that $\delta_{\text{var}} < \delta_{\text{bias}}$, which implies $L(\hat{\beta}_2^{\text{MTL}}) > L(\hat{\beta}_2^{\text{STL}})$. We can simplify (C.15) to

$$\Psi(\beta_1, \beta_2) = \frac{pd^2}{\sigma^2} > \Phi(\rho_1, \rho_2) \cdot (\alpha_-^2(\rho_1) - o(1))^{-1}, \quad (\text{C.16})$$

756 which gives the second statement of Proposition 3.3. \square

757 Next we consider the case where the two tasks have different noise variances $\sigma_1^2 \neq \sigma_2^2$. In particular,
758 we show Proposition C.3, which gives a transition threshold with respect to the difference between
759 the noise levels of the two tasks.

760 **Proposition C.3.** *In the isotropic model, assume that $\rho_1 > 40$ and $\mathbb{E}[\|\beta_1 - \beta_2\|^2] < \frac{1}{2}\sigma_2^2 \cdot \Phi(\rho_1, \rho_2)$.
761 Then we have the following transition with respect to σ_1^2 :*

- 762 • If $\sigma_1^2 < -\nu^{1/2}\rho_1 \cdot pd^2 + (1 + \nu^{-1/2}\rho_1\Phi(\rho_1, \rho_2)) \cdot \sigma_2^2$, then w.h.p. $L(\hat{\beta}_2^{\text{MTL}}) < L(\hat{\beta}_2^{\text{STL}})$.
- 763 • If $\sigma_1^2 > -\nu^{-1/2}\rho_1 \cdot pd^2 + (1 + \nu^{1/2}\rho_1\Phi(\rho_1, \rho_2)) \cdot \sigma_2^2$, then w.h.p. $L(\hat{\beta}_2^{\text{MTL}}) > L(\hat{\beta}_2^{\text{STL}})$.

764 As a corollary, if $\sigma_1^2 \leq \sigma_2^2$, then we always get positive transfer.

765 *Proof.* In the setting of Proposition C.3, the test loss is given by (A.6). In the isotropic model, using
766 again the concentration result, Lemma E.14, we can rewrite $L(\hat{\beta}_2^{\text{MTL}})$ as

$$\begin{aligned} L(\hat{\beta}_2^{\text{MTL}}) = & \hat{v}^2 \left[d^2 + (\hat{v} - 1)^2 \kappa^2 \right] \text{Tr} \left[(\hat{v}^2 X_1^\top X_1 + X_2^\top X_2)^{-2} (X_1^\top X_1)^2 \right] \cdot \left(1 + O(p^{-1/2+\epsilon}) \right) \\ & + \sigma_2^2 \cdot \text{Tr} \left[(\hat{v}^2 X_1^\top X_1 + X_2^\top X_2)^{-1} \right] + (\sigma_1^2 - \sigma_2^2) \cdot \text{Tr} \left[(\hat{v}^2 X_1^\top X_1 + X_2^\top X_2)^{-2} \hat{v}^2 X_1^\top X_1 \right] \end{aligned}$$

767 with high probability for any constant $\epsilon > 0$.

768 In the current setting, we can also show that (C.6) holds for \hat{v} . Since the proof is almost the same as
769 the one for Lemma C.2, we omit the details. Thus under the choice of parameters in (C.1), $L(\hat{\beta}_2^{\text{MTL}})$
770 can be simplified as in (C.2):

$$\begin{aligned} L(\hat{\beta}_2^{\text{MTL}}) = & (1 + O(n^{-\epsilon})) \cdot d^2 \text{Tr} \left[(X_1^\top X_1 + X_2^\top X_2)^{-2} (X_1^\top X_1)^2 \right] \\ & + (1 + O(n^{-\epsilon})) \cdot \sigma_2^2 \text{Tr} \left[(X_1^\top X_1 + X_2^\top X_2)^{-1} \right] \\ & + (1 + O(n^{-\epsilon})) \cdot (\sigma_1^2 - \sigma_2^2) \text{Tr} \left[(X_1^\top X_1 + X_2^\top X_2)^{-2} X_1^\top X_1 \right]. \end{aligned} \quad (\text{C.17})$$

Then we have

$$L(\hat{\beta}_2^{\text{STL}}) - L(\hat{\beta}_2^{\text{MTL}}) = \delta_{\text{var}} - \delta_{\text{bias}} - \delta_{\text{var}}^{(2)},$$

where

$$\delta_{\text{var}} := \sigma_2^2 \text{Tr}[(X_2^\top X_2)^{-1}] - (1 + O(n^{-\varepsilon})) \cdot \sigma_2^2 \text{Tr}[(X_1^\top X_1 + X_2^\top X_2)^{-1}]$$

satisfies (C.10) with σ^2 replaced by σ_2^2 ,

$$\delta_{\text{bias}} := (1 + O(n^{-\varepsilon})) \cdot d^2 \text{Tr}[(X_1^\top X_1 + X_2^\top X_2)^{-2} (X_1^\top X_1)^2]$$

771 satisfies (C.11), and $\delta_{\text{var}}^{(2)}$ is defined as

$$\delta_{\text{var}}^{(2)} := (1 + O(n^{-\varepsilon})) \cdot (\sigma_1^2 - \sigma_2^2) \text{Tr}[(X_1^\top X_1 + X_2^\top X_2)^{-2} X_1^\top X_1].$$

772 To estimate this new term $\delta_{\text{var}}^{(2)}$, we use the same arguments as in the proof of Lemma B.6: we first
 773 replace $X_1^\top X_1$ with $n_1 \text{Id}$ up to some error using (B.14), and then apply Lemma B.3 to calculate
 774 $\text{Tr}[(X_1^\top X_1 + X_2^\top X_2)^{-2}]$. This process leads to the following estimates on $\delta_{\text{var}}^{(2)}$:

$$\alpha_-(\rho_1) - o(1) \leq \delta_{\text{var}}^{(2)} / \Delta_{\text{var}}^{(2)} \leq \alpha_+(\rho_1) + o(1), \quad (\text{C.18})$$

where

$$\Delta_{\text{var}}^{(2)} := (\sigma_1^2 - \sigma_2^2) \frac{\rho_1(\rho_1 + \rho_2)}{(\rho_1 + \rho_2 - 1)^3}.$$

775 Next we compare δ_{var} with $\delta_{\text{bias}} + \delta_{\text{var}}^{(2)}$. Our main focus is to see how the extra $\delta_{\text{var}}^{(2)}$ affects the
 776 information transfer in this case.

777 Note that the condition $\mathbb{E}[\|\beta_1 - \beta_2\|^2] < \frac{1}{2}\sigma_2^2 \cdot \Phi(\rho_1, \rho_2)$ for $\rho_1 > 40$ gives that $\delta_{\text{var}} > \delta_{\text{bias}}$ by
 778 Proposition 3.3. Hence if $\sigma_1^2 \leq \sigma_2^2$, then $\delta_{\text{var}}^{(2)} < 0$ and we always have $\delta_{\text{var}} > \delta_{\text{bias}} + \delta_{\text{var}}^{(2)}$, which gives
 779 $L(\hat{\beta}_2^{\text{MTL}}) < L(\hat{\beta}_2^{\text{STL}})$. It remains to consider the case $\sigma_1^2 \geq \sigma_2^2$.

780 **Positive transfer.** By (C.10), (C.11) and (C.18), if the following inequality holds,

$$\begin{aligned} & \sigma_2^2 \cdot \frac{\rho_1}{(\rho_2 - 1)(\rho_1 + \rho_2 - 1)} \cdot (1 - o(1)) \\ & > pd^2 \cdot \frac{\rho_1^2(\rho_1 + \rho_2)}{(\rho_1 + \rho_2 - 1)^3} \alpha_+^2(\rho_1) + (\sigma_1^2 - \sigma_2^2) \cdot \frac{\rho_1(\rho_1 + \rho_2)}{(\rho_1 + \rho_2 - 1)^3} \alpha_+(\rho_1), \end{aligned} \quad (\text{C.19})$$

781 then we have $\delta_{\text{var}} > \delta_{\text{bias}} + \delta_{\text{var}}^{(2)}$ w.h.p., which gives $L(\hat{\beta}_t^{\text{MTL}}) < L(\hat{\beta}_t^{\text{STL}})$. We can solve (C.19) to get

$$\sigma_1^2 < -pd^2 \cdot \rho_1 \alpha_+(\rho_1) + \sigma_2^2 [1 + \rho_1 \Phi(\rho_1, \rho_2) \alpha_+^{-1}(\rho_1)] \cdot (1 - o(1)).$$

782 This proves the first claim of Proposition C.3 using $\nu \geq \alpha_+^2(\rho_1) + o(1)$.

783 **Negative transfer.** On the other hand, if the following inequality holds,

$$\begin{aligned} & \sigma_2^2 \cdot \frac{\rho_1}{(\rho_2 - 1)(\rho_1 + \rho_2 - 1)} \cdot (1 + o(1)) \\ & < pd^2 \cdot \frac{\rho_1^2(\rho_1 + \rho_2)}{(\rho_1 + \rho_2 - 1)^3} \alpha_-^2(\rho_1) + (\sigma_1^2 - \sigma_2^2) \cdot \frac{\rho_1(\rho_1 + \rho_2)}{(\rho_1 + \rho_2 - 1)^3} \alpha_-(\rho_1), \end{aligned} \quad (\text{C.20})$$

784 then we have $\delta_{\text{var}} < \delta_{\text{bias}} + \delta_{\text{var}}^{(2)}$ w.h.p., which gives $L(\hat{\beta}_t^{\text{MTL}}) > L(\hat{\beta}_t^{\text{STL}})$. We can solve (C.20) to get

$$\sigma_1^2 > -pd^2 \cdot \rho_1 \alpha_-(\rho_1) + \sigma_2^2 [1 + \rho_1 \Phi(\rho_1, \rho_2) \alpha_-^{-1}(\rho_1)] \cdot (1 + o(1)).$$

785 This proves the second claim of Proposition C.3. □

786 C.2 Missing Proofs regarding Sample Size

787 We first prove Proposition 3.4, which describes the effect of source/task data ratio on the information
 788 transfer.

789 *Proof of Proposition 3.4.* Following the proof of Proposition 3.3, we see that $L(\hat{\beta}_2^{\text{MTL}}) < L(\hat{\beta}_2^{\text{STL}})$
 790 w.h.p. if (C.14) holds, while $L(\hat{\beta}_2^{\text{MTL}}) > L(\hat{\beta}_2^{\text{STL}})$ w.h.p. if (C.16) holds.

791 We first explain the meaning of the condition

$$\Psi(\beta_1, \beta_2) > 2/(\rho_2 - 1). \quad (\text{C.21})$$

Notice that the function

$$\Phi(\rho_1, \rho_2) = \frac{(\rho_1 + \rho_2 - 1)^2}{\rho_1(\rho_1 + \rho_2)(\rho_2 - 1)} = \frac{1}{\rho_2 - 1} \left(1 + \frac{\rho_2 - 2}{\rho_1} + \frac{1}{\rho_1(\rho_1 + \rho_2)} \right)$$

is strictly decreasing with respect to ρ_1 as long as $\rho_2 > 2$, and $\Phi(\rho_1, \rho_2)$ converges to $(\rho_2 - 1)^{-1}$ as $\rho_1 \rightarrow \infty$. Moreover, we notice that $(\alpha_-^2(\rho_1) - o(1))^{-1} < 2$ for $\rho_1 > 40$. Hence (C.21) implies that (C.16) holds for all large enough ρ_1 . The transition from positive transfer when ρ_1 is small to negative transfer when ρ_1 is large is described by the two bounds in Proposition 3.4.

The two bounds follows directly from (C.14) and (C.16). We will use the following trivial inequalities

$$\frac{(\rho_2 - 1)\rho_1}{\rho_1 + \rho_2 - 2} \cdot \left(1 - \frac{1}{(\rho_1 + \rho_2 - 2)^2} \right) \leq \Phi(\rho_1, \rho_2) \leq \frac{(\rho_2 - 1)\rho_1}{\rho_1 + \rho_2 - 2}. \quad (\text{C.22})$$

Positive transfer. With (C.22), we see that (C.14) is implied by the following inequality:

$$\Psi(\beta_1, \beta_2) \cdot \frac{(\rho_2 - 1)\rho_1}{\rho_1 + \rho_2 - 2} < (\alpha_+^2(\rho_1) + o(1))^{-1}. \quad (\text{C.23})$$

Then we can solve (C.23) to get

$$\rho_1 < \frac{\rho_2 - 2}{\Psi(\beta_1, \beta_2) \cdot (\rho_2 - 1) (\alpha_+^2(\rho_1) + o(1)) - 1}. \quad (\text{C.24})$$

This gives the first statement of Proposition 3.4 using $\nu \geq \alpha_+^2(\rho_1) + o(1)$.

Note that if we require the RHS of (C.24) to be larger than 40, that is, (C.24) is not a null condition. Then together with (C.21), we get

$$\rho_2 - 2 > [2(\alpha_+^2(\rho_1) + o(1)) - 1] \rho_1.$$

Plugging into $\rho_1 > 40$, we get $\rho_2 \geq 106$. This gives a constraint on ρ_2 .

Negative transfer. With (C.22), we see that (C.16) is implied by the following inequality:

$$\Psi(\beta_1, \beta_2) \frac{(\rho_2 - 1)\rho_1}{\rho_1 + \rho_2 - 2} \left(1 - \frac{1}{(\rho_1 + \rho_2 - 2)^2} \right) > \Psi(\beta_1, \beta_2) \frac{(\rho_2 - 1.5)\rho_1}{\rho_1 + \rho_2 - 2} > (\alpha_-^2(\rho_1) - o(1))^{-1}. \quad (\text{C.25})$$

where we used $(1 - (\rho_1 + \rho_2 - 2)^{-2})(\rho_2 - 1) > \rho_2 - 1.5$ for $\rho_1 > 40$ and $\rho_2 > 110$. Then we can solve (C.25) to get

$$\rho_1 > \frac{(\rho_2 - 2)\sigma^2}{\Psi(\beta_1, \beta_2) \cdot (\rho_2 - 1.5) (\alpha_-^2(\rho_1) - o(1)) - 1}, \quad (\text{C.26})$$

which gives the second statement of Proposition 3.4. We remark that condition (C.21) implies $\Psi(\beta_1, \beta_2) \cdot (\rho_2 - 1.5) (\alpha_-^2(\rho_1) - o(1)) > 1$, so (C.26) does not give a trivial bound. \square

Next we state Proposition C.4, which gives precise upper and lower bounds on the data efficiency ratio for Taskonomy.

Proposition C.4. *In the isotropic model, assume that $\rho_1, \rho_2 \geq 9$ and $\Psi(\beta_1, \beta_2) < (5(\rho_1 - 1))^{-1} + (5(\rho_2 - 1))^{-1}$. Then the data efficiency ratio x^* satisfies*

$$x_l \leq x^* \leq \frac{1}{\rho_1 + \rho_2} \left(\frac{2}{(\rho_1 - 1)^{-1} + (\rho_2 - 1)^{-1} - 5\Psi(\beta_1, \beta_2)} + 1 \right), \quad (\text{C.27})$$

where we denoted

$$x_l := \frac{1}{\rho_1 + \rho_2} \left(\frac{2}{(\rho_1 - 1)^{-1} + (\rho_2 - 1)^{-1}} + 1 \right).$$

Proof. Suppose we have reduced number of datapoints— x_{n_1} for task 1 and x_{n_2} for task 2 with $n_1 = \rho_1 p$ and $n_2 = \rho_2 p$. Then all the results in the proof of Proposition 3.3 still hold, except that we need to replace (ρ_1, ρ_2) with $(x\rho_1, x\rho_2)$. More precisely, we have

$$\begin{aligned} a_1 &= \frac{\rho_1(x\rho_1 + x\rho_2 - 1)}{x(\rho_1 + \rho_2)^2}, & a_2 &= \frac{\rho_2(x\rho_1 + x\rho_2 - 1)}{x(\rho_1 + \rho_2)^2}, \\ a_3 &= \frac{\rho_2}{(\rho_1 + \rho_2)(x\rho_1 + x\rho_2 - 1)}, & a_4 &= \frac{\rho_1}{(\rho_1 + \rho_2)(x\rho_1 + x\rho_2 - 1)}. \end{aligned}$$

814 Moreover, with high probability,

$$L_i(\hat{\beta}_i^{\text{MTL}}(x)) = \frac{\sigma^2}{x(\rho_1 + \rho_2) - 1} (1 + o(1)) + \delta_{\text{bias}}^{(i)}, \quad i = 1, 2. \quad (\text{C.28})$$

815 Here the model shift biases $\delta_{\text{bias}}^{(i)}$ satisfy that

$$\alpha_-^2(\alpha\rho_i) - o(1) \leq \delta_{\text{bias}}^{(i)} / \Delta_{\text{bias}}^{(i)} \leq \alpha_+^2(\alpha\rho_i) + o(1), \quad i = 1, 2,$$

816 where $\Delta_{\text{bias}}^{(i)}$ are defined as

$$\Delta_{\text{bias}}^{(i)} := pd^2 \frac{(x\rho_i)^2 \cdot x(\rho_1 + \rho_2)}{[x(\rho_1 + \rho_2) - 1]^3}, \quad i = 1, 2, .$$

817 On the other hand, using Lemma B.1 we have w.h.p.,

$$L_i(\hat{\beta}_i^{\text{STL}}) = \frac{\sigma^2}{\rho_i - 1} (1 + o(1)), \quad i = 1, 2. \quad (\text{C.29})$$

Comparing (C.28) and (C.29), we immediately obtain the lower bound $x^* \geq x_l$. In fact, one can see that if $x < x_l$, then we have

$$\frac{2\sigma^2}{x(\rho_1 + \rho_2) - 1} > \frac{\sigma^2}{\rho_1 - 1} + \frac{\sigma^2}{\rho_2 - 1},$$

818 that is, $L_1(\hat{\beta}_1^{\text{MTL}}(x)) + L_2(\hat{\beta}_2^{\text{MTL}}(x))$ is larger than $L_1(\hat{\beta}_1^{\text{STL}}) + L_2(\hat{\beta}_2^{\text{STL}})$ even if we do not take into
819 account the model shift bias terms $\delta_{\text{bias}}^{(i)}$.

820 Then we try to obtain an upper bound on x^* . In the following discussions, we only consider x such
821 that $x > x_l$. In particular, we have $x\rho > x_l\rho \geq \min(\rho_1, \rho_2)$, where we abbreviated $\rho := \rho_1 + \rho_2$.

822 **The upper bound.** From (C.28) and (C.29), we see that $x^* \leq x$ if x satisfies

$$(1 + o(1)) \cdot \sum_{i=1}^2 pd^2 \frac{(x\rho_i)^2 \cdot x\rho}{(x\rho - 1)^3} \left(1 + \sqrt{\frac{1}{x\rho_i}}\right)^4 \leq \frac{\sigma^2}{\rho_1 - 1} + \frac{\sigma^2}{\rho_2 - 1} - \frac{2\sigma^2}{x\rho - 1}.$$

823 We rewrite the inequality as

$$(1 + o(1)) \cdot \frac{\Psi(\beta_1, \beta_2)}{[1 - (x\rho)^{-1}]^3} \sum_{i=1}^2 \left(\sqrt{\frac{\rho_i}{\rho}} + \sqrt{\frac{1}{x\rho}}\right)^4 \leq \frac{1}{\rho_1 - 1} + \frac{1}{\rho_2 - 1} - \frac{2}{x\rho - 1}. \quad (\text{C.30})$$

With $x\rho \geq \min(\rho_1, \rho_2) \geq 9$, we can get the simple bound

$$\frac{1 + o(1)}{[1 - (x\rho)^{-1}]^3} \sum_{i=1}^2 \left(\sqrt{\frac{\rho_i}{\rho}} + \sqrt{\frac{1}{x\rho}}\right)^4 < 5.$$

824 Inserting it into (C.30), we can solve for the upper bound in (C.27).

We can get better bounds if the values of ρ_1 and ρ_2 increase. For example, if we consider the case $\min(\rho_1, \rho_2) \geq 100$, then with some basic calculations, one can show that in this case

$$\frac{1}{[1 - (x\rho)^{-1}]^3} \sum_{i=1}^2 \left(\sqrt{\frac{\rho_i}{\rho}} + \sqrt{\frac{1}{x\rho}}\right)^4 < \frac{\rho_1^2 + \rho_2^2}{\rho^2} + 0.52.$$

825 Thus the following inequality implies (C.30):

$$\left(\frac{\rho_1^2 + \rho_2^2}{\rho^2} + 0.52\right) \Psi(\beta_1, \beta_2) < \frac{1}{\rho_1 - 1} + \frac{1}{\rho_2 - 1} - \frac{2}{x\rho - 1},$$

826 from which we can solve for the following upper bound on x^* :

$$x^* < \frac{1}{\rho} \frac{2}{\frac{1}{\rho_1 - 1} + \frac{1}{\rho_2 - 1} - \left(\frac{\rho_1^2 + \rho_2^2}{\rho^2} + 0.52\right) \Psi(\beta_1, \beta_2)} + \frac{1}{\rho}.$$

827 Similarly, we can get a better lower bound. From (C.28) and (C.29), we see that $x^* \geq x$ if x satisfies

$$(1 - o(1)) \cdot \frac{\Psi(\beta_1, \beta_2)}{[1 - (x\rho)^{-1}]^3} \sum_{i=1}^2 \left(\sqrt{\frac{\rho_i}{\rho}} - \sqrt{\frac{1}{x\rho}} \right)^4 \geq \frac{1}{\rho_1 - 1} + \frac{1}{\rho_2 - 1} - \frac{2}{x\rho - 1}. \quad (\text{C.31})$$

Then in the case $\min(\rho_1, \rho_2) \geq 100$, with some basic calculations, one can show that the sum on the left-hand side of (C.31) satisfies

$$\frac{1}{[1 - (x\rho)^{-1}]^3} \sum_{i=1}^2 \left(\sqrt{\frac{\rho_i}{\rho}} - \sqrt{\frac{1}{x\rho}} \right)^4 > \frac{\rho_1^2 + \rho_2^2}{\rho^2} - 0.33.$$

828 Thus the following inequality implies (C.31):

$$\left(\frac{\rho_1^2 + \rho_2^2}{\rho^2} - 0.33 \right) p d^2 > \frac{\sigma^2}{\rho_1 - 1} + \frac{\sigma^2}{\rho_2 - 1} - \frac{2\sigma^2}{x\rho - 1}, \quad (\text{C.32})$$

829 from which we can solve for the following lower bound on x^* :

$$x^* > \frac{1}{\rho} \frac{2}{\frac{1}{\rho_1 - 1} + \frac{1}{\rho_2 - 1} - \left(\frac{\rho_1^2 + \rho_2^2}{\rho^2} - 0.33 \right) \Psi(\beta_1, \beta_2)} + \frac{1}{\rho}.$$

830 This gives a lower bound above x_l . □

831 C.3 Missing Proofs regarding Covariate Shift

832 We now prove Proposition 3.5, which shows that $L(\hat{\beta}^{\text{MTL}})$ is minimized approximately when M is a
833 scalar matrix where there is enough source data.

Proof of Proposition 3.5. Let

$$M_0 := \arg \min_{M \in \mathcal{S}_\mu} g(M).$$

834 We now calculate $g(M_0)$. With the same arguments as in Lemma C.2, we can show that (C.6) holds.
835 Moreover, if the parameters are chosen such that $p^{-1+c_0}\sigma^2 \leq \kappa^2 \leq p^{-\varepsilon_0-c_0}\sigma^2$ as in (C.1), we can
836 simplify

$$g(M_0) = (1 + O(p^{-\varepsilon})) \cdot \sigma^2 \text{Tr} [\Sigma_2(X_1^\top X_1 + X_2^\top X_2)^{-1}],$$

837 with high probability for some constant $\varepsilon > 0$. In fact, Lemma C.2 was proved assuming that
838 $M = \text{Id}$, but its proof can be easily extended to the case with general $M \in \mathcal{S}_\mu$ by using that
839 $\mu_{\min} \leq \lambda_p(M) \leq \lambda_1(M) \leq \mu_{\max}$. We omit the details here.

840 Now using Lemma B.2, we obtain that with high probability,

$$g(M_0) = \frac{\sigma^2}{\rho_1 + \rho_2} \cdot \frac{1}{p} \text{Tr} \left(\frac{1}{a_1(M_0) \cdot M_0^\top M_0 + a_2(M_0)} \right) \cdot (1 + O(p^{-\varepsilon})). \quad (\text{C.33})$$

841 From equation (B.3), it is easy to obtain the following estimates on $a_1(M)$ and $a_2(M)$ for any
842 $M \in \mathcal{S}_\mu$:

$$\frac{\rho_1 - 1}{\rho_1 + \rho_2} < a_1(M) < \frac{\rho_1 + \rho_2 - 1}{\rho_1 + \rho_2}, \quad a_2(M) < \frac{\rho_2}{\rho_1 + \rho_2}. \quad (\text{C.34})$$

843 Inserting (C.34) into (C.33) and using $M_0^\top M_0 \succeq \mu_{\min}^2$, we obtain that with high probability,

$$\left(1 + \frac{\rho_2}{(\rho_1 - 1)\mu_{\min}^2} \right)^{-1} h(M_0) \cdot (1 - O(p^{-\varepsilon})) \leq g(M_0) \leq h(M_0) \cdot (1 + O(p^{-\varepsilon})), \quad (\text{C.35})$$

where

$$h(M_0) := \frac{\sigma^2}{(\rho_1 + \rho_2)a_1(M_0)} \cdot \frac{1}{p} \text{Tr} \left(\frac{1}{M_0^\top M_0} \right).$$

By AM-GM inequality, we observe that

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

844 is minimized when $\lambda_1 = \dots \lambda_p = \mu$ under the restriction $\prod_{i=1}^p \lambda_i \leq \mu^p$. Hence we get that

$$h(M_0) \leq \frac{\sigma^2}{\mu^2(\rho_1 + \rho_2)a_1(M_0)}. \quad (\text{C.36})$$

845 On the other hand, when $M = \mu \text{Id}$, applying Lemma B.2 we obtain that with high probability,

$$\begin{aligned} g(\mu \text{Id}) &= \frac{\sigma^2}{\rho_1 + \rho_2} \cdot \frac{1}{p} \text{Tr} \left(\frac{1}{\mu^2 a_1(\mu \text{Id}) + a_2(\mu \text{Id})} \right) \cdot (1 + O(p^{-\varepsilon})) \\ &\leq \frac{\sigma^2}{\mu^2(\rho_1 + \rho_2)a_1(\mu \text{Id})}. \end{aligned} \quad (\text{C.37})$$

846 Combining (C.34), (C.35), (C.36) and (C.37), we conclude the proof. \square

847 **D Proof for Many Tasks**

848 *Proof of Theorem 3.6.* In this setting, we need to study the following loss function:

$$f(B; W_1, \dots, W_t) = \sum_{i=1}^t \|X B W_i - Y_i\|^2. \quad (\text{D.1})$$

849 For any fixed $W_1, W_2, \dots, W_t \in \mathbb{R}^r$, we can derive a closed form solution for B as

$$\begin{aligned} \hat{B}(W_1, \dots, W_t) &= (X^\top X)^{-1} X^\top \left(\sum_{i=1}^t Y_i W_i^\top \right) (\mathcal{W} \mathcal{W}^\top)^{-1} \\ &= (B^* \mathcal{W}^\top) (\mathcal{W} \mathcal{W}^\top)^{-1} + (X^\top X)^{-1} X^\top \left(\sum_{i=1}^t \varepsilon_i W_i^\top \right) (\mathcal{W} \mathcal{W}^\top)^{-1}, \end{aligned}$$

850 where we denote $\mathcal{W} \in \mathbb{R}^{r \times t}$ as $\mathcal{W} = [W_1, W_2, \dots, W_t]$. Then as in (A.5), we pick N independent
851 samples of the training set for each task with $N \geq n^{1-\varepsilon_0}$, and use concentration to get the validation
852 loss as

$$g(\mathcal{W}) = N [\text{val}(\mathcal{W}) + t\sigma^2] \cdot \left(1 + O(p^{-(1-\varepsilon_0)/2+\varepsilon}) \right). \quad (\text{D.2})$$

Here $\text{val}(\mathcal{W})$ is defined as

$$\text{val}(\mathcal{W}) := \mathbb{E}_{\varepsilon_j, \forall 1 \leq j \leq t} \left[\sum_{i=1}^t \left\| \Sigma^{1/2} (\hat{B} W_i - \beta_i) \right\|^2 \right] = \delta_{\text{bias}}(\mathcal{W}) + \delta_{\text{var}}(\mathcal{W}),$$

853 where the model shift bias term $\delta_{\text{bias}}(\mathcal{W})$ is given by

$$\delta_{\text{bias}}(\mathcal{W}) := \sum_{i=1}^t \left\| \Sigma^{1/2} ((B^* \mathcal{W}^\top) (\mathcal{W} \mathcal{W}^\top)^{-1} W_i - \beta_i) \right\|^2,$$

854 and the variance term $\delta_{\text{var}}(\mathcal{W})$ can be calculated as

$$\delta_{\text{var}}(\mathcal{W}) := \sigma^2 \cdot \text{Tr} [\Sigma (X^\top X)^{-1}].$$

855 It suffices to minimize $\delta_{\text{bias}}(\mathcal{W})$ over \mathcal{W} , since both $t\sigma^2$ and δ_{var} do not depend on \mathcal{W} .

856 We denote $Q := \mathcal{W}^\top (\mathcal{W} \mathcal{W}^\top)^{-1} \mathcal{W} \in \mathbb{R}^{k \times k}$, whose (i, j) -th entry is equal to $W_i^\top (\mathcal{W} \mathcal{W}^\top)^{-1} W_j$.

857 Now we can write $\delta_{\text{bias}}(\mathcal{W})$ succinctly as

$$\delta_{\text{bias}}(\mathcal{W}) = \left\| \Sigma^{1/2} B^* (Q - \text{Id}) \right\|_F^2.$$

858 From this equation we can solve the minimizer optimally as $Q_0 \equiv \mathcal{W}_0^\top (\mathcal{W}_0 \mathcal{W}_0^\top)^{-1} \mathcal{W}_0 = U_r U_r^\top$.

859 On the other hand, let $\hat{\mathcal{W}}$ be the minimizer of g , and denote $\hat{Q} := \hat{\mathcal{W}}^\top (\hat{\mathcal{W}} \hat{\mathcal{W}}^\top)^{-1} \hat{\mathcal{W}}$. We claim that

860 \hat{Q} satisfies

$$\|Q_0^{-1} \hat{Q} - \text{Id}\| = o(1) \quad \text{w.h.p.} \quad (\text{D.3})$$

In fact, if (D.3) does not hold, then using the condition $\lambda_{\min}((B^*)^\top \Sigma B^*) \gtrsim \sigma^2$ and that $\delta_{\text{var}}(\mathcal{W}) = O(\sigma^2)$ by (B.14), we obtain that

$$\text{val}(\hat{\mathcal{W}}) + t\sigma^2 > (\text{val}(\mathcal{W}_0) + t\sigma^2) \cdot (1 + o(1)) \Rightarrow g(\hat{\mathcal{W}}) > g(\mathcal{W}_0),$$

that is, $\hat{\mathcal{W}}$ is not a minimizer. This leads to a contradiction.

In sum, we have solved that $\hat{\beta}_i^{\text{MTL}} = B^* (U_r U_r(i) + o(1))$. Inserting it into the definition of the test loss, we get that

$$\begin{aligned} L(\hat{\beta}_t^{\text{MTL}}) &= \left\| \Sigma^{1/2} \left((B^* \hat{\mathcal{W}}^\top)(\hat{\mathcal{W}} \hat{\mathcal{W}}^\top)^{-1} \hat{\mathcal{W}}_t - \beta_t \right) \right\|^2 + \sigma^2 \hat{\mathcal{W}}_t^\top (\hat{\mathcal{W}} \hat{\mathcal{W}}^\top)^{-1} \hat{\mathcal{W}}_t \cdot \text{Tr} [\Sigma (X^\top X)^{-1}] \\ &= \left\| \Sigma^{1/2} (B^* U_r U_r(t) - \beta_t) \right\|^2 + o(\|B^*\|^2) + \sigma^2 \|U_r(t)\|^2 \text{Tr} [\Sigma (X^\top X)^{-1}] \cdot (1 + o(1)) \\ &= \left\| \Sigma^{1/2} (B^* U_r U_r(t) - \beta_t) \right\|^2 + \frac{\sigma^2}{\rho - 1} \|U_r(t)\|^2 + o(\|B^*\|^2 + \sigma^2), \end{aligned}$$

with high probability, where we used Lemma B.1 in the last step. Similar, by Lemma B.1 we have

$$L(\hat{\beta}_t^{\text{STL}}) = \frac{\sigma^2}{\rho - 1} \cdot (1 + o(1)).$$

Combining the above two estimates, we conclude the proof. \square

E Proofs of the Bias and Variance Bounds

In random matrix theory, it is more convenient to rescale the matrices Z_1 and Z_2 such that their entries have variance n^{-1} , where $n := n_1 + n_2$. The advantage of this scaling is that the singular eigenvalues of Z_1 and Z_2 all lie in a bounded support that does grow with n .

Basic setting. We denote the two sample covariance matrices by $\mathcal{Q}_1 := X_1^\top X_1$ and $\mathcal{Q}_2 := X_2^\top X_2$. We assume that $Z_1 = (z_{ij}^{(1)})$ and $Z_2 = (z_{ij}^{(2)})$ are $n_1 \times p$ and $n_2 \times p$ random matrices with i.i.d. entries satisfying

$$\mathbb{E} z_{ij}^{(\alpha)} = 0, \quad \mathbb{E} |z_{ij}^{(\alpha)}|^2 = n^{-1}. \quad (\text{E.1})$$

Moreover, we assume that the fourth moments exist:

$$\mathbb{E} |\sqrt{n} z_{ij}^{(\alpha)}|^4 \leq C \quad (\text{E.2})$$

for some constant $C > 0$. Let $0 < \tau < 1$ be a small constant. We assume that the aspect ratios $d_1 := p/n_1$ and $d_2 := p/n_2$ satisfy that

$$0 \leq d_1 \leq \tau^{-1}, \quad 1 + \tau \leq d_2 \leq \tau^{-1}. \quad (\text{E.3})$$

Here the lower bound $1 + \tau \leq d_2$ is to ensure that the sample covariance matrix \mathcal{Q}_2 is non-singular with high probability; see Lemma E.4 below.

We assume that Σ_1 and Σ_2 have eigendecompositions

$$\Sigma_1 = O_1 \Lambda_1 O_1^\top, \quad \Sigma_2 = O_2 \Lambda_2 O_2^\top, \quad \Lambda_1 = \text{diag}(\sigma_1^{(1)}, \dots, \sigma_n^{(1)}), \quad \Lambda_2 = \text{diag}(\sigma_1^{(2)}, \dots, \sigma_N^{(2)}), \quad (\text{E.4})$$

where the eigenvalues satisfy that

$$\tau^{-1} \geq \sigma_1^{(1)} \geq \sigma_2^{(1)} \geq \dots \geq \sigma_p^{(1)} \geq 0, \quad \tau^{-1} \geq \sigma_1^{(2)} \geq \sigma_2^{(2)} \geq \dots \geq \sigma_p^{(2)} \geq \tau. \quad (\text{E.5})$$

We assume that $M = \Sigma_1^{1/2} \Sigma_2^{-1/2}$ has singular value decomposition

$$M = U \Lambda V^\top, \quad \Lambda = \text{diag}(\sigma_1, \dots, \sigma_p), \quad (\text{E.6})$$

where the singular values satisfy that

$$\tau \leq \sigma_p \leq \sigma_1 \leq \tau^{-1}. \quad (\text{E.7})$$

We summarize our basic assumptions here for future reference. Note that this assumption is in accordance with Assumption A.1, except that we rescale the entries of Z_1 and Z_2 here.

883 **Assumption E.1.** We assume that Z_1 and Z_2 are independent $n_1 \times p$ and $n_2 \times p$ random matrices
 884 with real i.i.d. entries satisfying (E.1) and (E.2), Σ_1 and Σ_2 are deterministic non-negative definite
 885 symmetric matrices satisfying (E.4)-(E.7), and $d_{1,2}$ satisfy (E.3).

886 We will use the following notion of stochastic domination, which was first introduced in [67] and
 887 subsequently used in many works on random matrix theory. It simplifies the presentation of the results
 888 and their proofs by systematizing statements of the form “ ξ is bounded by ζ with high probability up
 889 to a small power of n ”.

890 **Definition E.2** (Stochastic domination). (i) Let

$$\xi = \left(\xi^{(n)}(u) : n \in \mathbb{N}, u \in U^{(n)} \right), \quad \zeta = \left(\zeta^{(n)}(u) : n \in \mathbb{N}, u \in U^{(n)} \right)$$

891 be two families of nonnegative random variables, where $U^{(n)}$ is a possibly n -dependent parameter
 892 set. We say ξ is stochastically dominated by ζ , uniformly in u , if for any fixed (small) $\varepsilon > 0$ and
 893 (large) $D > 0$,

$$\sup_{u \in U^{(n)}} \mathbb{P} \left[\xi^{(n)}(u) > n^\varepsilon \zeta^{(n)}(u) \right] \leq n^{-D}$$

894 for large enough $n \geq n_0(\varepsilon, D)$, and we shall use the notation $\xi \prec \zeta$. If for some complex family ξ
 895 we have $|\xi| \prec \zeta$, then we will also write $\xi \prec \zeta$ or $\xi = O_\prec(\zeta)$.

896 (ii) We say an event Ξ holds with high probability if for any constant $D > 0$, $\mathbb{P}(\Xi) \geq 1 - n^{-D}$ for
 897 large enough n . We say Ξ holds with high probability on an event Ω if for any constant $D > 0$,
 898 $\mathbb{P}(\Omega \setminus \Xi) \leq n^{-D}$ for large enough n .

899 Then we introduce the following bounded support condition.

900 **Definition E.3.** We say a random matrix Z satisfies the bounded support condition with q , if

$$\max_{i,j} |Z_{ij}| \prec q. \quad (\text{E.8})$$

901 Here $q \equiv q(n)$ is a deterministic parameter and usually satisfies $n^{-1/2} \leq q \leq n^{-\phi}$ for some (small)
 902 constant $\phi > 0$. Whenever (E.8) holds, we say that X has support q .

903 Note that if the entries of $\sqrt{n}Z$ have finite moments up to any order as in (A.1), then using Markov’s
 904 inequality one can show that Z has bounded support $n^{-1/2}$.

905 Then we state the following lemma on the eigenvalues of $Z_1^\top Z_1$ and $Z_2^\top Z_2$, which are denoted as
 906 $\lambda_1(Z_1^\top Z_1) \geq \dots \geq \lambda_p(Z_1^\top Z_1)$ and $\lambda_1(Z_2^\top Z_2) \geq \dots \geq \lambda_p(Z_2^\top Z_2)$. We have used it in our previous
 907 proofs; see (B.14).

908 **Lemma E.4.** Suppose Assumption E.1 holds, and Z_1, Z_2 satisfy the bounded support condition (E.8)
 909 for some deterministic parameter $q \equiv q(n)$ satisfying $n^{-1/2} \leq q \leq n^{-\phi}$ for some (small) constant
 910 $\phi > 0$. Then for any constant $\varepsilon > 0$, we have with high probability,

$$\lambda_1(Z_1^\top Z_1) \leq (1 + \sqrt{d_1})^2 + n^\varepsilon q, \quad (\text{E.9})$$

911 and

$$(1 - \sqrt{d_2})^2 - n^\varepsilon q \leq \lambda_p(Z_2^\top Z_2) \leq \lambda_1(Z_2^\top Z_2) \leq (1 + \sqrt{d_2})^2 + n^\varepsilon q. \quad (\text{E.10})$$

912 *Proof.* This lemma essentially follows from [21, Theorem 2.10], although the authors considered
 913 the case with $q \prec n^{-1/2}$ only. The results for larger q follows from [68, Lemma 3.12], but only the
 914 bounds for largest eigenvalues are given there in order to avoid the issue with the smallest eigenvalue
 915 when d_2 is close to 1. However, under the assumption (E.3), the lower bound for the smallest
 916 eigenvalue follows from the same arguments as in [68]. Hence we omit the details. \square

917 In Section E.1, we introduce the concept of resolvent, and give an almost optimal convergent estimate
 918 on it—Theorem E.7. This estimate is conventionally called *local law* in random matrix theory
 919 literature. Based on Theorem E.7, we then complete the proof of Lemma B.2 and Lemma B.3. The
 920 proof of Theorem E.7 is presented in Section E.2.

921 E.1 Resolvent and Local Law

922 Our main goal is to study the matrix inverse $(\mathcal{Q}_1 + \mathcal{Q}_2)^{-1}$. Using (E.6), we can rewrite it as

$$(\mathcal{Q}_1 + \mathcal{Q}_2)^{-1} = \Sigma_2^{-1/2} V (\Lambda U^\top Z_1^\top Z_1 U \Lambda + V^\top Z_2^\top Z_2 V)^{-1} V^\top \Sigma_2^{-1/2}. \quad (\text{E.11})$$

923 For this purpose, we shall study the following matrix for $z \in \mathbb{C}_+$,

$$\mathcal{G}(z) := (\Lambda U^\top Z_1^\top Z_1 U \Lambda + V^\top Z_2^\top Z_2 V - z)^{-1}, \quad z \in \mathbb{C}_+, \quad (\text{E.12})$$

924 which we shall refer to as resolvent (or Green's function).

925 Next we introduce a convenient self-adjoint linearization trick. It has been proved to be useful in
 926 studying the local laws of random matrices of the Gram type [22, 69, 70]. We define the following
 927 $(p+n) \times (p+n)$ self-adjoint block matrix, which is a linear function of Z_1 and Z_2 :

$$H \equiv H(Z_1, Z_2) := \begin{pmatrix} 0 & \Lambda U^\top Z_1^\top & V^\top Z_2^\top \\ Z_1 U \Lambda & 0 & 0 \\ Z_2 V & 0 & 0 \end{pmatrix}. \quad (\text{E.13})$$

928 Then we define its resolvent (Green's function) as

$$G \equiv G(Z_1, Z_2, z) := \left[H(Z_1, Z_2) - \begin{pmatrix} z I_{p \times p} & 0 & 0 \\ 0 & I_{n_1 \times n_1} & 0 \\ 0 & 0 & I_{n_2 \times n_2} \end{pmatrix} \right]^{-1}, \quad z \in \mathbb{C}_+. \quad (\text{E.14})$$

For simplicity of notations, we define the index sets

$$\mathcal{I}_1 := \llbracket 1, p \rrbracket, \quad \mathcal{I}_2 := \llbracket p+1, p+n_1 \rrbracket, \quad \mathcal{I}_3 := \llbracket p+n_1+1, p+n_1+n_2 \rrbracket, \quad \mathcal{I} := \mathcal{I}_1 \cup \mathcal{I}_2 \cup \mathcal{I}_3.$$

We will consistently use the latin letters $i, j \in \mathcal{I}_1$, greek letters $\mu, \nu \in \mathcal{I}_2 \cup \mathcal{I}_3$, and $\mathfrak{a}, \mathfrak{b} \in \mathcal{I}$. We label the indices of the matrices according to

$$Z_1 = (z_{\mu i} : i \in \mathcal{I}_1, \mu \in \mathcal{I}_2), \quad Z_2 = (z_{\nu i} : i \in \mathcal{I}_1, \nu \in \mathcal{I}_3).$$

929 Then we denote the $\mathcal{I}_1 \times \mathcal{I}_1$ block of $G(z)$ by $\mathcal{G}_L(z)$, the $\mathcal{I}_1 \times (\mathcal{I}_2 \cup \mathcal{I}_3)$ block by \mathcal{G}_{LR} , the $(\mathcal{I}_2 \cup \mathcal{I}_3) \times \mathcal{I}_1$
 930 block by \mathcal{G}_{RL} , and the $(\mathcal{I}_2 \cup \mathcal{I}_3) \times (\mathcal{I}_2 \cup \mathcal{I}_3)$ block by \mathcal{G}_R . For simplicity, we abbreviate $Y_1 := Z_1 U \Lambda$,
 931 $Y_2 := Z_2 V$ and $W := (Y_1^\top, Y_2^\top)$. By Schur complement formula, one can find that

$$\mathcal{G}_L = (W W^\top - z)^{-1} = \mathcal{G}, \quad \mathcal{G}_{LR} = \mathcal{G}_{RL}^\top = \mathcal{G} W, \quad \mathcal{G}_R = z (W^\top W - z)^{-1}. \quad (\text{E.15})$$

932 Thus a control of G yields directly a control of the resolvent \mathcal{G} . We also introduce the following
 933 random quantities (some partial traces and weighted partial traces):

$$\begin{aligned} m(z) &:= \frac{1}{p} \sum_{i \in \mathcal{I}_1} G_{ii}(z), \quad m_1(z) := \frac{1}{p} \sum_{i \in \mathcal{I}_1} \sigma_i^2 G_{ii}(z), \\ m_2(z) &:= \frac{1}{n_1} \sum_{\mu \in \mathcal{I}_2} G_{\mu\mu}(z), \quad m_3(z) := \frac{1}{n_2} \sum_{\mu \in \mathcal{I}_3} G_{\mu\mu}(z). \end{aligned} \quad (\text{E.16})$$

934 Our proof will use the spectral decomposition of G . Let $W = \sum_{k=1}^p \sqrt{\lambda_k} \xi_k \zeta_k^\top$ be a singular value
 935 decomposition of W , where $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_p \geq 0 = \lambda_{p+1} = \dots = \lambda_n$ are the eigenvalues,
 936 $\{\xi_k\}_{k=1}^p$ are the left-singular vectors, and $\{\zeta_k\}_{k=1}^n$ are the right-singular vectors. Then using (E.15),
 937 we get that for $i, j \in \mathcal{I}_1$ and $\mu, \nu \in \mathcal{I}_2 \cup \mathcal{I}_3$,

$$G_{ij} = \sum_{k=1}^p \frac{\xi_k(i) \xi_k^\top(j)}{\lambda_k - z}, \quad G_{\mu\nu} = z \sum_{k=1}^n \frac{\zeta_k(\mu) \zeta_k^\top(\nu)}{\lambda_k - z}, \quad G_{i\mu} = G_{\mu i} = \sum_{k=1}^p \frac{\sqrt{\lambda_k} \xi_k(i) \zeta_k^\top(\mu)}{\lambda_k - z}. \quad (\text{E.17})$$

938 We now describe the asymptotic limit of $\mathcal{G}(z)$. First define the deterministic limits of $(m_2(z), m_3(z))$,
 939 denoted by $(m_{2c}(z), m_{3c}(z))$, as the (unique) solution to the following system of equations

$$\frac{1}{m_{2c}} = \frac{\gamma_n}{p} \sum_{i=1}^p \frac{\sigma_i^2}{z + \sigma_i^2 r_1 m_{2c} + r_2 m_{3c}} - 1, \quad \frac{1}{m_{3c}} = \frac{\gamma_n}{p} \sum_{i=1}^p \frac{1}{z + \sigma_i^2 r_1 m_{2c} + r_2 m_{3c}} - 1, \quad (\text{E.18})$$

such that $(m_{2c}(z), m_{3c}(z)) \in \mathbb{C}_+^2$ for $z \in \mathbb{C}_+$, where, for simplicity, we introduce the parameters

$$\gamma_n := \frac{p}{n}, \quad r_1 \equiv r_1(n) := \frac{n_1}{n}, \quad r_2 \equiv r_2(n) := \frac{n_2}{n}. \quad (\text{E.19})$$

We then define the matrix limit of $G(z)$ as

$$\Pi(z) := \begin{pmatrix} -(z + r_1 m_{2c} \Lambda^2 + r_2 m_{3c})^{-1} & 0 & 0 \\ 0 & m_{2c}(z) I_{n_1} & 0 \\ 0 & 0 & m_{3c}(z) I_{n_2} \end{pmatrix}. \quad (\text{E.20})$$

In particular, the matrix limit of $\mathcal{G}(z)$ is given by $-(z + r_1 m_{2c} \Lambda^2 + r_2 m_{3c})^{-1}$.

If $z = 0$, then the equations (E.18) are reduced to

$$r_1 b_2 + r_2 b_3 = 1 - \gamma_n, \quad b_2 + \frac{1}{n} \sum_{i=1}^p \frac{\sigma_i^2 b_2}{\sigma_i^2 r_1 b_2 + (1 - \gamma_n - r_1 b_2)} = 1. \quad (\text{E.21})$$

where $b_2 := -m_{2c}(0)$ and $b_3 := -m_{3c}(0)$. Note that the function

$$f(b_2) := b_2 + \frac{1}{n} \sum_{i=1}^p \frac{\sigma_i^2 b_2}{\sigma_i^2 b_2 + (1 - \gamma_n - r_1 b_2)}$$

is a strictly increasing function on $[0, r_1^{-1}(1 - \gamma_n)]$. Moreover, we have $f(0) = 0 < 1$ and $f(r_1^{-1}(1 - \gamma_n)) = 1 + \gamma_n > 1$. Hence by mean value theorem, there exists a unique solution $b_2 \in (0, r_1^{-1}(1 - \gamma_n))$. Moreover, it is easy to check that $f'(a) = O(1)$ for $a \in [0, r_1^{-1}(1 - \gamma_n)]$, and $f(1) > 1$ if $1 \leq r_1^{-1}(1 - \gamma_n)$. Hence there exists a constant $\tau > 0$, such that

$$r_1 \tau \leq r_1 b_2 < \min\{(1 - \gamma_n) - r_1 \tau, r_1(1 - \tau)\}, \quad \tau < r_2 b_3 \leq 1 - \gamma_n - r_1 \tau. \quad (\text{E.22})$$

For general z around $z = 0$, the existence and uniqueness of the solution $(m_{2c}(z), m_{3c}(z))$ is given by the following lemma. Moreover, we will also include some basic estimates on it.

Lemma E.5. *There exist constants $c_0, C_0 > 0$ depending only on τ in (E.3), (E.5), (E.7) and (E.22) such that the following statements hold. There exists a unique solution to (E.18) under the conditions*

$$|z| \leq c_0, \quad |m_{2c}(z) - m_{2c}(0)| + |m_{3c}(z) - m_{3c}(0)| \leq c_0. \quad (\text{E.23})$$

Moreover, the solution satisfies

$$\max_{\alpha=2}^3 |m_{\alpha c}(z) - m_{\alpha c}(0)| \leq C_0 |z|. \quad (\text{E.24})$$

The proof is a standard application of the contraction principle. For reader's convenience, we will include its proof in Appendix E.2.4. As a byproduct of the contraction mapping argument there, we also obtain the following stability result that will be used in the proof of Theorem E.7.

Lemma E.6. *There exist constants $c_0, C_0 > 0$ depending only on τ in (E.3), (E.5), (E.7) and (E.22) such that the self-consistent equations in (E.18) are stable in the following sense. Suppose $|z| \leq c_0$ and $m_\alpha : \mathbb{C}_+ \mapsto \mathbb{C}_+$, $\alpha = 2, 3$, are analytic functions of z such that*

$$|m_2(z) - m_{2c}(0)| + |m_3(z) - m_{3c}(0)| \leq c_0.$$

Suppose they satisfy the system of equations

$$\frac{1}{m_2} + 1 - \frac{1}{n} \sum_{i=1}^p \frac{\sigma_i^2}{z + \sigma_i^2 r_1 m_2 + r_2 m_3} = \mathcal{E}_2, \quad \frac{1}{m_3} + 1 - \frac{1}{n} \sum_{i=1}^p \frac{1}{z + \sigma_i^2 r_1 m_2 + r_2 m_3} = \mathcal{E}_3, \quad (\text{E.25})$$

for some (random) errors satisfying $\max_{\alpha=2}^3 |\mathcal{E}_\alpha| \leq \delta(z)$, where $\delta(z)$ is a deterministic z -dependent function with $\delta(z) \leq (\log n)^{-1}$. Then we have

$$\max_{\alpha=2}^3 |m_\alpha(z) - m_{\alpha c}(z)| \leq C_0 \delta(z). \quad (\text{E.26})$$

962 In the following proof, we choose a sufficiently small constants $c_0 > 0$ such that Lemma E.5 and
 963 Lemma E.6 hold. Then we define a domain of the spectral parameter z as

$$\mathbf{D} := \{z = E + i\eta \in \mathbb{C}_+ : |z| \leq (\log n)^{-1}\}. \quad (\text{E.27})$$

964 The following theorem gives an almost optimal estimate on the resolvent G , which is conventionally
 965 called the anisotropic local law.

966 **Theorem E.7.** *Suppose Assumption E.1 holds, and Z_1, Z_2 satisfy the bounded support condition*
 967 *(E.8) for a deterministic parameter $q \equiv q(n)$ satisfying $n^{-1/2} \leq q \leq n^{-\phi}$ for some (small) constant*
 968 *$\phi > 0$. Then there exists a sufficiently small constant $c_0 > 0$ such that the following **anisotropic***
 969 ***local law** holds uniformly for all $z \in \mathbf{D}$. For any deterministic unit vectors $\mathbf{u}, \mathbf{v} \in \mathbb{R}^{\mathcal{I}}$, we have*

$$|\mathbf{u}^\top (G(z) - \Pi(z)) \mathbf{v}| \prec q. \quad (\text{E.28})$$

970 The proof of this theorem will be given in Section E.2. We now use it to complete the proof of Lemma
 971 B.2 and Lemma B.3.

Proof of Lemma B.2. In the setting of Lemma B.2, we write

$$\mathcal{R} := (X_1^\top X_1 + X_2^\top X_2)^{-1} = n^{-1} \left(\Sigma_1^{1/2} Z_1^\top Z_1 \Sigma_1^{1/2} + \Sigma_2^{1/2} Z_2^\top Z_2 \Sigma_2^{1/2} \right)^{-1},$$

where the extra n^{-1} is due to the choice of the scaling—in the setting of Lemma B.2 the variances of the entries of $Z_{1,2}$ are equal to 1, while here they are taken to be n^{-1} . Then as in (E.11), we can write

$$\mathcal{R} = n^{-1} \Sigma_2^{-1/2} V \mathcal{G}(0) V^\top \Sigma_2^{-1/2}, \quad \mathcal{G}(0) = (\Lambda U^\top Z_1^\top Z_1 U \Lambda + V^\top Z_2^\top Z_2 V)^{-1}.$$

972 If the entries of $\sqrt{n} Z_1$ and $\sqrt{n} Z_2$ have arbitrarily high moments as in (A.1), then Z_1 and Z_2 have
 973 bounded support $q = n^{-1/2}$. Using Theorem E.7, we obtain that for any small constant $\varepsilon > 0$,

$$\max_{1 \leq i \leq p} |(\mathcal{A}\mathcal{R} - n^{-1} \Lambda \Sigma_2^{-1/2} V \Pi(0) V^\top \Sigma_2^{-1/2})_{ii}| \prec n^{-3/2} \|\mathcal{A}\|, \quad (\text{E.29})$$

where by (E.20), we have

$$\Pi(0) = -(r_1 m_{2c}(0) \Lambda^2 + r_2 m_{3c}(0))^{-1} = (r_1 b_2 V^\top M^\top M V + r_2 b_3)^{-1},$$

with (b_2, b_3) satisfying (E.21). Thus from (E.29) we get that

$$\text{Tr}(\mathcal{A}\mathcal{R}) = n^{-1} \text{Tr}(r_1 b_2 M^\top M + r_2 b_3)^{-1} + \mathcal{O}_\prec(n^{-1/2} \|\mathcal{A}\|).$$

974 This concludes (B.2) if we rename $r_1 b_2 \rightarrow a_1$ and $r_2 b_3 \rightarrow a_2$.

975 Note that if we set $n_1 = 0$ and $n_2 = n$, then $a_1 = 0$ and $a_2 = (n_2 - p)/n_2$ is the solution to (B.3).

976 This gives (B.1) using (B.2). \square

977 *Proof of Lemma B.3.* In the setting of Lemma B.3, we can write

$$\Delta := n^2 \left\| \Sigma_2^{1/2} (X_1^\top X_1 + X_2^\top X_2)^{-1} \beta \right\|^2 = \beta^\top \Sigma_2^{-1/2} (M^\top Z_1^\top Z_1 M + Z_2^\top Z_2)^{-2} \Sigma_2^{-1/2} \beta.$$

978 Here again the n^2 factor disappears due to the choice of scaling. With (E.6), we can write the above
 979 expression as $\Delta := \mathbf{v}^\top (\mathcal{G}^2)(0) \mathbf{v}$ where $\mathbf{v} := V^\top \Sigma_2^{-1/2} \beta$. Note that $\mathcal{G}^2(0) = \partial_z \mathcal{G}|_{z=0}$. Now using
 980 Cauchy's integral formula and Theorem E.7, we get that

$$\begin{aligned} \mathbf{v}^\top \mathcal{G}^2(0) \mathbf{v} &= \frac{1}{2\pi i} \oint_{\mathcal{C}} \frac{\mathbf{v}^\top \mathcal{G}(z) \mathbf{v}}{z^2} dz = \frac{1}{2\pi i} \oint_{\mathcal{C}} \frac{\mathbf{v}^\top \Pi(z) \mathbf{v}}{z^2} dz + \mathcal{O}_\prec(n^{-1/2} \|\beta\|^2) \\ &= \mathbf{v}^\top \Pi'(0) \mathbf{v} + \mathcal{O}_\prec(n^{-1/2} \|\beta\|^2), \end{aligned} \quad (\text{E.30})$$

981 where \mathcal{C} is the contour $\{z \in \mathbb{C} : |z| \leq (\log n)^{-1}\}$. Hence it remains to study the derivatives

$$\mathbf{v}^\top \Pi'(0) \mathbf{v} = \mathbf{v}^\top \frac{1 + r_1 m'_{2c}(0) \Lambda^2 + r_2 m'_{3c}(0)}{(r_1 m_{2c}(0) \Lambda^2 + r_2 m_{3c}(0))^2} \mathbf{v}, \quad (\text{E.31})$$

982 where we need to calculate the derivatives $m'_{2c}(0)$ and $m'_{3c}(0)$.

983 By the implicit differentiation of (E.18), we obtain that

$$\begin{aligned}\frac{1}{m_{2c}^2(0)}m'_{2c}(0) &= \frac{1}{n} \sum_{i=1}^p \frac{\sigma_i^2 (1 + \sigma_i^2 r_1 m'_{2c}(0) + r_2 m'_{3c}(0))}{(\sigma_i^2 r_1 m_{2c}(0) + r_2 m_{3c}(0))^2}, \\ \frac{1}{m_{3c}^2(0)}m'_{3c}(0) &= \frac{1}{n} \sum_{i=1}^p \frac{1 + \sigma_i^2 r_1 m'_{2c}(0) + r_2 m'_{3c}(0)}{(\sigma_i^2 r_1 m_{2c}(0) + r_2 m_{3c}(0))^2}.\end{aligned}$$

984 If we rename $-r_1 m_{2c}(0) \rightarrow a_1$, $-r_2 m_{3c}(0) \rightarrow a_2$, $r_2 m'_{3c}(0) \rightarrow a_3$ and $r_1 m'_{2c}(0) \rightarrow a_4$, then this
985 equation becomes

$$\begin{aligned}\left(\frac{r_2}{a_2^2} - \frac{1}{n} \sum_{i=1}^p \frac{1}{(\sigma_i^2 a_1 + a_2)^2}\right) a_3 - \left(\frac{1}{n} \sum_{i=1}^p \frac{\sigma_i^2}{(\sigma_i^2 a_1 + a_2)^2}\right) a_4 &= \frac{1}{n} \sum_{i=1}^p \frac{1}{(\sigma_i^2 a_1 + a_2)^2}, \\ \left(\frac{r_1}{a_1^2} - \frac{1}{n} \sum_{i=1}^p \frac{\sigma_i^4}{(\sigma_i^2 a_1 + a_2)^2}\right) a_4 - \left(\frac{1}{n} \sum_{i=1}^p \frac{\sigma_i^2}{(\sigma_i^2 a_1 + a_2)^2}\right) a_3 &= \frac{1}{n} \sum_{i=1}^p \frac{\sigma_i^2}{(\sigma_i^2 a_1 + a_2)^2}.\end{aligned}\tag{E.32}$$

986 Then by (E.30) and (E.31), we get

$$\Delta = \beta^\top \Sigma_2^{-1/2} V \frac{1 + a_3 + a_4 \Lambda^2}{(a_1 \Lambda^2 + a_2)} V^\top \Sigma_2^{-1/2} \beta = \beta^\top \Sigma_2^{-1/2} \frac{1 + a_3 + a_4 M^\top M}{(a_1 M^\top M + a_2)} \Sigma_2^{-1/2} \beta,$$

987 where we used $M^\top M = V \Lambda^2 V^\top$ in the second step. This concludes Lemma B.3. \square

988 Using a simple cutoff argument, it is easy to obtain from Theorem E.7 the following corollary under
989 weaker moment assumptions.

990 **Corollary E.8.** *Suppose Assumption E.1 holds. Moreover, assume that the entries of Z_1 and Z_2 are*
991 *i.i.d. random variables satisfying (E.1) and*

$$\max_{i,j} \mathbb{E} |\sqrt{n} z_{ij}^{(\alpha)}|^a = O(1), \quad \alpha = 1, 2, \tag{E.33}$$

992 for some fixed $a > 4$. Then (E.28) holds for $q = n^{2/a-1/2}$ on an event with probability $1 - o(1)$.

Proof of Corollary E.8. Fix any sufficiently small constant $\varepsilon > 0$. We choose $q = n^{-c_a+\varepsilon}$ with
 $c_a = 1/2 - 2/a$. Then we introduce the truncated matrices \tilde{Z}_1 and \tilde{Z}_2 , with entries

$$\tilde{z}_{ij}^{(\alpha)} := \mathbf{1} \left\{ |\tilde{z}_{ij}^{(\alpha)}| \leq q \right\} \cdot z_{ij}^{(\alpha)}, \quad \alpha = 1, 2.$$

993 By the moment conditions (E.33) and a simple union bound, we have

$$\mathbb{P}(\tilde{Z}_1 = Z_1, \tilde{Z}_2 = Z_2) = 1 - O(n^{-a\varepsilon}). \tag{E.34}$$

994 Using (E.33) and integration by parts, it is easy to verify that

$$|\mathbb{E} \tilde{z}_{ij}^{(\alpha)}| = O(n^{-2-\varepsilon}), \quad \mathbb{E} |\tilde{z}_{ij}^{(\alpha)}|^2 = n^{-1} + O(n^{-2-\varepsilon}), \quad \alpha = 1, 2, . \tag{E.35}$$

Then we can centralize and rescale \tilde{Z}_1 and \tilde{Z}_2 as $\hat{Z}_\alpha := (\tilde{Z}_\alpha - \mathbb{E} \tilde{Z}_\alpha) / (\mathbb{E} |\tilde{z}_{11}^{(\alpha)}|^2)^{1/2}$, $\alpha = 1, 2$. Now
 \hat{Z}_1 and \hat{Z}_2 satisfy the assumptions in Theorem E.7 with $q = n^{-c_a+\varepsilon}$, and (E.28) gives that

$$\left| \mathbf{u}^\top (G(\hat{Z}_1, \hat{Z}_2, z) - \Pi(z)) \mathbf{v} \right| \prec q.$$

Then using (E.35) and (E.37) below, we obtain that

$$\left| \mathbf{u}^\top (G(\hat{Z}_1, \hat{Z}_2, z) - G(\tilde{Z}_1, \tilde{Z}_2, z)) \mathbf{v} \right| \prec n^{-1-\varepsilon},$$

995 where we also used the bound $\|\mathbb{E} \tilde{Z}_\alpha\| = O(n^{-1-\varepsilon})$ by (E.35). This shows that (E.28) also holds for
996 $G(\tilde{Z}_1, \tilde{Z}_2, z)$ with $q = n^{-c_a+\varepsilon}$, and hence concludes the proof by (E.34). \square

997 With this corollary, we can easily extend Lemma B.2 and Lemma B.3 to the case with weaker moment
998 assumptions. Due to length constraint, we will not go into further details here.

999 E.2 Proof of the Anisotropic Local Law

The main difficulty for the proof of Theorem E.7 is due to the fact that the entries of $Y_1 = Z_1 U \Lambda$ and $Y_2 = Z_2 V$ are not independent. However, notice that if the entries of $Z_1 \equiv Z_1^{Gauss}$ and $Z_2 \equiv Z_2^{Gauss}$ are i.i.d. Gaussian, then by the rotational invariance of the multivariate Gaussian distribution, we have

$$Z_1^{Gauss} U \Lambda \stackrel{d}{=} Z_1^{Gauss} \Lambda, \quad Z_2^{Gauss} V \stackrel{d}{=} Z_2^{Gauss}.$$

1000 In this case, the problem is reduced to proving the anisotropic local law for G with $U = \text{Id}$ and
 1001 $V = \text{Id}$, such that the entries of Y_1 and Y_2 are independent. This can be handled using the standard
 1002 resolvent methods as in e.g. [21, 45, 71]. To go from the Gaussian case to the general X case, we
 1003 will adopt a continuous self-consistent comparison argument developed in [22].
 1004 For the case $U = \text{Id}$ and $V = \text{Id}$, we need to deal with the following resolvent:

$$G_0(z) := \begin{pmatrix} -zI_{p \times p} & \Lambda Z_1^\top & Z_2^\top \\ Z_1 \Lambda & -I_{n_1 \times n_1} & 0 \\ Z_2 & 0 & -I_{n_2 \times n_2} \end{pmatrix}^{-1}, \quad z \in \mathbb{C}_+, \quad (\text{E.36})$$

1005 and prove the following result.

1006 **Proposition E.9.** *Suppose Assumption E.1 holds, and Z_1, Z_2 satisfy the bounded support condition*
 1007 *(E.8) with $q = n^{-1/2}$. Suppose U and V are identity. Then the estimate (E.28) holds for $G_0(z)$.*

1008 This section is organized as follows. In Section E.2.1, we collect some basic estimates and resolvent
 1009 identities that will be used in the proof of Theorem E.7 and Proposition E.9. Then in Section E.2.2
 1010 we give the proof of Proposition E.9, which concludes Theorem E.7 for i.i.d. Gaussian Z_1 and Z_2 . In
 1011 Section E.2.3, we describe how to extend the result in Theorem E.7 from the Gaussian case to the
 1012 case with generally distributed entries of Z_1 and Z_2 . Finally, in Section E.2.4, we give the proof of
 1013 Lemma E.5 and Lemma E.6. In the proof, we always denote the spectral parameter by $z = E + i\eta$.

1014 E.2.1 Basic Estimates

1015 The estimates in this section work for general G , that is, we do not require U and V to be identity.
 1016 First with Lemma E.4, we can obtain the following a priori estimate on the resolvent $G(z)$ for $z \in \mathbf{D}$.

1017 **Lemma E.10.** *Suppose the assumptions of Lemma E.4 holds. Then there exists a constant $C > 0$*
 1018 *such that the following estimates hold uniformly in $z, z' \in \mathbf{D}$ with high probability:*

$$\|G(z)\| \leq C, \quad (\text{E.37})$$

1019 and for any deterministic unit vectors $\mathbf{u}, \mathbf{v} \in \mathbb{R}^{\mathcal{I}}$,

$$|\mathbf{u}^\top [G(z) - G(z')] \mathbf{v}| \leq C|z - z'|. \quad (\text{E.38})$$

1020 *Proof.* As in (E.17), we let $\{\lambda_k\}_{1 \leq k \leq p}$ be the eigenvalues of WW^\top . By Lemma E.4 and the
 1021 assumption (E.3), we obtain that $\lambda_p \geq \lambda_p(Z_2^\top Z_2) \gtrsim 1$, which further implies the estimate that
 1022 $\inf_{z \in \mathbf{D}} \min_{1 \leq k \leq p} |\lambda_k - z| \gtrsim 1$. Together with (E.17), we obtain (E.37) and (E.38). \square

1023 The following lemma collects basic properties of stochastic domination \prec , which will be used tacitly
 1024 in the proof.

1025 **Lemma E.11** (Lemma 3.2 in [21]). *Let ξ and ζ be families of nonnegative random variables.*

1026 (i) *Suppose that $\xi(u, v) \prec \zeta(u, v)$ uniformly in $u \in U$ and $v \in V$. If $|V| \leq n^C$ for some constant C ,*
 1027 *then $\sum_{v \in V} \xi(u, v) \prec \sum_{v \in V} \zeta(u, v)$ uniformly in u .*

1028 (ii) *If $\xi_1(u) \prec \zeta_1(u)$ and $\xi_2(u) \prec \zeta_2(u)$ uniformly in $u \in U$, then $\xi_1(u)\xi_2(u) \prec \zeta_1(u)\zeta_2(u)$*
 1029 *uniformly in u .*

1030 (iii) *Suppose that $\Psi(u) \geq n^{-C}$ is deterministic and $\xi(u)$ satisfies $\mathbb{E}\xi(u)^2 \leq n^C$. If $\xi(u) \prec \Psi(u)$*
 1031 *uniformly in u , then we also have $\mathbb{E}\xi(u) \prec \Psi(u)$ uniformly in u .*

1032 Now we introduce the concept of minors, which are defined by removing certain rows and columns
 1033 of the matrix H .

1034 **Definition E.12 (Minors).** For any $(p+n) \times (p+n)$ matrix \mathcal{A} and $\mathbb{T} \subseteq \mathcal{I}$, we define the minor
1035 $\mathcal{A}^{(\mathbb{T})} := (\mathcal{A}_{ab} : a, b \in \mathcal{I} \setminus \mathbb{T})$ as the $(p+n-|\mathbb{T}|) \times (p+n-|\mathbb{T}|)$ matrix obtained by removing
1036 all rows and columns indexed by \mathbb{T} . Note that we keep the names of indices when defining $\mathcal{A}^{(\mathbb{T})}$, i.e.
1037 $(\mathcal{A}^{(\mathbb{T})})_{ab} = \mathcal{A}_{ab}$ for $a, b \notin \mathbb{T}$. Correspondingly, we define the resolvent minor as (recall (E.15))

$$G^{(\mathbb{T})} := \left[\left(H - \begin{pmatrix} zI_p & 0 \\ 0 & I_n \end{pmatrix} \right)^{(\mathbb{T})} \right]^{-1} = \begin{pmatrix} \mathcal{G}^{(\mathbb{T})} & \mathcal{G}^{(\mathbb{T})} W^{(\mathbb{T})} \\ (W^{(\mathbb{T})})^\top \mathcal{G}^{(\mathbb{T})} & \mathcal{G}_R^{(\mathbb{T})} \end{pmatrix},$$

1038 and the partial traces $m^{(\mathbb{T})}$, $m_1^{(\mathbb{T})}$, $m_2^{(\mathbb{T})}$ and $m_3^{(\mathbb{T})}$ by replacing G with $G^{(\mathbb{T})}$ in (E.16). For convenience,
1039 we will adopt the convention that for any minor $\mathcal{A}^{(\mathbb{T})}$ defined as above, $\mathcal{A}_{ab}^{(\mathbb{T})} = 0$ if $a \in \mathbb{T}$ or
1040 $b \in \mathbb{T}$. Moreover, we will abbreviate $(\{a\}) \equiv (a)$ and $(\{a, b\}) \equiv (ab)$.

1041 The following resolvent identities and the concentration bounds are the main tools for our proof.

1042 **Lemma E.13.** We have the following resolvent identities.

1043 (i) For $i \in \mathcal{I}_1$ and $\mu \in \mathcal{I}_2 \cup \mathcal{I}_3$, we have

$$\frac{1}{G_{ii}} = -z - \left(W G^{(i)} W^\top \right)_{ii}, \quad \frac{1}{G_{\mu\mu}} = -1 - \left(W^\top G^{(\mu)} W \right)_{\mu\mu}. \quad (\text{E.39})$$

1044 (ii) For $i \in \mathcal{I}_1$, $\mu \in \mathcal{I}_2 \cup \mathcal{I}_3$, $\mathbf{a} \in \mathcal{I} \setminus \{i\}$ and $\mathbf{b} \in \mathcal{I} \setminus \{\mu\}$, we have

$$G_{i\mathbf{a}} = -G_{ii} \left(W G^{(i)} \right)_{i\mathbf{a}}, \quad G_{\mu\mathbf{b}} = -G_{\mu\mu} \left(W^\top G^{(\mu)} \right)_{\mu\mathbf{b}}. \quad (\text{E.40})$$

1045 (iii) For $\mathbf{a} \in \mathcal{I}$ and $\mathbf{b}, \mathbf{c} \in \mathcal{I} \setminus \{\mathbf{a}\}$,

$$G_{\mathbf{b}\mathbf{c}}^{(\mathbf{a})} = G_{\mathbf{b}\mathbf{c}} - \frac{G_{\mathbf{b}\mathbf{a}} G_{\mathbf{a}\mathbf{c}}}{G_{\mathbf{a}\mathbf{a}}}, \quad \frac{1}{G_{\mathbf{b}\mathbf{b}}} = \frac{1}{G_{\mathbf{b}\mathbf{b}}^{(\mathbf{a})}} - \frac{G_{\mathbf{b}\mathbf{a}} G_{\mathbf{a}\mathbf{b}}}{G_{\mathbf{b}\mathbf{b}}^{(\mathbf{a})} G_{\mathbf{a}\mathbf{a}}}. \quad (\text{E.41})$$

1046 *Proof.* All these identities can be proved directly using Schur's complement formula. The reader can
1047 also refer to, for example, [22, Lemma 4.4]. \square

1048 **Lemma E.14** (Lemma 3.8 of [72]). Let (x_i) , (y_j) be independent families of centered and inde-
1049 pendent random variables, and (A_i) , (B_{ij}) be families of deterministic complex numbers. Suppose
1050 the entries x_i , y_j have variances at most n^{-1} and satisfy the bounded support condition (E.8) with
1051 $q \leq n^{-\phi}$ for some constant $\phi > 0$. Then we have the following bounds:

$$\left| \sum_i A_i x_i \right| \prec q \max_i |A_i| + \frac{1}{\sqrt{n}} \left(\sum_i |A_i|^2 \right)^{1/2}, \quad \left| \sum_{i,j} x_i B_{ij} y_j \right| \prec q^2 B_d + q B_o + \frac{1}{n} \left(\sum_{i \neq j} |B_{ij}|^2 \right)^{1/2},$$

$$\left| \sum_i \bar{x}_i B_{ii} x_i - \sum_i (\mathbb{E}|x_i|^2) B_{ii} \right| \prec q B_d, \quad \left| \sum_{i \neq j} \bar{x}_i B_{ij} x_j \right| \prec q B_o + \frac{1}{n} \left(\sum_{i \neq j} |B_{ij}|^2 \right)^{1/2},$$

1052 where $B_d := \max_i |B_{ii}|$ and $B_o := \max_{i \neq j} |B_{ij}|$. Moreover, if all the moments of $\sqrt{n}x_i$ and $\sqrt{n}y_j$
1053 exist in the sense of (A.1), then we have stronger bounds

$$\left| \sum_i A_i x_i \right| \prec \frac{1}{\sqrt{n}} \left(\sum_i |A_i|^2 \right)^{1/2}, \quad \left| \sum_{i,j} x_i B_{ij} y_j \right| \prec \frac{1}{n} \left(\sum_{i \neq j} |B_{ij}|^2 \right)^{1/2},$$

$$\left| \sum_i \bar{x}_i B_{ii} x_i - \sum_i (\mathbb{E}|x_i|^2) B_{ii} \right| \prec \frac{1}{n} \left(\sum_i |B_{ii}|^2 \right)^{1/2}, \quad \left| \sum_{i \neq j} \bar{x}_i B_{ij} x_j \right| \prec \frac{1}{n} \left(\sum_{i \neq j} |B_{ij}|^2 \right)^{1/2}.$$

1054 E.2.2 Entrywise Local Law

1055 The main goal of this subsection is to prove the following entrywise local law. The anisotropic local
1056 law (E.28) then follows from the entrywise local law combined with a polynomialization method as
1057 we will explain later. Recall that in the setting of Proposition E.9, we have $q = n^{-1/2}$ and

$$W = (\Lambda Z_1^\top, Z_2^\top). \quad (\text{E.42})$$

1058 **Lemma E.15.** Suppose the assumptions in Proposition E.9 hold. Then the following estimate holds
 1059 uniformly for $z \in \mathbf{D}$:

$$\max_{\mathbf{a}, \mathbf{b} \in \mathcal{I}} |(G_0)_{\mathbf{ab}}(z) - \Pi_{\mathbf{ab}}(z)| \prec n^{-1/2}. \quad (\text{E.43})$$

1060 *Proof.* The proof of Lemma E.15 is divided into three steps. For simplicity, we will still denote
 1061 $G \equiv G_0$ in the following proof, while keeping in mind that W takes the form in (E.42).

1062 **Step 1: Large deviations estimates.** In this step, we prove some (almost) optimal large deviation
 1063 estimates on the off-diagonal entries of G , and on the following Z variables. In analogy to [72,
 1064 Section 3] and [22, Section 5], we introduce the Z variables

$$Z_{\mathbf{a}}^{(\mathbb{T})} := (1 - \mathbb{E}_{\mathbf{a}})(G_{\mathbf{aa}}^{(\mathbb{T})})^{-1}, \quad \mathbf{a} \notin \mathbb{T},$$

1065 where $\mathbb{E}_{\mathbf{a}}[\cdot] := \mathbb{E}[\cdot \mid H^{(\mathbf{a})}]$, i.e. it is the partial expectation over the randomness of the \mathbf{a} -th row and
 1066 column of H . Using (E.39), we get that for $i \in \mathcal{I}_1$, $\mu \in \mathcal{I}_2$ and $\nu \in \mathcal{I}_3$,

$$Z_i = \sigma_i^2 \sum_{\mu, \nu \in \mathcal{I}_2} G_{\mu\nu}^{(i)} \left(\frac{1}{n} \delta_{\mu\nu} - z_{\mu i} z_{\nu i} \right) + \sum_{\mu, \nu \in \mathcal{I}_3} G_{\mu\nu}^{(i)} \left(\frac{1}{n} \delta_{\mu\nu} - z_{\mu i} z_{\nu i} \right), \quad (\text{E.44})$$

$$Z_{\mu} = \sum_{i, j \in \mathcal{I}_1} \sigma_i \sigma_j G_{ij}^{(\mu)} \left(\frac{1}{n} \delta_{ij} - z_{\mu i} z_{\mu j} \right), \quad Z_{\nu} = \sum_{i, j \in \mathcal{I}_1} G_{ij}^{(\nu)} \left(\frac{1}{n} \delta_{ij} - z_{\nu i} z_{\nu j} \right). \quad (\text{E.45})$$

1067 For simplicity, we introduce the random error $\Lambda_o := \max_{\mathbf{a} \neq \mathbf{b}} |G_{\mathbf{aa}}^{-1} G_{\mathbf{ab}}|$. The following lemma
 1068 gives the desired large deviations estimates on Λ_o and the Z variables.

1069 **Lemma E.16.** Suppose the assumptions in Proposition E.9 hold. Then the following estimates hold
 1070 uniformly for all $z \in \mathbf{D}$:

$$\Lambda_o + \max_{\mathbf{a} \in \mathcal{I}} |Z_{\mathbf{a}}| \prec n^{-1/2}. \quad (\text{E.46})$$

1071 *Proof.* Note that for any $\mathbf{a} \in \mathcal{I}$, $H^{(\mathbf{a})}$ and $G^{(\mathbf{a})}$ also satisfies the assumptions for Lemma E.10. Hence
 1072 (E.37) and (E.38) also hold for $G^{(\mathbf{a})}$. Now applying Lemma E.14 to (E.44) and (E.45), and using the
 1073 a priori bound (E.37), we get that for any $i \in \mathcal{I}_1$,

$$|Z_i| \lesssim \sum_{\alpha=2}^3 \left| \sum_{\mu, \nu \in \mathcal{I}_{\alpha}} G_{\mu\nu}^{(i)} \left(\frac{1}{n} \delta_{\mu\nu} - z_{\mu i} z_{\nu i} \right) \right| \prec n^{-1/2} + \frac{1}{n} \left(\sum_{\mu, \nu \in \mathcal{I}_2 \cup \mathcal{I}_3} |G_{\mu\nu}^{(i)}|^2 \right)^{1/2} \prec n^{-1/2},$$

1074 where in the last step we used (E.37) to get that for any μ ,

$$\sum_{\nu \in \mathcal{I}_2 \cup \mathcal{I}_3} |G_{\mu\nu}^{(i)}|^2 \leq \sum_{\mathbf{a} \in \mathcal{I}} |G_{\mu\mathbf{a}}^{(i)}|^2 = [G^{(i)}(G^{(i)})^*]_{\mu\mu} = O(1). \quad (\text{E.47})$$

1075 Similarly, applying Lemma E.14 to Z_{μ} and Z_{ν} in (E.45) and using (E.37), we obtain the same bound.
 1076 we have

$$G_{i\mathbf{a}} = -G_{ii} \left(W G^{(i)} \right)_{i\mathbf{a}}, \quad G_{\mu\mathbf{b}} = -G_{\mu\mu} \left(W^{\top} G^{(\mu)} \right)_{\mu\mathbf{b}}. \quad (\text{E.48})$$

1077 Then we prove the off-diagonal estimate on Λ_o . For $i \in \mathcal{I}_1$ and $\mathbf{a} \in \mathcal{I} \setminus \{i\}$, using (E.40), Lemma
 1078 E.14 and (E.37), we obtain that

$$|G_{ii}^{-1} G_{i\mathbf{a}}| \prec n^{-1/2} + \frac{1}{\sqrt{n}} \left(\sum_{\mu \in \mathcal{I}_2 \cup \mathcal{I}_3} |G_{\mu\mathbf{a}}^{(i)}|^2 \right)^{1/2} \prec n^{-1/2}.$$

1079 We have a similar estimate for $|G_{\mu\mu}^{-1} G_{\mu\mathbf{b}}|$ with $\mu \in \mathcal{I}_2 \cup \mathcal{I}_3$ and $\mathbf{b} \in \mathcal{I} \setminus \{\mu\}$. Thus we obtain that
 1080 $\Lambda_o \prec n^{-1/2}$, which concludes (E.46). \square

1081 Note that combining (E.37) and (E.46), we immediately conclude (E.43) for $\mathbf{a} \neq \mathbf{b}$.

1082 **Step 2: Self-consistent equations.** This is the key step of the proof for Proposition E.15, which
 1083 derives approximate self-consistent equations satisfied by $m_2(z)$ and $m_3(z)$. More precisely, we

will show that $(m_2(z), m_3(z))$ satisfies (E.25) for some small error $|\mathcal{E}_{2,3}| \prec n^{-1/2}$. Then in Step 3 we will apply Lemma E.6 to show that $(m_2(z), m_3(z))$ is close to $(m_{2c}(z), m_{3c}(z))$. We define the following z -dependent event

$$\Xi(z) := \left\{ |m_2(z) - m_{2c}(z)| + |m_3(z) - m_{3c}(z)| \leq (\log n)^{-1/2} \right\}. \quad (\text{E.49})$$

Note that by (E.24), we have $|m_{2c} + b_2| \lesssim (\log n)^{-1}$ and $|m_{3c} + b_3| \lesssim (\log n)^{-1}$. Together with (E.18), (E.22) and (E.7), we obtain the following basic estimates

$$|m_{2c}| \sim |m_{3c}| \sim 1, \quad |z + \sigma_i^2 r_1 m_{2c} + r_2 m_{3c}| \sim 1, \quad |1 + \gamma_n m_c| \sim |1 + \gamma_n m_{1c}| \sim 1, \quad (\text{E.50})$$

uniformly in $z \in \mathbf{D}$, where we abbreviated

$$m_c(z) := -\frac{1}{p} \sum_{i \in \mathcal{I}_1} \frac{1}{z + \sigma_i^2 r_1 m_{2c} + r_2 m_{3c}}, \quad m_{1c}(z) := -\frac{1}{p} \sum_{i \in \mathcal{I}_1} \frac{\sigma_i^2}{z + \sigma_i^2 r_1 m_{2c} + r_2 m_{3c}}.$$

Plugging (E.50) into (E.20), we get

$$|\Pi_{\mathbf{a}\mathbf{a}}(z)| \sim 1 \quad \text{uniformly in } z \in \mathbf{D}, \mathbf{a} \in \mathcal{I}. \quad (\text{E.51})$$

Then we claim the following result.

Lemma E.17. *Suppose the assumptions in Proposition E.9 hold. Then the following estimates hold uniformly in $z \in \mathbf{D}$:*

$$\begin{aligned} \mathbf{1}(\Xi) \left| \frac{1}{m_2} + 1 - \frac{1}{n} \sum_{i=1}^p \frac{\sigma_i^2}{z + \sigma_i^2 r_1 m_2 + r_2 m_3} \right| &\prec n^{-1/2}, \\ \mathbf{1}(\Xi) \left| \frac{1}{m_3} + 1 - \frac{1}{n} \sum_{i=1}^p \frac{1}{z + \sigma_i^2 r_1 m_2 + r_2 m_3} \right| &\prec n^{-1/2}. \end{aligned} \quad (\text{E.52})$$

Proof. By (E.39), (E.44) and (E.45), we obtain that for $i \in \mathcal{I}_1$, $\mu \in \mathcal{I}_2$ and $\nu \in \mathcal{I}_3$,

$$\frac{1}{G_{ii}} = -z - \frac{\sigma_i^2}{n} \sum_{\mu \in \mathcal{I}_2} G_{\mu\mu}^{(i)} - \frac{1}{n} \sum_{\mu \in \mathcal{I}_3} G_{\mu\mu}^{(i)} + Z_i = -z - \sigma_i^2 r_1 m_2 - r_2 m_3 + \varepsilon_i, \quad (\text{E.53})$$

$$\frac{1}{G_{\mu\mu}} = -1 - \frac{1}{n} \sum_{i \in \mathcal{I}_1} \sigma_i^2 G_{ii}^{(\mu)} + Z_\mu = -1 - \gamma_n m_1 + \varepsilon_\mu, \quad (\text{E.54})$$

$$\frac{1}{G_{\nu\nu}} = -1 - \frac{1}{n} \sum_{i \in \mathcal{I}_1} G_{ii}^{(\nu)} + Z_\nu = -1 - \gamma_n m + \varepsilon_\nu, \quad (\text{E.55})$$

where we recall Definition E.12, and

$$\varepsilon_i := Z_i + \sigma_i r_1 (m_2 - m_2^{(i)}) + r_2 (m_3 - m_3^{(i)}), \quad \varepsilon_\mu := \begin{cases} Z_\mu + \gamma_n (m_1 - m_1^{(\mu)}), & \text{if } \mu \in \mathcal{I}_2 \\ Z_\mu + \gamma_n (m - m^{(\mu)}), & \text{if } \mu \in \mathcal{I}_3 \end{cases}.$$

By (E.41) we can bound that

$$|m_2 - m_2^{(i)}| \leq \frac{1}{n_1} \sum_{\mu \in \mathcal{I}_2} \left| \frac{G_{\mu i} G_{i\mu}}{G_{ii}} \right| \prec n^{-1},$$

where we used (E.46) in the second step. Similarly, we can get that

$$|m - m^{(\mu)}| + |m_1 - m_1^{(\mu)}| + |m_2 - m_2^{(i)}| + |m_3 - m_3^{(i)}| \prec n^{-1} \quad (\text{E.56})$$

for any $i \in \mathcal{I}_1$ and $\mu \in \mathcal{I}_2 \cup \mathcal{I}_3$. Together with (E.46), we obtain that for all i and μ ,

$$|\varepsilon_i| + |\varepsilon_\mu| \prec n^{-1/2}. \quad (\text{E.57})$$

With (E.50) and the definition of Ξ , we get that $\mathbf{1}(\Xi) |z + \sigma_i^2 r_1 m_2 + r_2 m_3| \sim 1$. Hence using (E.53), (E.57) and (E.46), we obtain that

$$\mathbf{1}(\Xi) G_{ii} = \mathbf{1}(\Xi) \left[-\frac{1}{z + \sigma_i^2 r_1 m_2 + r_2 m_3} + O_{\prec} \left(n^{-1/2} \right) \right]. \quad (\text{E.58})$$

1099 Plugging it into the definitions of m and m_1 in (E.16), we get

$$\mathbf{1}(\Xi)m = \mathbf{1}(\Xi) \left[-\frac{1}{p} \sum_{i \in \mathcal{I}_1} \frac{1}{z + \sigma_i^2 r_1 m_2 + r_2 m_3} + O_{\prec}(n^{-1/2}) \right], \quad (\text{E.59})$$

$$\mathbf{1}(\Xi)m_1 = \mathbf{1}(\Xi) \left[-\frac{1}{p} \sum_{i \in \mathcal{I}_1} \frac{\sigma_i^2}{z + \sigma_i^2 r_1 m_2 + r_2 m_3} + O_{\prec}(n^{-1/2}) \right]. \quad (\text{E.60})$$

1100 As a byproduct, we obtain from these two estimates that

$$\mathbf{1}(\Xi) (|m - m_c| + |m_1 - m_{1c}|) \lesssim (\log n)^{-1/2}, \quad \text{with high probability.} \quad (\text{E.61})$$

1101 Together with (E.50), we get that

$$|1 + \gamma_n m_1| \sim 1, \quad |1 + \gamma_n m| \sim 1, \quad \text{with high probability on } \Xi. \quad (\text{E.62})$$

1102 Now using (E.54), (E.55), (E.57), (E.46) and (E.62), we obtain that for $\mu \in \mathcal{I}_2$ and $\nu \in \mathcal{I}_3$,

$$\mathbf{1}(\Xi) \left(G_{\mu\mu} + \frac{1}{1 + \gamma_n m_1} \right) = O_{\prec}(n^{-1/2}), \quad \mathbf{1}(\Xi) \left(G_{\nu\nu} + \frac{1}{1 + \gamma_n m} \right) = O_{\prec}(n^{-1/2}). \quad (\text{E.63})$$

1103 Taking average over $\mu \in \mathcal{I}_2$ and $\nu \in \mathcal{I}_3$, we get that with high probability,

$$\mathbf{1}(\Xi) \left(m_2 + \frac{1}{1 + \gamma_n m_1} \right) = O_{\prec}(n^{-1/2}), \quad \mathbf{1}(\Xi) \left(m_3 + \frac{1}{1 + \gamma_n m} \right) = O_{\prec}(n^{-1/2}). \quad (\text{E.64})$$

1104 Finally, plugging (E.59) and (E.60) into (E.64), we conclude (E.52). \square

1105 **Step 3: Ξ holds with high probability.** In this step, we show that the event $\Xi(z)$ in fact holds with
 1106 high probability for all $z \in \mathbf{D}$. Once we have proved this fact, then applying Lemma E.6 to (E.52)
 1107 immediately shows that $(m_2(z), m_3(z))$ is equal to $(m_{2c}(z), m_{3c}(z))$ up to an error of order $n^{-1/2}$.
 1108 We claim that it suffices to show

$$|m_2(0) - m_{2c}(0)| + |m_3(0) - m_{3c}(0)| \prec n^{-1/2}. \quad (\text{E.65})$$

1109 Once we know (E.65), then by (E.24) and (E.38), we get $\max_{\alpha=2}^3 |m_{\alpha c}(z) - m_{\alpha c}(0)| =$
 1110 $O((\log n)^{-1})$ and $\max_{\alpha=2}^3 |m_{\alpha}(z) - m_{\alpha}(0)| = O((\log n)^{-1})$ with high probability for all $z \in \mathbf{D}$.
 1111 Together with (E.65), we obtain that

$$\sup_{z \in \mathbf{D}} (|m_2(z) - m_{2c}(z)| + |m_3(z) - m_{3c}(z)|) \lesssim (\log n)^{-1} \quad \text{with high probability,} \quad (\text{E.66})$$

1112 and

$$\sup_{z \in \mathbf{D}} (|m_2(z) - m_{2c}(0)| + |m_3(z) - m_{3c}(0)|) \lesssim (\log n)^{-1} \quad \text{with high probability.} \quad (\text{E.67})$$

1113 The condition (E.66) shows that Ξ holds with high probability, and the condition (E.67) verifies the
 1114 condition (E.23) of Lemma E.6. Then applying Lemma E.6 to (E.52), we obtain that

$$|m_2(z) - m_{2c}(z)| + |m_3(z) - m_{3c}(z)| \prec n^{-1/2} \quad (\text{E.68})$$

1115 for all $z \in \mathbf{D}$. Plugging (E.68) into (E.53)-(E.55), we get the diagonal estimate

$$\max_{a \in \mathcal{I}} |G_{aa}(z) - \Pi_{aa}(z)| \prec n^{-1/2}. \quad (\text{E.69})$$

1116 Together with the off-diagonal estimate in (E.46), we conclude (E.43). \square

1117 Now we give the proof of (E.65).

Proof of (E.65). By (E.17), we get

$$m(0) = \frac{1}{p} \sum_{i \in \mathcal{I}_1} G_{ii}(0) = \frac{1}{p} \sum_{k=1}^p \frac{|\xi_k(i)|^2}{\lambda_k} \geq \lambda_1^{-1} \gtrsim 1.$$

Similarly, we can also get that $m_1(0)$ is positive and has size $m_1(0) \sim 1$. Hence we have

$$1 + \gamma_n m_1(0) \sim 1, \quad 1 + \gamma_n m_1(0) \sim 1.$$

Together with (E.54), (E.55) and (E.57), we obtain that (E.64) holds at $z = 0$ even without the indicator function $\mathbf{1}(\Xi)$. Furthermore, it gives that

$$|\sigma_i^2 r_1 m_2(0) + r_2 m_3(0)| = \left| \frac{\sigma_i^2 r_1}{1 + \gamma_n m_1(0)} + \frac{r_2}{1 + \gamma_n m(0)} + O_{\prec}(n^{-1/2}) \right| \sim 1$$

1118 with high probability. Then using (E.53) and (E.57), we obtain that (E.59) and (E.60) hold at
 1119 $z = 0$ even without the indicator function $\mathbf{1}(\Xi)$. Finally, plugging (E.59) and (E.60) into (E.64), we
 1120 conclude (E.52) holds at $z = 0$, that is,

$$\begin{aligned} \left| \frac{1}{m_2(0)} + 1 - \frac{1}{n} \sum_{i=1}^p \frac{\sigma_i^2}{\sigma_i^2 r_1 m_2(0) + r_2 m_3(0)} \right| &\prec n^{-1/2}, \\ \left| \frac{1}{m_3(0)} + 1 - \frac{1}{n} \sum_{i=1}^p \frac{1}{\sigma_i^2 r_2 m_2(0) + r_2 m_3(0)} \right| &\prec n^{-1/2}. \end{aligned} \quad (\text{E.70})$$

Denoting $\omega_2 = -m_{2c}(0)$ and $\omega_3 = -m_{2c}(0)$. By (E.64), we have

$$\omega_2 = \frac{1}{1 + \gamma_n m_1(0)} + O_{\prec}(n^{-1/2}), \quad \omega_3 = \frac{1}{1 + \gamma_n m(0)} + O_{\prec}(n^{-1/2}).$$

1121 Hence there exists a sufficiently small constant $c > 0$ such that

$$c \leq \omega_2 \leq 1, \quad c \leq \omega_3 \leq 1, \quad \text{with high probability.} \quad (\text{E.71})$$

1122 Also one can verify from (E.70) that (ω_2, ω_3) satisfy approximately the same equations as (E.21):

$$r_1 \omega_2 + r_2 \omega_3 = 1 - \gamma_n + O_{\prec}(n^{-1/2}), \quad f(\omega_2) = 1 + O_{\prec}(n^{-1/2}). \quad (\text{E.72})$$

1123 The first equation and (E.71) together implies that $\omega_2 \in [0, r_1^{-1}(1 - \gamma_n)]$ with high probability. Since
 1124 f is strictly increasing and has bounded derivatives on $[0, r_1^{-1}(1 - \gamma_n)]$, by basic calculus the second
 1125 equation in (E.72) gives that $|\omega_2 - b_2| \prec n^{-1/2}$. Together with the first equation in (E.72), we get
 1126 $|\omega_3 - b_3| \prec n^{-1/2}$. This concludes (E.65). \square

1127 With Lemma E.15, we can complete the proof of Proposition E.9.

1128 *Proof of Proposition E.9.* With (E.43), one can use the polynomialization method in [21, Section 5]
 1129 to get the anisotropic local law (E.28) for G_0 with $q = n^{-1/2}$. The proof is exactly the same, except
 1130 for some minor differences in notations, so we omit the details. \square

1131 E.2.3 Anisotropic Local Law

1132 In this subsection, we finish the proof of Theorem E.7 for a general X satisfying the bounded support
 1133 condition (E.8) with $q \leq n^{-\phi}$ for some constant $\phi > 0$. Proposition E.9 implies that (E.28) holds for
 1134 Gaussian Z_1^{Gauss} and Z_2^{Gauss} as discussed before. Thus the basic idea is to prove that for Z_1 and Z_2
 1135 satisfying the assumptions in Theorem E.7,

$$\mathbf{u}^\top (G(Z, z) - G(Z^{Gauss}, z)) \mathbf{v} \prec q$$

1136 for any deterministic unit vectors $\mathbf{u}, \mathbf{v} \in \mathbb{C}^{\mathcal{I}}$ and $z \in \mathbf{D}$. Here we abbreviated $Z := \begin{pmatrix} Z_1 \\ Z_2 \end{pmatrix}$ and

1137 $Z^{Gauss} := \begin{pmatrix} Z_1^{Gauss} \\ Z_2^{Gauss} \end{pmatrix}$. We prove the above statement using a continuous comparison argument
 1138 introduced in [22]. The proof is similar to the ones in Sections 7-8 of [22], so we only give a rough
 1139 description of the basic idea, without writing down all the details.

1140 **Definition E.18** (Interpolation). We denote $Z^0 := Z^{Gauss}$ and $Z^1 := Z$. Let $\rho_{\mu i}^0$ and $\rho_{\mu i}^1$ be the laws
 1141 of $Z_{\mu i}^0$ and $Z_{\mu i}^1$, respectively. For $\theta \in [0, 1]$, we define the interpolated law $\rho_{\mu i}^\theta := (1 - \theta)\rho_{\mu i}^0 + \theta\rho_{\mu i}^1$.
 1142 We shall work on the probability space consisting of triples (Z^0, Z^θ, Z^1) of independent $n \times p$
 1143 random matrices, where the matrix $Z^\theta = (Z_{\mu i}^\theta)$ has law

$$\prod_{i \in \mathcal{I}_1} \prod_{\mu \in \mathcal{I}_2 \cup \mathcal{I}_3} \rho_{\mu i}^\theta(dZ_{\mu i}^\theta). \quad (\text{E.73})$$

1144 For $\lambda \in \mathbb{R}$, $i \in \mathcal{I}_1$ and $\mu \in \mathcal{I}_2 \cup \mathcal{I}_3$, we define the matrix $Z_{(\mu i)}^{\theta, \lambda}$ through

$$\left(Z_{(\mu i)}^{\theta, \lambda} \right)_{\nu j} := \begin{cases} Z_{\mu i}^\theta, & \text{if } (j, \nu) \neq (i, \mu) \\ \lambda, & \text{if } (j, \nu) = (i, \mu) \end{cases}.$$

1145 We also introduce the matrices $G^\theta(z) := G(Z^\theta, z)$, $G_{(\mu i)}^{\theta, \lambda}(z) := G(Z_{(\mu i)}^{\theta, \lambda}, z)$.

1146 We shall prove (E.28) through interpolation matrices Z^θ between Z^0 and Z^1 . We have seen that (E.28)
 1147 holds for Z^0 by Proposition E.9. Using (E.73) and fundamental calculus, we get the following basic
 1148 interpolation formula: for $F : \mathbb{R}^{n \times p} \rightarrow \mathbb{C}$,

$$\frac{d}{d\theta} \mathbb{E} F(Z^\theta) = \sum_{i \in \mathcal{I}_1} \sum_{\mu \in \mathcal{I}_2 \cup \mathcal{I}_3} \left[\mathbb{E} F \left(Z_{(\mu i)}^{\theta, Z_{\mu i}^1} \right) - \mathbb{E} F \left(Z_{(\mu i)}^{\theta, Z_{\mu i}^0} \right) \right] \quad (\text{E.74})$$

1149 provided all the expectations exist. We shall apply (E.74) to $F(Z) := F_{\mathbf{u}\mathbf{v}}^s(Z, z)$ for (large) $s \in 2\mathbb{N}$
 1150 and $F_{\mathbf{u}\mathbf{v}}(Z, z)$ defined as

$$F_{\mathbf{u}\mathbf{v}}(Z, z) := |\mathbf{u}^\top (G(Z, z) - \Pi(z)) \mathbf{v}|.$$

1151 The main part of the proof is to show the following self-consistent estimate for the right-hand side of
 1152 (E.74) for any fixed $s \in 2\mathbb{N}$ and constant $\varepsilon > 0$:

$$\sum_{i \in \mathcal{I}_1} \sum_{\mu \in \mathcal{I}_2 \cup \mathcal{I}_3} \left[\mathbb{E} F_{\mathbf{u}\mathbf{v}}^s \left(Z_{(\mu i)}^{\theta, Z_{\mu i}^1}, z \right) - \mathbb{E} F_{\mathbf{u}\mathbf{v}}^s \left(Z_{(\mu i)}^{\theta, Z_{\mu i}^0}, z \right) \right] = O((n^\varepsilon q)^s + \mathbb{E} F_{\mathbf{u}\mathbf{v}}^s(Z^\theta, z)) \quad (\text{E.75})$$

for all $\theta \in [0, 1]$. If (E.75) holds, then combining (E.74) with a Grönwall's argument we obtain that
 for any fixed $s \in 2\mathbb{N}$ and constant $\varepsilon > 0$:

$$\mathbb{E} |G_{\mathbf{u}\mathbf{v}}(Z^1, z) - \Pi_{\mathbf{u}\mathbf{v}}(z)|^p \leq (n^\varepsilon q)^p.$$

1153 Together with Markov's inequality, we conclude (E.28). Underlying the proof of (E.75) is an
 1154 expansion approach, which is very similar to the ones for Lemma 7.10 of [22] and Lemma 6.11 of
 1155 [45]. So we omit the details.

1156 E.2.4 Proofs of the Limiting Equations

1157 Finally, we give the proof of Lemma E.5 and Lemma E.6 using the contraction principle.

1158 *Proof of Lemma E.5.* One can check that the equations in (E.18) are equivalent to the following ones:

$$r_1 m_{2c} = -(1 - \gamma_n) - r_2 m_{3c} - z(m_{3c}^{-1} + 1), \quad g_z(m_{3c}(z)) = 1, \quad (\text{E.76})$$

where

$$g_z(m_{3c}) := -m_{3c} + \frac{1}{n} \sum_{i=1}^p \frac{m_{3c}}{z - \sigma_i^2(1 - \gamma_n) + (1 - \sigma_i^2)r_2 m_{3c} - \sigma_i^2 z(m_{3c}^{-1} + 1)}.$$

1160 We first show that there exists a unique solution $m_{3c}(z)$ to the equation $g_z(m_{3c}(z)) = 1$ under the
 1161 conditions in (E.23), and the solution satisfies (E.24). Now we abbreviate $\varepsilon(z) := m_{3c}(z) - m_{3c}(0)$,
 1162 and from (E.76) we obtain that

$$0 = [g_z(m_{3c}(z)) - g_0(m_{3c}(0)) - g'_z(m_{3c}(0))\varepsilon(z)] + g'_z(m_{3c}(0))\varepsilon(z),$$

1163 which implies

$$\varepsilon(z) = -\frac{g_z(m_{3c}(0)) - g_0(m_{3c}(0))}{g'_z(m_{3c}(0))} - \frac{g_z(m_{3c}(0) + \varepsilon(z)) - g_z(m_{3c}(0)) - g'_z(m_{3c}(0))\varepsilon(z)}{g'_z(m_{3c}(0))}.$$

1164 Inspired by this equation, we define iteratively a sequence $\varepsilon^{(k)} \in \mathbb{C}$ such that $\varepsilon^{(0)} = 0$, and

$$\varepsilon^{(k+1)} = -\frac{g_z(m_{3c}(0)) - g_0(m_{3c}(0))}{g'_z(m_{3c}(0))} - \frac{g_z(m_{3c}(0) + \varepsilon^{(k)}) - g_z(m_{3c}(0)) - g'_z(m_{3c}(0))\varepsilon^{(k)}}{g'_z(m_{3c}(0))}. \quad (\text{E.77})$$

1165 Then (E.77) defines a mapping $h : \mathbb{C} \rightarrow \mathbb{C}$, which maps $\varepsilon^{(k)}$ to $\varepsilon^{(k+1)} = h(\varepsilon^{(k)})$.

With direct calculation, one can get the derivative

$$g'_z(m_{3c}(0)) = -1 - \frac{1}{n} \sum_{i=1}^p \frac{\sigma_i^2(1 - \gamma_n) - z[1 - \sigma_i^2(2m_{3c}^{-1}(0) + 1)]}{[z - \sigma_i^2(1 - \gamma_n) + (1 - \sigma_i^2)r_2m_{3c}(0) - \sigma_i^2z(m_{3c}^{-1}(0) + 1)]^2}.$$

1166 Then it is easy to check that there exist constants $\tilde{C}, \tilde{C} > 0$ depending only on τ in (E.7) and (E.22)
1167 such that

$$|[g'_z(m_{3c}(0))]^{-1}| \leq \tilde{C}, \quad \left| \frac{g_z(m_{3c}(0)) - g_0(m_{3c}(0))}{g'_z(m_{3c}(0))} \right| \leq \tilde{C}|z|, \quad (\text{E.78})$$

1168 and

$$\left| \frac{g_z(m_{3c}(0) + \varepsilon_1) - g_z(m_{3c}(0) + \varepsilon_2) - g'_z(m_{3c}(0))(\varepsilon_1 - \varepsilon_2)}{g'_z(m_{3c}(0))} \right| \leq \tilde{C}|\varepsilon_1 - \varepsilon_2|^2, \quad (\text{E.79})$$

for all $|z| \leq \tilde{C}$ and $|\varepsilon_1| \leq \tilde{C}, |\varepsilon_2| \leq \tilde{C}$. Then with (E.78) and (E.79), it is easy to see that there exists a sufficiently small constant $\delta > 0$ depending only on \tilde{C} , such that h is a self-mapping

$$h : B_r \rightarrow B_r, \quad B_r := \{\varepsilon \in \mathbb{C} : |\varepsilon| \leq r\},$$

1169 as long as $r \leq \delta$ and $|z| \leq c_\delta$ for some constant $c_\delta > 0$ depending only on \tilde{C} and δ . Now it suffices
1170 to prove that h restricted to B_r is a contraction, which then implies that $\varepsilon := \lim_{k \rightarrow \infty} \varepsilon^{(k)}$ exists and
1171 $m_{3c}(0) + \varepsilon$ is a unique solution to the second equation of (E.76) subject to the condition $\|\varepsilon\|_\infty \leq r$.

1172 From the iteration relation (E.77), using (E.78) one can readily check that

$$\varepsilon^{(k+1)} - \varepsilon^{(k)} = h(\varepsilon^{(k)}) - h(\varepsilon^{(k-1)}) \leq \tilde{C}|\varepsilon^{(k)} - \varepsilon^{(k-1)}|^2. \quad (\text{E.80})$$

1173 Hence as long as r is chosen to be sufficiently small such that $2r\tilde{C} \leq 1/2$, then h is indeed
1174 a contraction mapping on B_r , which proves both the existence and uniqueness of the solution
1175 $m_{3c}(z) = m_{3c}(0) + \varepsilon$, if we choose c_0 in (E.23) as $c_0 = \min\{c_\delta, r\}$. After obtaining $m_{3c}(z)$, we
1176 can then find $m_{2c}(z)$ using the first equation in (E.76).

1177 Note that with (E.79) and $\varepsilon^{(0)} = 0$, we get from (E.77) that $|\varepsilon^{(1)}| \leq \tilde{C}|z|$. With the contraction
1178 mapping, we have the bound

$$|\varepsilon| \leq \sum_{k=0}^{\infty} |\varepsilon^{(k+1)} - \varepsilon^{(k)}| \leq 2\tilde{C}|z|. \quad (\text{E.81})$$

This gives the bound (E.24) for $m_{3c}(z)$. Using the first equation in (E.76), we immediately obtain the bound $r_1|m_{2c}(z) - m_{2c}(0)| \leq C|z|$. This gives (E.24) for $m_{2c}(z)$ as long as if $r_1 \gtrsim 1$. To deal with the small r_1 case, we go back to the first equation in (E.18) and treat $m_{2c}(z)$ as the solution to the following equation:

$$\tilde{g}_z(m_{2c}(z)) = 1, \quad \tilde{g}_z(x) := -x + \frac{\gamma_n}{p} \sum_{i=1}^p \frac{\sigma_i^2 x}{z + \sigma_i^2 r_1 x + r_2 m_{3c}(z)}.$$

1179 Then with similar arguments as above between (E.76) and (E.81), we can conclude (E.24) for $m_{2c}(z)$.
1180 This concludes the proof of Lemma E.5. \square

1181 *Proof of Lemma E.6.* Under (E.23), we can obtain equation (E.76) approximately up to some small
1182 error

$$r_1 m_{2c} = -(1 - \gamma_n) - r_2 m_{3c} - z(m_{3c}^{-1} + 1) + \mathcal{E}'_2(z), \quad g_z(m_{3c}(z)) = 1 + \mathcal{E}'_3(z), \quad (\text{E.82})$$

1183 with $|\mathcal{E}'_2(z)| + |\mathcal{E}'_3(z)| = O(\delta(z))$. Then we subtract the equations (E.76) from (E.82), and consider
1184 the contraction principle for the functions $\varepsilon(z) := m_3(z) - m_{3c}(z)$. The rest of the proof is exactly
1185 the same as the one for Lemma E.5, so we omit the details. \square

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  $\{x^{(k)}, x^{(k)}\}_{k=1}^i$  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
```

F Missing Details from the Experiments

F.1 Synthetic Settings

We describe the parameter settings used in the synthetic experiments (Figure 1). For all three synthetic experiments, we set the input feature dimension as $p = 200$.

- Task similarity: We use $\rho_1 = 90, \rho_2 = 30$ for sample sizes. The noise level is $\sigma = 5$. We set $\kappa = 1$ and vary model distance d from 0.01 to 0.2. The x -axis measures the function $\Phi(\beta_1, \beta_2)$ described in Section 3.2. The y -axis measures the improvement of prediction loss using MTL compared to STL.
- Sample size: We set $\kappa = 1$ and $d = 0.02$ for model distance. We use $\rho_2 = 500$ and vary ρ_1 from 50 to 800 for sample sizes.
- Covariate shift: We set $\kappa = 1$ and $d = 0$. We set $\rho_2 = 4$ and vary ρ_1 from 5 to 25 for sample sizes. We use the scale parameter $\lambda = 1$ for the curve without covariate shift and $\lambda = 2$ for the curve with covariate shift (cf. Section 3.4). Without loss of generality, we have rescaled the x and y axis for the ease of presentation. This can be achieved similarly by rescaling the task data.

F.2 Image and Text Classification Settings

For the text classification experiment, we encode each word using the GLoVe word embeddings.¹ We evaluate three model choices. For multi-layer perceptron (MLP), we apply an average pooling layer over the word embeddings. For LSTM and CNN, we add a shared feature representation layer on top of the word embeddings [34].

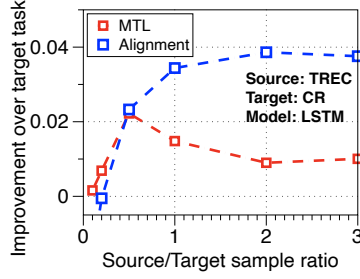
Predicting transfer effect via STL results. We simplify the setup of this experiment by fixing the sample sizes of every task pair. For sentiment analysis tasks, the sample size of the source task ranges in 500, 1000, 1500. We randomly sample these many data points from the task. The sample size of the target task is 1000. For image classification tasks, the training sample size is 10,000 for every task.

Mitigating negative transfer via incremental training. For the case of two tasks, we compare the incremental training scheduled described in Algorithm 1 to a round-robin training schedule baseline. We add 20% of source task samples for every $T = 2$ epochs. The total number of epochs is 20. We set the threshold τ as the validation accuracy of the target task using the baseline training schedule.

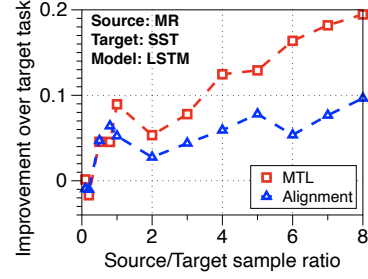
For the case of six tasks, we extend Algorithm 1 accordingly. Initially, we use 5% of samples from SST and 50% of samples from the other tasks. We add 19% of samples from SST and 5% of samples from the other tasks for every 2 epochs. We run 20 epochs in total.

Validating the Theoretical Results. We fill in the details of the experimental procedure used for the results in Figure 2.

¹<http://nlp.stanford.edu/data/wordvecs/glove.6B.zip>



(a) Task pair TREC and CR



(b) Task pair MR and SST

Figure 3: (a) For the task pair TREC and CR, adding the covariance alignment procedure provides more improvement when the source/target sample ratio is large. (b) For the task pair MR and SST, adding the covariance alignment procedure hurts performance. One explanation is that MR and SST are similar tasks, hence adding the alignment module is unnecessary.

- Task similarity: We select a similar and a dissimilar source task compared to the target task using domain knowledge. First pair: the customer review dataset (CR), which predicts whether a review is positive or negative, is more similar to SST (sentiment treebank) than MPQA (question type). Second pair: SST is more similar to MR since they both concern about positive or negative opinions expressed the text. TREC is less similar to MR because the task is about question types. Third pair: MPQA (opinion polarity) is more similar to TREC (question type)
- Sample size: We vary the sample size of the source task from 100 to 3000.
- Covariate shift: We implement the covariance alignment procedure following [15]. We fix the sample size of the target task as 1000.

Further results of the covariance alignment procedure. Our results in Figure 2c are averaged over all the task pairs. In Figure 3, we show two task pairs as examples. In Figure 3a, we observe that for the particular task pair, covariance alignment provides more significant gains when the sample ratio is large. In Figure 3b, we observe that covariance alignment does not always improve over the baseline multi-task learning model. One explanation is that MR and SST are similar tasks, hence adding the alignment module is unnecessary. An interesting question is to understand when adding the alignment module benefits the multi-task learning model. We leave this question for future work.