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 anwer the question in the high-dimensional linear regression setting. We show that the 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. And we validate the three effects on text classification tasks. Inspired by our theory, we show two practical connections of interest. First, single-task performance can help understand multi-task performance. 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 has often been observed to perform worse than single-task learning [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].

However, 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 task two. 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

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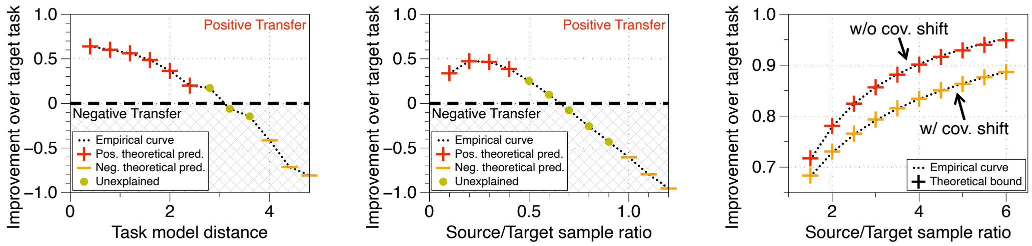


(a) Task similarity (b) Sample size (c) Covariate shift

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.

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

- **Task similarity:** Assume that both tasks follow a linear model with parameters $\beta_1, \beta_2 \in \mathbb{R}^p$, respectively. We measure the distance between them by $\|\beta_1 - \beta_2\|$.
- **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 both fixed values that do not grow with p. We measure the source/target sample ratio by ρ_1/ρ_2.
- **Covariate shift:** Assume that the task features are random vectors with positive semidefinite covariance matrix $\Sigma_1, \Sigma_2 \in \mathbb{R}^{p \times p}$, respectively. We define covariate shift as the matrix $\Sigma_1^{1/2}\Sigma_2^{-1/2}$.

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

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

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

- We provide conditions to predict the effect of transfer as a parameter of model distance $\|\beta_1 - \beta_2\|$ (Section 3.2). As model distance increases, the bias becomes larger, resulting in negative transfer.
- We provide conditions to predict transfer as a parameter of sample ratio n_1/n_2 (Section 3.3). Adding source task samples helps initially by reducing variance, but hurts eventually due to bias.
- For a special case of $\beta_1 = \beta_2$, we show that MTL performs best when the singular values of $\Sigma_1^{1/2}\Sigma_2^{-1/2}$ are the same (Section 3.4). Otherwise, the variance reduces less with covariate shift.

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

Our study also leads to several algorithmic consequences with practical interest. First, we show that single-task learning results can help predict positive or negative transfer for multi-task learning. We validate this observation on ChestX-ray14 [1] and sentiment analysis datasets [23]. Second, we propose a new multi-task training schedule by incrementally adding task data batches to the training procedure. This is inspired by our observation in Figure 1b where adding more source task data helps initially, but hurts eventually. Using our incremental training schedule, we reduce the computational cost by 65% compared to baseline multi-task training over six sentiment analysis dataset while keeping the accuracy the same. Third, we provide a fine-grained insight on a covariance alignment procedure proposed in [15]. We show that the alignment procedure provides more significant improvement when the source/target sample ratio is large. Finally, we validate our three theoretical 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 $X_k \in \mathbb{R}^{n_i \times p}$, consists 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 regularization effect. As observed in Proposition 1 of [15], if $r \geqslant t$, 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 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.
- Learning 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 $W_1, \dots, W_k$.

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

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

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

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 $\hat{\beta}_t^{\mathrm{MTL}}$ denote the multi-task estimator obtained from the procedure above. Our goal is to compare the prediction loss of $\hat{\beta}_t^{\mathrm{MTL}}$, defined by

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

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

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

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

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

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 $\hat{\beta}_t^{\mathrm{MTL}}$. 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 $\hat{\beta}_t^{\mathrm{MTL}}$ minus the variance of $\hat{\beta}_t^{\mathrm{STL}}$, 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 task models become 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 $\mathrm{Tr}[(X_2^\top X_2)^{-1}\Sigma_2]$ 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 $n_2 = \rho_2 \cdot$ 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 $\hat{\beta}_t^{MTL}$ equals*

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

where a_1, a_2 are solutions of the following equations:

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

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 $\mathrm{O}(p^{-1/2+o(1)})$ 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 C.3 in Appendix C). 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 $\rho_1 \gtrsim \delta^{-2} \cdot \lambda_{\min}(\Sigma_1^{1/2}\Sigma_2^{-1/2})^{-4}\|\Sigma_1\| \max(\|\beta_1\|^2, \|\beta_2\|^2)$, and . There exists 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 $\Delta_{bias} - \Delta_{var} < -\delta$, then w.h.p. over the randomness of X_1, X_2, we have $L(\hat{\beta}_t^{MTL}) < L(\hat{\beta}_t^{STL})$.*
- *If $\Delta_{bias} - \Delta_{var} > \delta$, then w.h.p. over the randomness of X_1, X_2, we have $L(\hat{\beta}_t^{MTL}) > L(\hat{\beta}_t^{STL})$.*

Theorem 3.2 applies to settings where large amounts of source task data is 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 C and the proof of Lemma 3.1 is in Appendix F.

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 $\Sigma_1 = \Sigma_2 = \mathrm{Id}$. Each task has sample size $n_1 = \rho_1 \cdot p$ and $n_2\rho_2 \cdot p$. Assume that for the target task, 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.

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

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

- *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, $L(\hat{\beta}_t^{MTL}) < L(\hat{\beta}_t^{STL})$.*
- *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, $L(\hat{\beta}_t^{MTL}) > L(\hat{\beta}_t^{STL})$.*

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

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

Algorithmic consequence. We can in fact extend the result to the cases where the noise variances are different. In this case, we will see that MTL is particularly effective. Concretely, suppose the 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 task provides a negative transfer to the target. If σ_1^2 is small, the source task is more helpful. We leave the result to Proposition D.2 in Appendix D.1. Inspired by the observation, we propose a single-task based metric to help understand MTL results using STL results.

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

3.3 Sample Size

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

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

- *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. $L(\hat{\beta}_t^{MTL}) < L(\hat{\beta}_t^{STL})$.*
- *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. $L(\hat{\beta}_t^{MTL}) > L(\hat{\beta}_t^{STL})$.*

Proposition 3.4 describes the bias-variance tradeoff in terms of the sample ratio n_1/n_2. We apply the result to the setting of Figure 1b (described in Appendix G.1). There are several unexplained observations near $y = 0$ caused by ν. The proof of Proposition 3.4 can be found in Appendix D.2.

Connection to Taskonomy. We use our tools to explain a key result of Taskonomy by Zamir et al. (2018) [2], which shows that MTL can reduce the amount of labeled data needed to achieve comparable performance to STL. For $i = 1, 2$, let $\hat{\beta}_i^{\text{MTL}}(x)$ denote the estimator trained using $x \cdot n_i$ datapoints from every task. The data efficiency ratio is defined as

$$\underset{x \in (0,1)}{\arg\min} \;\; L_1(\hat{\beta}_1^{\text{MTL}}(x)) + L_2(\hat{\beta}_2^{\text{MTL}}(x)) \leqslant L_1(\hat{\beta}_1^{\text{STL}}) + L_2(\hat{\beta}_2^{\text{STL}}).$$

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

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

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 constant multiple), the transfer is positive. Moreover, the data efficiency ratio quantifies how effective the positive transfer is using MTL. The result can be found in Proposition D.3 in Appendix D.2.

Algorithmic consequence. An interesting consequence of Proposition 3.4 is that $L(\hat{\beta}_t^{\mathrm{MTL}})$ is not monotone in ρ_1. In particular, Figure 1b (and our analysis) shows that $L(\hat{\beta}_t^{\mathrm{MTL}})$ behaves as a quadratic function over ρ_1. More generally, depending on how large $\Psi(\beta_1, \beta_2)$ is, $L(\hat{\beta}_t^{\mathrm{MTL}})$ 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 G 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 $M = \mathrm{Id}$; (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.

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

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*

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

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 D.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 Wu et al. (2020) [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 $1 \leqslant i \leqslant t$. Let $B^\star := [\beta_1, \beta_2, \dots, \beta_t]$ 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 $(B^\star)^\top \Sigma B^\star$. Assume that $\lambda_{\min}({B^\star}^\top \Sigma B^\star) \gtrsim \sigma^2$. Let v_i denote the i-th row vector of U_r. There exists a value $\delta = \mathrm{o}\left(\|B^\star\|^2 + \sigma^2\right)$ such that*

- *If $\left(1 - \|v_t\|^2\right) \frac{\sigma^2}{\rho - 1} - \|\Sigma(B^\star U_r v_t - \beta_t)\|^2 > \delta$, then w.h.p $L(\hat{\beta}_t^{MTL}) < L(\hat{\beta}_t^{STL})$.*
- *If $\left(1 - \|v_t\|^2\right) \frac{\sigma^2}{\rho - 1} - \|\Sigma(B^\star U_r v_t - \beta_t)\|^2 < -\delta$, 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. Specially, $(1 - \|v_t\|^2)\sigma^2/(\rho - 1)$ shows the amount of reduced variance and $\|\Sigma(B^\star U_r v_t - \beta_t)\|$ shows the bias of the multi-task estimator. The proof of 3.6 can be found in Appendix E.

4 Experiments

We validate our theory and algorithmic insights. First, we validate the single-task based metric on sentiment analysis and ChestX-ray14 datasets. We show that single-task learning results can help predict positive or negative transfer for both datasets. Second, our proposed incremental training schedule improves the training efficiency of standard multi-task training on sentiment analysis tasks. Third, when the sample ratio is large, performing the alignment procedure of [15] provides more improvement for MTL. Finally, we validate our theoretical results on text classification tasks.

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), sentence subjectivity (SUBJ), customer reviews polarity (CR), question type (TREC), opinion polarity (MPQA), and the Stanford sentiment treebank (SST) tasks. The question is to predict positive or negative sentiment expressed in the text. We use an embedding layer with GloVe embeddings followed by an LSTM, MLP or CNN layer proposed by [27].

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

For all models, we share the main module across all tasks and assign a separate regression or classification layer on top of the shared module for each tasks. The baseline training schedule for MTL is the round-robin training schedule. We measure the test accuracy of predicting a target task.

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 multi-task learning 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 2 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% accuracy 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. 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. Over six randomly selected 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 next result shows the incremental training schedule applies to multiple tasks as well. In Table 1, 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

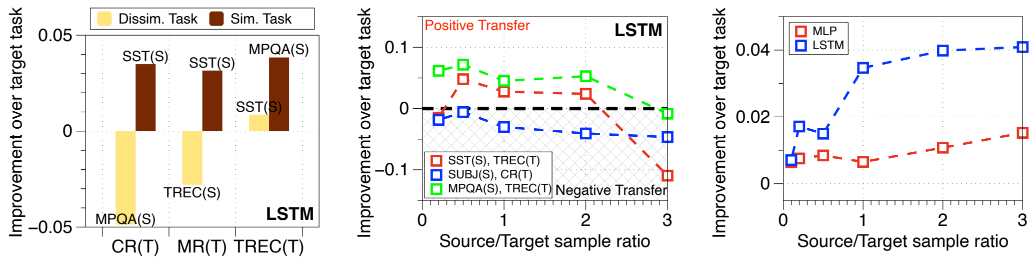
We validate our three theoretical results in Section 3 on the sentiment analysis tasks. In Figure 2a, we compare the performance training with a semantically similar task versus a dissimilar task with a target task. We select each task pair based on our domain knowledge. We observe that adding a similar task helps the target task whereas adding a dissimilar task hurts. In Figure 2b, we validate

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

Table 1: Efficiency of incremental training compared to baseline MTL.

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 2: Single-task learning results can help predict postive or negative transfer in multi-task learning.



(a) Task similarity (b) Data size (c) Covariate shift

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.

the phenomenon that adding more source data samples does not always improve performance on the target task. In Figure 2c, we measure the performance gains from performing the alignment procedure proposed in [15] minus baseline MTL performance. 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 G.2.

5 Related Work

We refer the interested readers to several excellent surveys on multi-task learning for a comprehensive survey [9, 10, 5, 28]. Below, we describe several lines of work that are most related to this work.

Multi-task learning theory. Some of the earliest works on multi-task learning are Baxter [11], Ben-David and Schuller [29]. Mauer [13] studies generalization bounds for linear separation settings of MTL. Ben-David et al. [30] provides uniform convergence bounds that combines source and target errors in an optimal way. The benefit of learning multi-task representations is studied for learning certain half-spaces [14] and sparse regression [31, 32]. 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 do not explain the phenomena of negative transfer.

Multi-task learning methodology. Ando and Zhang [12] introduces an alternating minimization framework for learning multiple tasks. Argyriou et al. [33] present a convex algorithm which learns common sparse representations across a pool of related tasks. Evgeniou et al. [34] develop a framework for multi-task learning in the context of kernel methods. The multi-task learning model that we have focused on is based on the idea of hard parameter sharing [35, 36, 10]. We believe that the technical tools we have developed can also be applied to many other multi-task learning models.

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 $\Sigma = \mathrm{Id}$, 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 [37]. On the other hand, one may derive the asymptotic result in Theorem 3.1 with error $\mathrm{o}(1)$ using the free addition of two independent random matrices in free probability theory [38]. 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 C.3) involves an error term that scales down with ρ_1. Tightening this error bound can potentially 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 study 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 bound the bias and variance. We relate the bounds to three properties of task data. We further provide guidance for detecting and mitigating negative transfer on image and text classification tasks.

Our theoretical framework has the potential to impact many other neighboring areas in the ML community. Multi-task learning connects to a wide range of areas [28]. To name a few, transfer learning, meta learning, multimodal learning, semi-supervised learning, and representation learning are all closely related areas to multi-task learning. Any learning scenario such as reinforcement learning [25] that combines multiple datasets to supervise a model is using multi-task learning. While the theoretical results that we have provided are not directly applicable to these different settings, we believe that the tools we have developed and the framework we have provided can inspire followup works in different settings. For one specific example, we have developed new concentration bounds that may apply to many settings such as soft parameter sharing [10] , kernel methods [34], and convex formulation of multi-task learning [39]. For another example, our results also allow extensions to transfer learning and domain adaptation [40]. The insights we have developed on positive and negative transfer can potentially find applications in multimodal learning, where the data sources are usually heterogeneous. Our fine-gained study on sample sizes have the potential to provide new insight in meta learning, where scarse labeled samples presents a significant challenge.

Our algorithmic consequences of our theory have the potential to impact downstream applications of multi-task learning. For 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 large amounts of labeled data are collected [3], in medical applications it is typically difficult to acquire large amounts of labeled data. For such settings, training multi-task models can be very challenging. Our insight on using single-task learning results to help understand multi-task learning can be valuable for helping practitioners understand their results.

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A Extended Related Work

McNamara and Balcan [41]

Bullins et al. [42]

Cavallanti et al. [43]

Daume and Marcu [44]

Zhao et al. [45]

B Missing Details of Problem Formulation

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

Assumption B.1. *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 matrices, 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*

$$\mathbb{E}|z_{ij}|^k \leqslant C_k, \quad 1 \leqslant i \leqslant n, \ 1 \leqslant j \leqslant p. \tag{B.1}$$

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: $\kappa(\Sigma) \leqslant C$, where $\kappa(\cdot)$ denotes the condition number.

Here we have assumed (B.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 $\mathrm{O}(p^{-\frac{1}{2}+\varepsilon})$ with $\mathrm{O}(p^{-\frac{1}{2}+\frac{2}{a}+\varepsilon})$ in some error bounds. We will not get deeper into this issue in this section, but refer the reader to Corollary F.8 below.

Then we make the following assumptions on the data models.

Assumption B.2. *For for some fixed $t \in \mathbb{N}$, let $Y_i = X_i\beta_i + \varepsilon_i$, $1 \leqslant i \leqslant t$, 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 B.1 with $\rho_i := n_i/p > 1$ being fixed constants, and $\varepsilon_i \in \mathbb{R}^{n_i}$ are random vectors with i.i.d. entries with mean zero, variance σ_i^2 and all moments as in* (B.1).

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

The multi-task learning estimator. From [15], we know that we need to explicitly restrict the capacity r of B so that there is transfer between the two tasks. for the rest of the section, we shall consider the case of two tasks with $r = 1$. Then equation (2.1) simplifies to

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

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

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

As a remark, when $w_1 = w_2 = 1$, we recover the linear regression estimator. The advantage of using $f(B; w_1, w_2)$ is that if β_1 is a scaling of β_2, then this case can be solved optimally using equation (B.2) [36].

Next we consider N_i independent samples of the training set $\{(\widetilde{x}_k^{(i)}, \widetilde{y}_k^{(i)}) : 1 \leqslant k \leqslant N_i\}$ from task-i, $i = 1, 2$. With these sample, we form the random matrices $\widetilde{X}_i \in \mathbb{R}^{N_i \times p}$ and $\widetilde{Y}_i \in \mathbb{R}^{N \times p}$,

$i = 1, 2$, whose row vectors are given by $\widetilde{x}_k^{(i)}$ and $\widetilde{y}_k^{(i)}$. Here we assume that N_1 and N_2 satisfies $N_1/N_2 = n_1/n_2$ and $N_i \geqslant n_i^{1-\varepsilon_0}$ for some constant $\varepsilon_0 > 0$. Then we define the validation loss as

$$\widetilde{f}(\hat{B}; w_1, w_2) = \left\| \widetilde{X}_1 \hat{B} w_1 - \widetilde{Y}_1 \right\|^2 + \left\| \widetilde{X}_2 \hat{B} w_2 - \widetilde{Y}_2 \right\|^2. \tag{B.4}$$

Inserting (B.3) into (B.4), one can see that $\widetilde{f}$ only depends on the ratio $v := w_1/w_2$. Hence we will also write $\widetilde{f}(\hat{B}; v)$ in the following discussion.

Let $\hat{v} = \hat{w}_1/\hat{w}_2$ be the global minimizer of $\widetilde{f}(\hat{B}; v)$. We will define the multi-task learning estimator for the target task as

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

where $t = 2$ since we are considering the two task case, and it also stands for the "target task". The intuition for deriving $\hat{\beta}_t^{\text{MTL}}$ is akin to performing multi-task training in practice. Then the test loss of using $\hat{\beta}_t^{\text{MTL}}$ for the target task is

$$\begin{aligned} L(\hat{\beta}_t^{\text{MTL}}) = \; & \hat{v}^2 \left\| \Sigma_2^{1/2} (\hat{v}^2 X_1^\top X_1 + X_2^\top X_2)^{-1} X_1^\top X_1 (\beta_1 - \hat{v}\beta_2) \right\|^2 \\ + \; & \operatorname{Tr}\left[\Sigma_2 (\hat{v}^2 X_1^\top X_1 + X_2^\top X_2)^{-2} \left(\sigma_1^2 \cdot \hat{v}^2 X_1^\top X_1 + \sigma_2^2 \cdot X_2^\top X_2 \right) \right], \end{aligned} \tag{B.5}$$

which is well-defined since it only depends on $\hat{v}$, but otherwise does not depend on $\hat{w}_1$ or $\hat{w}_2$ separately. Our goal is to study under model and covariate shifts, whether multi-task learning helps to learn the target task better than single-task learning. The baseline where we solve the target task with its own data is

$$L(\hat{\beta}_t^{\text{STL}}) = \sigma_2^2 \cdot \operatorname{Tr}\left[\Sigma_2 (X_2^\top X_2)^{-1} \right], \;\; \text{where} \;\; \hat{\beta}_t^{\text{STL}} = (X_2^\top X_2)^{-1} X_2^\top Y_2.$$

One may observe that we can reduce $\widetilde{f}$ to an expression that is easier to handle using concentration of random vectors with i.i.d. entries. Before doing that, we first need to fix the setting for the following discussions, because we want to keep track of the error rate carefully instead of obtaining an asymptotic result only.

Now suppose $Y_i = X_i \beta_i + \varepsilon_i$ and $\widetilde{Y}_i = \widetilde{X}_i \beta_i + \widetilde{\varepsilon}_i$, $i = 1, 2$, all satisfy Assumption B.2. Then we rewrite (B.4) as

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

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

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

with high probability. Thus we obtain that

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

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

$$\sum_{i=1}^{2} N_i \left\| \Sigma_i^{1/2} (\hat{B} w_1 - \beta_i) \right\|^2 = val(\hat{B}; v) \cdot \left(1 + \mathrm{O}(p^{-1/2+\varepsilon}) \right)$$

with high probability, where

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

In sum, we have obtained that

$$\widetilde{f}(\hat{B}; v) = \left[val(\hat{B}; v) + (N_1\sigma_1^2+N_2\sigma_2^2)\right]\cdot\left(1+\mathrm{O}(p^{-(1-\varepsilon_0)/2+\varepsilon})\right). \tag{B.6}$$

Hence to minimize $\widetilde{f}$, it suffices to minimize $val(\hat{B}; v)$ over v.

C Proof of Theorem 3.2

We now state several helper lemmas to get estimates on $L(\hat{\beta}_t^{\mathrm{STL}})$ and $L(\hat{\beta}_t^{\mathrm{MTL}})$. The first lemma, which is a folklore result in random matrix theory, helps to determine the asymptotic limit of $L(\hat{\beta}_t^{\mathrm{STL}})$, as $p\to\infty$. When the entries of X are multivariate Gaussian, this lemma recovers the classical result for the mean of inverse Wishart distribution [46]. For general non-Gaussian random matrices, it can be obtained from Stieltjes transform method; see e.g., Lemma 3.11 of [47]. Here we shall state a result obtained from Theorem 2.4 in [21], which gives an almost sharp error bound.

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

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

with high probability.

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

Lemma C.2. *Suppose $X_1 = Z_1\Sigma_1^{1/2}\in\mathbb{R}^{n_1\times p}$ and $X_2 = Z_2\Sigma_2^{1/2}\in\mathbb{R}^{n_2\times p}$ satisfy Assumption B.1 with $\rho_1 := n_1/p > 1$ and $\rho_2 := n_2/p > 1$ being fixed 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 $M^\top M$ in descending order. Let A be any $p\times p$ matrix that is independent of X_1 and X_2. We have that for any constant $\varepsilon>0$,*

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

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

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

Proof Overview. We first describe the proof of Theorem 3.1. We use the Stieltjes transform method (or the resolvent method) in random matrix theory [47, 48, 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, 37], we find the asymptotic limit, say $R_\infty(z)$, of $R(z)$ for any z as $p\to\infty$ with an almost optimal convergence rate. In particular, when $z=0$, $\mathrm{Tr}[R_\infty(0)]$ gives the expression inTheorem 3.1. The details can be found in Appendix F and F.3.

Finally, the last lemma describes the asymptotic limit of $(X_1^\top X_1+X_2^\top X_2)^{-1}\Sigma_2(X_1^\top X_1+X_2^\top X_2)^{-1}$, which will be needed when we estimate the first term on the right-hand side of (B.5).

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

$$\begin{aligned}&(n_1+n_2)^2 \left\| \Sigma_2^{1/2} (X_1^\top X_1 + X_2^\top X_2)^{-1} \beta \right\|^2 \\ &= \beta^\top \Sigma_2^{-1/2} \frac{(1+a_3)\,\mathrm{Id} + a_4 M^\top M}{(a_1 M^\top M + a_2)^2} \Sigma_2^{-1/2} \beta + \mathrm{O}(p^{-1/2+\varepsilon} \|\beta\|^2),\end{aligned} \tag{C.4}$$

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

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

Here b_0, b_1 and b_2 are defined as

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

The proof of Lemma C.2 and Lemma C.3 is a main focus of Section F. We remark that one can probably derive the same asymptotic result using free probability theory (see e.g. [38]), but our results (C.2) and (C.4) also give an almost sharp error bound $\mathrm{O}\left(p^{-1/2+\varepsilon}\right)$.

In this section, we state and prove the formal version of Theorem 3.2, which covers the two tasks case with $t = 2$. In this section, we consider the case where the entries of ε_1 and ε_2 have the same variance $\sigma_1^2 = \sigma_2^2 = \sigma^2$.

First, we introduce several quantities that will be used in our statement, and they are also related to the quantities in Lemma C.2 and Lemma C.3. Given the optimal ratio $\hat{v}$, let $\hat{M} = \hat{v}\Sigma_1^{1/2}\Sigma_2^{-1/2}$ denote the weighted covariate shift matrix, and $\hat{\lambda}_1 \geqslant \hat{\lambda}_2 \geqslant \ldots \geqslant \hat{\lambda}_p$ be the eigenvalues of $\hat{M}^\top \hat{M}$. Define $(\hat{a}_1, \hat{a}_2)$ as the solution to the following system of deterministic equations,

$$\hat{a}_1 + \hat{a}_2 = 1 - \frac{1}{\rho_1 + \rho_2}, \quad \hat{a}_1 + \frac{1}{\rho_1 + \rho_2} \cdot \frac{1}{p} \sum_{i=1}^p \frac{\hat{\lambda}_i^2 \hat{a}_1}{\hat{\lambda}_i^2 \hat{a}_1 + \hat{a}_2} = \frac{\rho_1}{\rho_1 + \rho_2}. \tag{C.6}$$

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

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

where we denoted

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

Then we introduce the following matrix

$$\Pi = \frac{\rho_1^2}{(\rho_1 + \rho_2)^2} \cdot \hat{M} \frac{(1 + \hat{a}_3)\,\mathrm{Id} + \hat{a}_4 \hat{M}^\top \hat{M}}{(\hat{a}_1 \hat{M}^\top \hat{M} + \hat{a}_2)^2} \hat{M}^\top. \tag{C.8}$$

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 [49]. 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

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

where $\lambda_{\min}(\hat{M})$ is the smallest singular value of $\hat{M}$. 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 C.4. *Consider two data models $Y_i = X_i\beta_i + \varepsilon_i$, $i = 1, 2$, that satisfy Assumption B.2. With high probability, we have*

$$L(\hat{\beta}_t^{\mathit{MTL}}) \leqslant L(\hat{\beta}_t^{\mathit{STL}}) \quad \textit{when:} \quad \Delta_{\mathit{var}} - \Delta_{\mathit{bias}} \geqslant \delta \tag{C.10}$$

$$L(\hat{\beta}_t^{\mathit{MTL}}) \geqslant L(\hat{\beta}_t^{\mathit{STL}}) \quad \textit{when:} \quad \Delta_{\mathit{var}} - \Delta_{\mathit{bias}} \leqslant -\delta, \tag{C.11}$$

where

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

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

For the isotropic model in Section 3, we actually have an easier and sharper bound than Theorem C.4 as follows.

Lemma C.5. *In the setting of Theorem C.4, assume that $\Sigma_1 = \operatorname{Id}$, 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 $(\beta_1 - \beta_2)$ is a random vector with i.i.d. entries with mean 0, variance d^2 and all moments. Denote $\Delta_{\mathit{bias}}^\star := \left((1-\hat{v})^2\kappa^2 + d^2\right) \operatorname{Tr}[\Pi]$. Then we have*

$$L(\hat{\beta}_t^{\mathit{MTL}}) \leqslant L(\hat{\beta}_t^{\mathit{STL}}) \quad \textit{when:} \quad \Delta_{\mathit{var}} \geqslant (\alpha_+^2(\rho_1) + \mathrm{o}(1)) \cdot \Delta_{\mathit{bias}}^\star,$$

$$L(\hat{\beta}_t^{\mathit{MTL}}) \geqslant L(\hat{\beta}_t^{\mathit{STL}}) \quad \textit{when:} \quad \Delta_{\mathit{var}} \leqslant (\alpha_-^2(\rho_1) - \mathrm{o}(1)) \cdot \Delta_{\mathit{bias}}^\star.$$

Now we give the proof of Theorem C.4 based on Lemma C.2 and Lemma C.3.

Proof of Theorem C.4. Note that

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

The proof is divided into the following four steps.

(i) We first consider $\hat{M} \equiv \hat{M}(v) = v\Sigma_1^{1/2}\Sigma_2^{-1/2}$ for a fixed $v \in \mathbb{R}$. Then we use Lemma C.1 and Lemma C.2 to calculate the variance reduction $\delta_{\mathrm{var}}(v)$, which will lead to the Δ_{var} term.

(ii) Using the approximate isometry property of X_1 (see (C.16) below), we will bound the bias term $\delta_{\mathrm{bias}}(v)$ through

$$\widetilde{\delta}_{\mathrm{bias}}(v) := v^2 n_1^2 \left\| \Sigma_2^{1/2} (v^2 X_1^\top X_1 + X_2^\top X_2)^{-1} \Sigma_1 (\beta_1 - v\beta_2) \right\|^2. \tag{C.14}$$

(iii) We use Lemma C.3 to calculate (C.14), which will lead to the Δ_{bias} term.

(iv) Finally we use a standard ε-net argument to extend the above results to $\hat{M} = \hat{v}\Sigma_1^{1/2}\Sigma_2^{-1/2}$ for a possibly random $\hat{v}$ which depends on Y_1 and Y_2.

Step I: Variance reduction. Let $\hat{M} = v\Sigma_1^{1/2}\Sigma_2^{-1/2}$ for any fixed constant $v \in \mathbb{R}$. Using Lemma C.2, we can obtain that for any constant $\varepsilon > 0$,

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

and

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

with high probability, where $\hat{a}_1$ and $\hat{a}_2$ satisfy (C.6). Combining them, we get

$$\delta_{\mathrm{var}}(v) = \Delta_{\mathrm{var}}(v) + \mathrm{O}(\sigma^2 p^{-1/2+e}) \quad \text{whp}, \tag{C.15}$$

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

Step II: Bounding the bias term. In this step, we shall use the following the following bounds on the singular values of Z_1: for any fixed $\varepsilon > 0$, we have

$$\alpha_-(\rho_1) - \mathrm{O}(p^{-1/2+e}) \preceq \frac{Z_1^T Z_1}{n_1} \preceq \alpha_+(\rho_1) + \mathrm{O}(p^{-1/2+e}) \tag{C.16}$$

with high probability. In fact, $Z_1^T Z_1$ is a standard sample covariance matrix, and it is well-known that its nonzero eigenvalues are all inside the support of the Marchenko-Pastur law $[\alpha_-(\rho_1) - \mathrm{o}(1), \alpha_+(\rho_1) + \mathrm{o}(1)]$ with probability $1 - \mathrm{o}(1)$ [50]. For the estimate (C.16) we used [21, Theorem 2.10] to get a stronger probability bound.

Next we shall use (C.16) to approximate $\delta_{\text{bias}}(v)$ with $\widetilde{\delta}_{\text{bias}}(v)$ in (C.14).

Lemma C.6. *In the setting of Theorem C.4, we denote by $K = (v^2 X_1^\top X_1 + X_2^\top X_1)^{-1}$, and*

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

Then we have whp,

$$\left| \delta_{bias}(v) - \widetilde{\delta}_{bias}(v) \right| \leqslant \left(\alpha_+^2(\rho_1) - 1 + \mathrm{O}(p^{-1/2+\varepsilon}) \right) \delta_\varepsilon.$$

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

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

Using (C.16), we can bound

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

Thus we can estimate that

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

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

Note by (C.16), we have with high probability,

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

for some small enough constant $c > 0$. Together with Lemma C.6, we get with high probability,

$$\left| \delta_{\text{bias}}(v) - \widetilde{\delta}_{\text{bias}}(v) \right| \leqslant (1 - c) \delta(v) \tag{C.18}$$

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

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

$$\widetilde{\delta}_{\text{bias}}(v) = \frac{\rho_1^2}{(\rho_1+\rho_2)^2} \cdot v^2(\beta_1 - v\beta_2)^\top \Sigma_1 \Sigma_2^{-1/2} \frac{(1+\hat{a}_3)\,\mathrm{Id} + \hat{a}_4 \hat{M}^\top \hat{M}}{(a_1 \hat{M}^\top \hat{M} + a_2)^2} \Sigma_2^{-1/2} \Sigma_1 (\beta_1 - v\beta_2) + \mathrm{O}(p^{-1/2+\varepsilon})$$
$$= (\beta_1 - v\beta_2)^\top \Sigma_1^{1/2} \Pi \Sigma_1^{1/2} (\beta_1 - v\beta_2) + \mathrm{O}(p^{-1/2+\varepsilon}) =: \Delta_{\text{bias}}(v) + \mathrm{O}(p^{-1/2+\varepsilon}),$$

with high probability. Together with and (C.15) and (C.18), we obtain that whp,

$$\begin{cases} \delta_{\text{var}}(v) > \delta_{\text{bias}}(v), & \text{if} \quad \Delta_{\text{var}}(v) - \Delta_{\text{bias}}(v) \geqslant \delta(v), \\ \delta_{\text{var}}(v) < \delta_{\text{bias}}(v), & \text{if} \quad \Delta_{\text{var}}(v) - \Delta_{\text{bias}}(v) \leqslant -\delta(v). \end{cases} \tag{C.19}$$

Step IV: An ε-net argument. Finally, it remains to extend the above result 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 (C.19) holds uniformly for all $v \in [-C_0, C_0]$. In fact, for a large constant $C_1 > 0$, we consider v belonging to a discrete set

$$V := \{v_k = kp^{-1} : -(C_0 p + 1) \leqslant k \leqslant C_0 p + 1\}.$$

Then using the arguments for the first three steps and a simple union bound, we get that (C.19) holds simultaneously for all $v \in V$ with high probability. On the other hand, by (C.16) 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 $v_k \leqslant v \leqslant v_{k+1}$ we have the following estimates:

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

Then a simple application of triangle inequality gives that the event

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

holds with high probability. On the other hand, on Ξ_1 one can see that for any small constant $\varepsilon > 0$,

$$|\delta_{\text{var}}(v) - \delta_{\text{var}}(C_0)| \leqslant \varepsilon\delta_{\text{var}}(C_0), \quad |\delta_{\text{bias}}(v) - \delta_{\text{bias}}(C_0)| \leqslant \varepsilon\delta_{\text{bias}}(C_0), \quad |\delta(v) - \delta(C_0)| \leqslant \varepsilon\delta(C_0),$$
$$|\Delta_{\text{bias}}(v) - \Delta_{\text{bias}}(C_0)| \leqslant \varepsilon\Delta_{\text{bias}}(C_0), \quad |\Delta_{\text{var}}(v) - \Delta_{\text{var}}(C_0)| \leqslant \varepsilon\Delta_{\text{var}}(C_0),$$

for all $v \geqslant C_0$ as long as C_0 is chosen large enough depending on ε. Similar estimates hold for $v \leqslant -C_0$ if we replace C_0 with $-C_0$ in the above estimates. Together with the estimate at $\pm C_0$, we get that (C.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. ☐

Remark C.7. One can see from the above proof that the main error, δ, of Theorem C.4 comes from approximating δ_{bias} by $\widetilde{\delta}_{\text{bias}}$ in (C.18). In order to improve this estimate and obtain an exact asymptotic result as for the δ_{var} term, one needs to study the singular value distribution of the following random matrix:

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

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; see e.g. [51]. However, since $\mathcal{X}$ is not symmetric, it is known that the singular values of $\mathcal{X}$ are different from its eigenvalues. To the best of our knowledge, the asymptotic singular value behavior of $\mathcal{X}$ is still unknown in random matrix theory literature, and the study of the singular values of $\mathcal{X} + v^2$ will be even harder. We leave this problem to future study.

By replacing (C.18) with a tighter bound in Step II of the above proof, we can conclude the proof of Lemma C.5.

Proof of Lemma C.5. 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 F.14, we get that for any constant $\varepsilon > 0$,

$$\left|\delta_{\text{bias}}(v) - [(1-v)^2\kappa^2 + d^2]\,\mathrm{Tr}(\mathcal{K}^\top\mathcal{K})\right|$$
$$= \left|(\beta_1 - v\beta_2)^\top \mathcal{K}^\top \mathcal{K} (\beta_1 - v\beta_2) - [(1-v)^2\kappa^2 + d^2]\,\mathrm{Tr}(\mathcal{K}^\top\mathcal{K})\right|$$
$$\leqslant p^{\varepsilon}[(1-v)^2\kappa^2 + d^2]\left\{\mathrm{Tr}\left[(\mathcal{K}^\top\mathcal{K})^2\right]\right\}^{1/2} \lesssim p^{1/2+\varepsilon}[(1-v)^2\kappa^2 + d^2], \tag{C.20}$$

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 $\|\mathcal{K}\| = \mathrm{O}(1)$ by (C.16). Now for $\mathrm{Tr}(\mathcal{K}^\top \mathcal{K})$, we rewrite it as

$$v^2[(1-v)^2\kappa^2 + d^2]\,\mathrm{Tr}\left[(v^2 X_1^\top X_1 + X_2^\top X_2)^{-1}\Sigma_2 (v^2 X_1^\top X_1 + X_2^\top X_2)^{-1}(X_1^\top X_1)^2\right].$$

Recalling that $\Sigma_1 = \mathrm{Id}$ and bounding $(X_1^\top X_1)^2 = (Z_1^\top Z_1)^2$ using (C.16) again, we obtain that

$$\delta^\star_{\text{bias}}(v)\cdot(\alpha_-^2(\rho_1) - \mathrm{O}(p^{-1/2+\varepsilon})) \leqslant [(1-v)^2\kappa^2 + d^2]\,\mathrm{Tr}(\mathcal{K}^\top\mathcal{K}) \leqslant \delta^\star_{\text{bias}}(v)\cdot(\alpha_+^2(\rho_1) + \mathrm{O}(p^{-1/2+\varepsilon})), \tag{C.21}$$

where

$$\delta^\star_{\text{bias}}(v) := n_1^2 v^2[(1-v)^2\kappa^2 + d^2]\,\mathrm{Tr}\left[(v^2 X_1^\top X_1 + X_2^\top X_2)^{-1}\Sigma_2(v^2 X_1^\top X_1 + X_2^\top X_2)^{-1}\right].$$

Note that $\delta^\star_{\text{bias}}(v) \sim 1$, hence combining (C.20) and (C.21) we get

$$\delta^\star_{\text{bias}}(v)\cdot(\alpha_-^2(\rho_1) - \mathrm{O}(p^{-1/2+\varepsilon})) \leqslant \delta_{\text{bias}}(v) \leqslant \delta^\star_{\text{bias}}(v)\cdot(\alpha_+^2(\rho_1) + \mathrm{O}(p^{-1/2+\varepsilon})). \tag{C.22}$$

Now we can replace the estimate (C.18) with this stronger estimate, and repeat all the other parts of the proof of Theorem C.4 to conclude Lemma C.5. In particular, one can calculate $\delta^\star_{\text{bias}}(v)$ using Lemma C.3 and get the $\Delta^\star_{\text{bias}}(v)$ term, We omit the details. $\square$

D Proofs for Isotropic and Covariate Shifted Settings

D.1 Missing Proofs of Section 3.2

We define the function

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

For the isotropic model with $\sigma_1^2 = \sigma_2^2 = \sigma^2$, using concentration for random vectors with i.i.d. entries, Lemma F.14, we can obtain that $val(\hat{B}; w_1, w_2) = val(v)\cdot\left(1 + \mathrm{O}(p^{-1/2+\varepsilon})\right)$. Hence the validation loss in (B.6) reduces to

$$\widetilde{f}(\hat{B}; v) = \left[N_2\cdot val(v) + (N_1\sigma_1^2 + N_2\sigma_2^2)\right]\cdot\left(1 + \mathrm{O}(p^{-(1-\varepsilon_0)/2+\varepsilon})\right) \tag{D.1}$$

with high probability for any constant $\varepsilon > 0$. Thus for the following discussions, it suffices to focus on the behavior of $val(v)$. Let $\hat{w}$ the minimizer of $val(v)$. The proof will consist of two main steps.

- First, we show that $\hat{w}$ is close to 1, and then (D.1) implies that $\hat{v}$ is also close to 1.
- Second, we plug $\hat{v}$ back into $L(\hat{\beta}_2^{\text{MTL}})$ and use Lemma C.5 to show the result.

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

Lemma D.1. *For the isotropic model, the minimizer for $val(v)$ satisfies*

$$|\hat{w} - 1| \leqslant C\left(\frac{d^2}{\kappa^2} + \frac{\sigma^2}{p\kappa^2}\right) \quad \textit{whp} \tag{D.2}$$

for some constant $C > 0$.

Proof. To be consistent with the notation $\hat{w}$, we shall change the name of the argument to w in the proof. First it is easy to observe that $val(w) < val(-w)$ for $w > 0$. Hence it suffices to assume that $w \geqslant 0$.

We first consider the case $w \geqslant 1$. We write

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

Notice that

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

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

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

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 (C.16), we get that $\mathcal{A}$ is lower bounded as

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

as long as

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

Hence $val'(w) > 0$ on (w_1, ∞), i.e. $val(w)$ is strictly increasing for $w > w_1$. Hence we must have $\hat{w} \leqslant w_1$.

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

$$\begin{aligned} val'(w) \leqslant{}& \frac{\rho_1}{\rho_2}\left[2\,(w-1)\,\kappa^2\right] \cdot \mathrm{Tr}\left[(w^2 X_1^\top X_1 + X_2^\top X_2)^{-2} (X_2^\top X_2)^2\right] \\ &+ \left[2wd^2 + 2w\,(w-1)\,(2w-1)\kappa^2\right] \cdot \mathrm{Tr}\left[(w^2 X_1^\top X_1 + X_2^\top X_2)^{-2} (X_1^\top X_1)^2\right] \\ &+ \frac{\rho_1}{\rho_2}(2w\sigma^2) \cdot \mathrm{Tr}\left[(w^2 X_1^\top X_1 + X_2^\top X_2)^{-2} X_2^\top X_2\right] \\ &= \frac{\rho_1}{\rho_2}\,\mathrm{Tr}\left[(w^2 X_1^\top X_1 + X_2^\top X_2)^{-1} \mathcal{B}\right], \end{aligned} \tag{D.3}$$

where the matrix $\mathcal{B}$ is

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

Using the estimate (C.16), we get that $\mathcal{B}$ is upper bounded as

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

as long as

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

Hence $val'(w) < 0$ on $[0, w_2)$, i.e. $val(w)$ is strictly decreasing for $w < w_2$. Hence we must have $\hat{w} \geqslant w_2$.

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

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

which concludes the proof. □

For the rest of this section, we choose the parameters that satisfy the following relations:

$$pd^2 \sim \sigma^2 \sim 1, \quad p^{-1+c_0}\sigma^2 \leqslant \kappa^2 \leqslant p^{-\varepsilon_0 - c_0}\sigma^2, \tag{D.4}$$

for some small constant $c_0 > 0$. We will explain below why we make this choice. Before that, we first show the following estimate on the optimizer $\hat{v}$: with high probability,

$$|\hat{v} - 1| = \mathrm{O}\left(\mathcal{E}\right), \quad \mathcal{E} := \frac{d^2}{\kappa^2} + \frac{\sigma^2}{p\kappa^2} + p^{-1/2+\varepsilon_0/2+2\varepsilon}. \tag{D.5}$$

In fact, from the proof of Lemma D.1 above, one can check that if $C\mathcal{E} \leqslant |w - \hat{w}| \leqslant 2C\mathcal{E}$ for a large enough constant $C > 1$, then $|val'(w)| \gtrsim pd^2$. Moreover, under the choice (D.4) we have

$$val(w) = \mathrm{O}(pd^2), \quad \text{for} \quad |w - \hat{w}| \leqslant 2C\mathcal{E}.$$

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

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

which leads to $\widetilde{f}(\hat{B}; w) > \widetilde{f}(\hat{B}; \hat{w})$ whp by (D.1). Thus w cannot be a minimizer of $\widetilde{f}(\hat{B}; v)$, and we must have $|\hat{v} - \hat{w}| \leqslant 2C\mathcal{E}$. Together with (D.2), we conclude (D.5).

Inserting (D.5) into (B.5) and applying Lemma F.14 to $(\beta_1 - \hat{v}\beta_s)$ again, we get whp,

$$\begin{aligned} L(\hat{\beta}_t^{\text{MTL}}) = &(1 + \mathrm{O}(\mathcal{E})) \cdot \left[d^2 + \mathrm{O}\left(\mathcal{E}^2\kappa^2\right)\right] \mathrm{Tr}\left[(X_1^\top X_1 + X_2^\top X_2)^{-2}(X_1^\top X_1)^2\right] \\ &+ (1 + \mathrm{O}(\mathcal{E})) \cdot \sigma^2 \,\mathrm{Tr}\left[(X_1^\top X_1 + X_2^\top X_2)^{-1}\right]. \end{aligned} \tag{D.6}$$

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 (C.16), we see that

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

Hence we need to choose that $p \cdot d^2 \sim \sigma^2$. On the other hand, we want the error term $\mathcal{E}^2\kappa^2$ to be much 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 lead to the choices of parameters in (D.4). Moreover, under (D.4) we can simplify (D.6) to

$$\begin{aligned} L(\hat{\beta}_2^{\text{MTL}}) = &(1 + \mathrm{O}(n^{-\varepsilon})) \cdot d^2 \,\mathrm{Tr}\left[(X_1^\top X_1 + X_2^\top X_2)^{-2}(X_1^\top X_1)^2\right] \\ &+ (1 + \mathrm{O}(n^{-\varepsilon})) \cdot \sigma^2 \,\mathrm{Tr}\left[(X_1^\top X_1 + X_2^\top X_2)^{-1}\right] \end{aligned} \tag{D.7}$$

whp for some constant $\varepsilon > 0$.

With (D.7) and Lemma C.5, we can prove Proposition 3.3, which gives a transition threshold with respect to the ratio between the model bias and the noise level. With slight abuse of notations, we shall write $\hat{a}_i$, $\hat{b}_k$ and $\hat{M}$ as a_i, b_k and M throughout the rest of this section.

Proof of Proposition 3.3. In the setting of Proposition 3.3, we have $M = \Sigma_1^{1/2}\Sigma_2^{-1/2} = \mathrm{Id}$. Then solving equations (C.6) and (C.7) with $\hat{\lambda}_i = 1$, we get that

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

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

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

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

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

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

we can get from Lemma C.5 (or rather the proof of it) that

$$\alpha_-^2(\rho_1) - \mathrm{o}(1) \leqslant \frac{\delta_{\text{bias}}}{\Delta_{\text{bias}}} \leqslant \alpha_+^2(\rho_1) + \mathrm{o}(1), \tag{D.11}$$

where

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

Note that

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

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

Positive transfer. With (D.10) and (D.11), we conclude that if

$$pd^2 \cdot \frac{\rho_1^2(\rho_1+\rho_2)}{(\rho_1+\rho_2-1)^3} \cdot \left(\alpha_+^2(\rho_1) + \mathrm{o}(1)\right) < \sigma^2 \cdot \frac{\rho_1}{(\rho_2-1)(\rho_1+\rho_2-1)}, \tag{D.13}$$

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

$$\frac{pd^2}{\sigma^2} < \Phi(\rho_1,\rho_2) \cdot \left(\alpha_+^2(\rho_1) + \mathrm{o}(1)\right)^{-1}, \tag{D.14}$$

Since $\Psi(\beta_1,\beta_2) = pd^2/\sigma^2$, it gives the first statement of Proposition 3.3.

Negative transfer. On the other hand, if

$$pd^2 \cdot \frac{\rho_1^2(\rho_1+\rho_2)}{(\rho_1+\rho_2-1)^3} \cdot \left(\alpha_-^2(\rho_1) - \mathrm{o}(1)\right) > \sigma^2 \cdot \frac{\rho_1}{(\rho_2-1)(\rho_1+\rho_2-1)}, \tag{D.15}$$

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

$$\Psi(\beta_1,\beta_2) = \frac{pd^2}{\sigma^2} > \Phi(\rho_1,\rho_2) \cdot \left(\alpha_-^2(\rho_1) - \mathrm{o}(1)\right)^{-1}, \tag{D.16}$$

which gives the second statement of Proposition 3.3. □

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

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

- *If* $\sigma_1^2 < -\gamma_+^{1/2}\rho_1 \cdot pd^2 + \left(1 + \gamma_+^{-1/2}\rho_1\Phi(\rho_1,\rho_2)\right) \cdot \sigma_2^2$, *then whp* $L(\hat{\beta}_2^{MTL}) < L(\hat{\beta}_2^{STL})$.
- *If* $\sigma_1^2 > -\gamma_-^{1/2}\rho_1 \cdot pd^2 + \left(1 + \gamma_-^{-1/2}\rho_1\Phi(\rho_1,\rho_2)\right) \cdot \sigma_2^2$, *then whp* $L(\hat{\beta}_2^{MTL}) > L(\hat{\beta}_2^{STL})$.

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

Proof of Proposition D.2. In the setting of Proposition D.2, the test loss is given by (B.5). In the isotropic model, using again the concentration of random vector with i.i.d. entries, Lemma F.14, we can rewrite $L(\hat{\beta}_2^{\mathrm{MTL}})$ as

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

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

In the current setting, we can also show that (D.5) holds for $\hat{v}$. Since the proof is almost the same as the one for Lemma D.1, we omit the details. Thus under the choice parameters in (D.4), $L(\hat{\beta}_2^{\mathrm{MTL}})$ can be simplified as in (D.7):

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

Then we write

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

where

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

satisfies (D.10) but with σ^2 replaced with σ_2^2,

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

satisfies (D.11), and

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

To estimate this new term $\delta_{\mathrm{var}}^{(2)}$, we use the same arguments as in the proof of Lemma C.5: we first replace $X_1^\top X_1$ with $n_1 \operatorname{Id}$ up to some error using (C.16), and then apply Lemma C.3 to calcualte $\operatorname{Tr}\left[(X_1^\top X_1 + X_2^\top X_2)^{-2}\right]$. This process leads to the following estimates on $\delta_{\mathrm{var}}^{(2)}$:

$$\alpha_-(\rho_1) - \mathrm{o}(1) \leqslant \frac{\delta_{\mathrm{var}}^{(2)}}{\Delta_{\mathrm{var}}^{(2)}} \leqslant \alpha_+(\rho_1) + \mathrm{o}(1), \tag{D.18}$$

where

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

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

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

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

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

then we have $\delta_{\mathrm{var}} > \delta_{\mathrm{bias}} + \delta_{\mathrm{var}}^{(2)}$ whp, which gives $L(\hat{\beta}_t^{\mathrm{MTL}}) < L(\hat{\beta}_t^{\mathrm{STL}})$. We can solve (D.19) to get

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

This proves the first claim of Proposition D.2 for positive transfer.

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

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

then we have $\delta_{\mathrm{var}} < \delta_{\mathrm{bias}} + \delta_{\mathrm{var}}^{(2)}$ whp, which gives $L(\hat{\beta}_t^{\mathrm{MTL}}) > L(\hat{\beta}_t^{\mathrm{STL}})$. We can solve (D.20) to get

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

This proves the second claim of Proposition D.2 for negative transfer. $\square$

D.2 Missing Proofs of Section 3.3

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

Proof of Proposition 3.4. Following the above proof of Proposition 3.3, we see that $L(\hat{\beta}_2^{\mathrm{MTL}}) < L(\hat{\beta}_2^{\mathrm{STL}})$ whp if (D.14) holds, while $L(\hat{\beta}_2^{\mathrm{MTL}}) > L(\hat{\beta}_2^{\mathrm{STL}})$ whp if (D.16) holds.

We first explain the meaning of the condition

$$\Psi(\beta_1, \beta_2) > 2/(\rho_2 - 1). \tag{D.21}$$

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 $\rho_1 \to \infty$. Moreover, we notice that $\left(\alpha_-^2(\rho_1) - \mathrm{o}(1)\right)^{-1} < 2$ for $\rho_1 > 40$. Hence (D.21) implies that (D.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 (D.14) and (D.16). We will use the following trivial inequalities

$$\frac{(\rho_2 - 1)\rho_1}{\rho_1 + \rho_2 - 2} \cdot \left(1 - \frac{1}{(\rho_1 + \rho_2 - 2)^2}\right) \leqslant \Phi(\rho_1, \rho_2) \leqslant \frac{(\rho_2 - 1)\rho_1}{\rho_1 + \rho_2 - 2}. \tag{D.22}$$

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

$$\Psi(\beta_1, \beta_2) \cdot \frac{(\rho_2 - 1)\rho_1}{\rho_1 + \rho_2 - 2} < \gamma_+^{-1}. \tag{D.23}$$

then we can solve (D.23) to get

$$\rho_1 < \frac{\rho_2 - 2}{\Psi(\beta_1, \beta_2) \cdot \gamma_+(\rho_2 - 1) - 1}. \tag{D.24}$$

This gives the first statement of Proposition 3.4.

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

$$\rho_2 - 2 > (2\gamma_+ - 1)\rho_1.$$

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

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

$$\Psi(\beta_1, \beta_2) \cdot \frac{(\rho_2 - 1)\rho_1}{\rho_1 + \rho_2 - 2}\left(1 - \frac{1}{(\rho_1 + \rho_2 - 2)^2}\right) > \Psi(\beta_1, \beta_2) \cdot \frac{(\rho_2 - 1.5)\rho_1}{\rho_1 + \rho_2 - 2} > \gamma_-^{-1}. \tag{D.25}$$

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 (D.25) to get

$$\rho_1 > \frac{(\rho_2 - 2)\sigma^2}{\Psi(\beta_1, \beta_2) \cdot \gamma_-(\rho_2 - 1.5) - 1}, \tag{D.26}$$

which gives the second statement of Proposition 3.4. We remark that condition (D.21) implies $\Psi(\beta_1, \beta_2) \cdot \gamma_-(\rho_2 - 1.5) > 1$, so (D.26) does not give a trivial bound. □

Next we state Proposition D.3, which gives precise upper and lower bounds on the data efficiency ratio for taskonomy.

Proposition D.3 (Labeled data efficiency)**.** *In the isotropic model, assume that $\rho_1, \rho_2 \geqslant 9$ and $\Psi(\beta_1, \beta_2) < (5(\rho_1 - 1))^{-1} + (5(\rho_2 - 1))^{-1}$. Then the data efficiency ratio $x^\star$ satisfies*

$$x_l \leqslant x^\star \leqslant \frac{1}{\rho_1 + \rho_2}\left(\frac{2}{(\rho_1 - 1)^{-1} + (\rho_2 - 1)^{-1} - 5\Psi(\beta_1, \beta_2)} + 1\right), \tag{D.27}$$

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 of Proposition D.3. Suppose we have reduced number of datapoints—xn_1 for task 1 and xn_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

$$a_1 = \frac{\rho_1(x\rho_1 + x\rho_2 - 1)}{x(\rho_1+\rho_2)^2}, \quad a_2 = \frac{\rho_2(x\rho_1 + \alpha\rho_2 - 1)}{x(\rho_1+\rho_2)^2},$$
$$a_3 = \frac{\rho_2}{(\rho_1+\rho_2)(x\rho_1 + x\rho_2 - 1)}, \quad a_4 = \frac{\rho_1}{(\rho_1+\rho_2)(x\rho_1 + x\rho_2 - 1)}.$$

Moreover, with high probability,

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

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

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

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

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

On the other hand, using Lemma C.1 we have whp,

$$L_i(\hat{\beta}_i^{\mathrm{STL}}) = \frac{\sigma^2}{\rho_i - 1}\left(1 + \mathrm{o}(1)\right), \quad i = 1, 2. \tag{D.29}$$

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

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

that is, $L_1(\hat{\beta}(\alpha)) + L_2(\hat{\beta}(\alpha))$ is larger than $L_1(\hat{\beta}_t^{\mathrm{STL}}) + L_2(\hat{\beta}_t^{\mathrm{STL}})$ even if we do not take into account the model shift bias terms $\delta_{\text{bias}}^{(i)}$.

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

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

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

We rewrite the inequality as

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

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

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

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

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

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

Thus the following inequality implies (D.30):

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

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

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

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

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

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

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

Thus the following inequality implies (D.31):

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

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

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

This gives a lower bound above x_l. □

D.3 Missing Proofs of Section 3.4

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

Proof of Proposition 3.5. Let

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

We now calculate $g(M_0)$. With the same arguments as in Lemma D.1 we can show that (D.5) holds. Moreover, if the parameters are chosen such that $p^{-1+c_0}\sigma^2\leqslant\kappa^2\leqslant p^{-\varepsilon_0-c_0}\sigma^2$ as in (D.4), we can simplify

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

with high probability for some constant $\varepsilon>0$. In fact, Lemma D.1 was proved assuming that $M=\mathrm{Id}$, but its proof can be easily extended to the case with general $M\in\mathcal{S}_\mu$ by using that $\mu_{\min}\leqslant\lambda_p(M)\leqslant\lambda_1(M)\leqslant\mu_{\max}$. We omit the details here.

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

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

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

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

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

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

where

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

By AM-GM inequality, we observe that

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

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

$$h(M_0) \leqslant \frac{\sigma^2}{\mu^2(\rho_1+\rho_2)a_1(M_0)}. \tag{D.36}$$

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

$$\begin{aligned} g(\mu\,\mathrm{Id}) &= \frac{\sigma^2}{\rho_1+\rho_2} \cdot \frac{1}{p} \operatorname{Tr}\left(\frac{1}{\mu^2 a_1(\mu\,\mathrm{Id}) + a_2(\mu\,\mathrm{Id})}\right) \cdot \left(1 + \mathrm{O}(p^{-\varepsilon})\right) \\ &\leqslant \frac{\sigma^2}{\mu^2(\rho_1+\rho_2)a_1(\mu\,\mathrm{Id})}. \end{aligned} \tag{D.37}$$

Combining (D.34), (D.35), (D.36) and (D.37), we conclude the proof. □

E Proof of Theorem 3.6

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

$$f(B; W_1, \ldots, W_t) = \sum_{i=1}^{t} \|XBW_i - Y_i\|^2. \tag{E.1}$$

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

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

where we denote $\mathcal{W} \in \mathbb{R}^{r\times t}$ as $\mathcal{W} = [W_1, W_2, \ldots, W_t]$. Then as in (B.6), we pick N independent samples of the training set for each task with $N \geqslant n^{1-\varepsilon_0}$, and use concentration to get the validation loss as

$$\widetilde{f}(\hat{B}; \mathcal{W}) = N\left[val(\mathcal{W}) + t\sigma^2\right] \cdot \left(1 + \mathrm{O}(p^{-(1-\varepsilon_0)/2+\varepsilon})\right). \tag{E.2}$$

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

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

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

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

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

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

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

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 $W_i^\top(\mathcal{W}\mathcal{W}^\top)^{-1}W_j$. Now we can write $\delta_{\text{bias}}(\mathcal{W})$ succinctly as

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

From this equation we can solve the minimizer optimally as $Q_0 = U_r U_r^\top$. On the other hand, let $\hat{\mathcal{W}}$ be the minimizer of $\widetilde{f}$, and denote $\hat{Q} := \hat{\mathcal{W}}^\top(\hat{\mathcal{W}}\hat{\mathcal{W}}^\top)^{-1}\hat{\mathcal{W}}$. We claim that $\hat{Q}$ satisfies

$$\|Q_0^{-1}\hat{Q} - \mathrm{Id}\,\| = \mathrm{o}(1) \quad \text{whp.} \tag{E.3}$$

In fact, if (E.3) does not hold, then using the condition $\lambda_{\min}((B^\star)^\top\Sigma B^\star) \gtrsim \sigma^2$ and that $\delta_{\text{var}}(\mathcal{W}) = \mathrm{O}(\sigma^2)$ by (C.16), we obtain that

$$val(\hat{\mathcal{W}}) + t\sigma^2 > (val(\mathcal{W}_0) + t\sigma^2)\cdot(1+\mathrm{o}(1)) \;\Rightarrow\; \widetilde{f}(\hat{B};\hat{\mathcal{W}}) > \widetilde{f}(\hat{B};\mathcal{W}_0),$$

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

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

$$\begin{aligned}
L(\hat{\beta}_t^{\text{MTL}}) &= \left\|\Sigma^{1/2}\left((B^\star\hat{\mathcal{W}}^\top)(\hat{\mathcal{W}}\hat{\mathcal{W}}^\top)^{-1}\hat{W}_t - \beta_2\right)\right\|^2 + \sigma^2\hat{W}_t^\top(\hat{\mathcal{W}}\hat{\mathcal{W}}^\top)^{-1}\hat{W}_t\cdot\mathrm{Tr}\left[\Sigma(X^\top X)^{-1}\right] \\
&= \left\|\Sigma^{1/2}\left(B^\star U_r U_r(t) - \beta_2\right)\right\|^2 + \mathrm{o}\left(\|B^\star\|^2\right) + \sigma^2\|U_r(t)\|^2\,\mathrm{Tr}\left[\Sigma(X^\top X)^{-1}\right]\cdot(1+\mathrm{o}(1)) \\
&= \left\|\Sigma^{1/2}\left(B^\star U_r U_r(t) - \beta_2\right)\right\|^2 + \frac{\sigma^2}{\rho-1}\|U_r(t)\|^2 + \mathrm{o}\left(\|B^\star\|^2 + \sigma^2\right),
\end{aligned}$$

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

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

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

F Proof of Lemma C.2 and Lemma C.3

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.

F.1 Notations and basic tools

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

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

Moreover, we assume that the fourth moments exist:

$$\mathbb{E}|\sqrt{n}z_{ij}^{(\alpha)}|^4 \leqslant C \tag{F.2}$$

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

$$0 \leqslant d_1 \leqslant \tau^{-1}, \quad 1+\tau \leqslant d_2 \leqslant \tau^{-1}. \tag{F.3}$$

Here the lower bound $1+\tau \leqslant d_2$ is to ensure that the sample covariance matrix $\mathcal{Q}_2$ is non-singular with high probability; see Lemma F.10 below.

We assume that Σ_1 and Σ_2 have eigendecompositions

$$\Sigma_1 = O_1\Lambda_1 O_1^\top,\;\; \Sigma_2 = O_2\Lambda_2 O_2^\top,\;\; \Lambda_1 = \mathrm{diag}(\sigma_1^{(1)},\ldots,\sigma_n^{(1)}),\;\; \Lambda_2 = \mathrm{diag}(\sigma_1^{(2)},\ldots,\sigma_N^{(2)}), \tag{F.4}$$

where the eigenvalues satisfy that

$$\tau^{-1} \geqslant \sigma_1^{(1)} \geqslant \sigma_2^{(1)} \geqslant \ldots \geqslant \sigma_p^{(1)} \geqslant 0, \quad \tau^{-1} \geqslant \sigma_1^{(2)} \geqslant \sigma_2^{(2)} \geqslant \ldots \geqslant \sigma_p^{(2)} \geqslant \tau. \tag{F.5}$$

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

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

where the singular values satisfy that

$$\tau \leqslant \sigma_p \leqslant \sigma_1 \leqslant \tau^{-1}. \tag{F.7}$$

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

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

We will use the following notion of stochastic domination, which was first introduced in [52] and subsequently used in many works on random matrix theory. It simplifies the presentation of the results and their proofs by systematizing statements of the form "ξ is bounded by ζ with high probability up to a small power of n".

Definition F.2 (Stochastic domination)**.** *(i) Let*

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

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

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

for large enough $n \geqslant n_0(\varepsilon, D)$, and we shall use the notation $\xi \prec \zeta$. If for some complex family ξ we have $|\xi| \prec \zeta$, then we will also write $\xi \prec \zeta$ or $\xi = \mathrm{O}_\prec(\zeta)$.

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

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

Lemma F.3 (Lemma 3.2 in [21])**.** *Let ξ and ζ be families of nonnegative random variables.*

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

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

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

Definition F.4 (Bounded support condition)**.** *We say a random matrix Z satisfies the bounded support condition with q, if*

$$\max_{i,j} |x_{ij}| \prec q. \tag{F.8}$$

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

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

$$(\mathcal{Q}_1 + \mathcal{Q}_2)^{-1} = \Sigma_2^{-1/2} V \left(\Lambda U^\top Z_1^\top Z_1 U \Lambda + V^\top Z_2^\top Z_2 V\right)^{-1} V^\top \Sigma_2^{-1/2}. \tag{F.9}$$

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

$$\mathcal{G}(z) := \left(\Lambda U^\top Z_1^\top Z_1 U \Lambda + V^\top Z_2^\top Z_2 V - z\right)^{-1}, \quad z \in \mathbb{C}_+, \tag{F.10}$$

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

Next we introduce a convenient self-adjoint linearization trick. It has been proved to be useful in studying the local laws of random matrices of the Gram type [22, 53, 54]. We define the following $(p+n)\times(p+n)$ self-adjoint block matrix, which is a linear function of Z_1 and Z_2:

$$H \equiv H(Z_1, Z_2) := \begin{pmatrix} 0 & \Lambda U^\top Z_1^\top & V^\top Z_2^\top \\ Z_1 U \Lambda & 0 & 0 \\ Z_2 V & 0 & 0 \end{pmatrix}. \tag{F.11}$$

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

$$G \equiv G(Z_1, Z_2, z) := \left[H(Z_1, Z_2) - \begin{pmatrix} zI_{p\times p} & 0 & 0 \\ 0 & I_{n_1\times n_1} & 0 \\ 0 & 0 & I_{n_2\times n_2} \end{pmatrix} \right]^{-1}, \quad z \in \mathbb{C}_+. \tag{F.12}$$

For simplicity of notations, we define the index sets

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

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

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

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 $(\mathcal{I}_2 \cup \mathcal{I}_3) \times \mathcal{I}_1$ 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 $Y_1 := Z_1 U \Lambda$, $Y_2 := Z_2 V$ and $W := (Y_1^\top, Y_2^\top)$. By Schur complement formula, one can find that

$$\mathcal{G}_L = \left(WW^\top - z\right)^{-1} = \mathcal{G}, \quad \mathcal{G}_{LR} = \mathcal{G}_{RL}^\top = \mathcal{G}W, \quad \mathcal{G}_R = z\left(W^\top W - z\right)^{-1}. \tag{F.13}$$

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

$$\begin{aligned} m(z) &:= \frac{1}{p}\sum_{i\in\mathcal{I}_1} G_{ii}(z), \quad m_1(z) := \frac{1}{p}\sum_{i\in\mathcal{I}_1} \sigma_i^2 G_{ii}(z), \\ m_2(z) &:= \frac{1}{n_1}\sum_{\mu\in\mathcal{I}_2} G_{\mu\mu}(z), \quad m_3(z) := \frac{1}{n_2}\sum_{\mu\in\mathcal{I}_3} G_{\mu\mu}(z). \end{aligned} \tag{F.14}$$

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 decomposition of W, where $\lambda_1 \geqslant \lambda_2 \geqslant \ldots \geqslant \lambda_p \geqslant 0 = \lambda_{p+1} = \ldots = \lambda_n$ are the eigenvalues, $\{\xi_k\}_{k=1}^p$ are the left-singular vectors, and $\{\zeta_k\}_{k=1}^n$ are the right-singular vectors. Then using (F.13), we get that for $i, j \in \mathcal{I}_1$ and $\mu, \nu \in \mathcal{I}_2 \cup \mathcal{I}_3$,

$$G_{ij} = \sum_{k=1}^p \frac{\xi_k(i)\xi_k^\top(j)}{\lambda_k - z}, \quad G_{\mu\nu} = z\sum_{k=1}^n \frac{\zeta_k(\mu)\zeta_k^\top(\nu)}{\lambda_k - z}, \quad G_{i\mu} = G_{\mu i} = \sum_{k=1}^p \frac{\sqrt{\lambda_k}\xi_k(i)\zeta_k^\top(\mu)}{\lambda_k - z}. \tag{F.15}$$

F.2 Local laws

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

$$\frac{1}{m_{2c}} = \frac{\gamma_n}{p}\sum_{i=1}^p \frac{\sigma_i^2}{z + \sigma_i^2 r_1 m_{2c} + r_2 m_{3c}} - 1, \quad \frac{1}{m_{3c}} = \frac{\gamma_n}{p}\sum_{i=1}^p \frac{1}{z + \sigma_i^2 r_1 m_{2c} + r_2 m_{3c}} - 1, \tag{F.16}$$

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

$$\gamma_n := \frac{p}{n}, \quad r_1 \equiv r_1(n) := \frac{n_1}{n}, \quad r_2 \equiv r_2(n) := \frac{n_2}{n}. \tag{F.17}$$

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

$$\Pi(z) := \begin{pmatrix} -(z + r_1 m_{2c}\Lambda^2 + r_2 m_{3c})^{-1} & 0 & 0 \\ 0 & m_{2c}(z) I_{n_1} & 0 \\ 0 & 0 & m_{3c}(z) I_{n_2} \end{pmatrix}. \tag{F.18}$$

In particular, the matrix limit of $\mathcal{G}(z)$ is given by $-(z+r_1m_{2c}\Lambda^2+r_2m_{3c})^{-1}$.

If $z=0$, then the equations (F.16) in are reduced to

$$r_1b_2+r_2b_3=1-\gamma_n,\quad b_2+\frac{1}{n}\sum_{i=1}^{p}\frac{\sigma_i^2b_2}{\sigma_i^2r_1b_2+(1-\gamma_n-r_1b_2)}=1. \tag{F.19}$$

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

$$f(b_2):=b_2+\frac{1}{n}\sum_{i=1}^{p}\frac{\sigma_i^2b_2}{\sigma_i^2b_2+(1-\gamma_n-r_1b_2)}$$

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 $f'(a)=\mathrm{O}(1)$ for $a\in[0,r_1^{-1}(1-\gamma_n)]$, and $f(1)>1$ if $1\leqslant r_1^{-1}(1-\gamma_n)$. Hence there exists a constant $\tau>0$, such that

$$r_1\tau\leqslant r_1b_2<\min\{(1-\gamma_n)-r_1\tau,r_1(1-\tau)\},\quad \tau<r_2b_3\leqslant 1-\gamma_n-r_1\tau. \tag{F.20}$$

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 F.5. *There exist constants $c_0,C_0>0$ depending only on τ in* (F.3)*,* (F.5)*,* (F.7) *and* (F.20) *such that the following statements hold. There exists a unique solution to* (F.16) *under the conditions*

$$|z|\leqslant c_0,\quad |m_{2c}(z)-m_{2c}(0)|+|m_{3c}(z)-m_{3c}(0)|\leqslant c_0. \tag{F.21}$$

Moreover, the solution satisfies

$$\max_{\alpha=2}^{3}|m_{\alpha c}(z)-m_{\alpha c}(0)|\leqslant C_0|z|. \tag{F.22}$$

The proof is a standard application of the contraction principle. For reader's convenience, we will include its proof in Appendix F.3.4. As a byproduct of the contraction mapping argument there, we also obtain the following stability result that will be useful for our proof of Theorem F.7 below.

Lemma F.6. *There exist constants $c_0,C_0>0$ depending only on τ in* (F.3)*,* (F.5)*,* (F.7) *and* (F.20) *such that the self-consistent equations in* (F.16) *are stable in the following sense. Suppose $|z|\leqslant c_0$ and $m_\alpha:\mathbb{C}_+\mapsto\mathbb{C}_+$, $\alpha=2,3$, are analytic functions of z such that*

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

Suppose they satisfy the system of equations

$$\frac{1}{m_2}+1-\frac{1}{n}\sum_{i=1}^{p}\frac{\sigma_i^2}{z+\sigma_i^2r_1m_2+r_2m_3}=\mathcal{E}_2,\quad \frac{1}{m_3}+1-\frac{1}{n}\sum_{i=1}^{p}\frac{1}{z+\sigma_i^2r_1m_2+r_2m_3}=\mathcal{E}_3, \tag{F.23}$$

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

$$\max_{\alpha=2}^{3}|m_\alpha(z)-m_{\alpha c}(z)|\leqslant C_0\delta(z). \tag{F.24}$$

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

$$\mathbf{D}:=\left\{z=E+\mathrm{i}\eta\in\mathbb{C}_+:|z|\leqslant(\log n)^{-1}\right\}. \tag{F.25}$$

The following theorem gives almost optimal estimates on the resolvent G, which are conventionally called local laws.

Theorem F.7. *Suppose Assumption F.1 holds, and Z_1,Z_2 satisfy the bounded support condition* (F.8) *for a deterministic parameter $q\equiv q(n)$ satisfying $n^{-1/2}\leqslant q\leqslant n^{-\phi}$ for some (small) constant $\phi>0$. Then there exists a sufficiently small constant $c_0>0$ such that the following* **anisotropic 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*

$$\left|\mathbf{u}^\top(G(z)-\Pi(z))\mathbf{v}\right|\prec q. \tag{F.26}$$

The proof of this theorem will be given in Section F.3. We now use it to complete the proof of Lemma C.2 and Lemma C.3.

Proof of Lemma C.2. In the setting of Lemma C.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 C.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 (F.9), we can write

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

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

$$\max_{1 \leqslant i \leqslant p} |(A\mathcal{R} - n^{-1} A \Sigma_2^{-1/2} V \Pi(0) V^\top \Sigma_2^{-1/2})_{ii}| \prec n^{-3/2}\|A\|, \tag{F.27}$$

where by (F.18), 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 (F.19). Thus from (F.27) we get that

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

This concludes (C.2) if we rename $r_1 b_2 \to a_1$ and $r_2 b_3 \to a_2$.

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 (C.3). This gives (C.1) using (C.2). $\square$

Proof of Lemma C.3. In the setting of Lemma C.3, we can write

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

Here again the n^2 factor disappears due to the choice of scaling. With (F.6), we can write the above 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 Cauchy's integral formula and Theorem F.7, we get that

$$\begin{aligned}\mathbf{v}^\top \mathcal{G}^2(0)\,\mathbf{v} = \frac{1}{2\pi \mathrm{i}}\oint_{\mathcal{C}} \frac{\mathbf{v}^\top \mathcal{G}(z)\,\mathbf{v}}{z^2}\mathrm{d}z &= \frac{1}{2\pi \mathrm{i}}\oint_{\mathcal{C}} \frac{\mathbf{v}^\top \Pi(z)\,\mathbf{v}}{z^2}\mathrm{d}z + \mathrm{O}_\prec(n^{-1/2}\|\beta\|^2) \\ &= \mathbf{v}^\top \Pi'(0)\,\mathbf{v} + \mathrm{O}_\prec(n^{-1/2}\|\beta\|^2),\end{aligned} \tag{F.28}$$

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

$$\mathbf{v}^\top \Pi'(0)\,\mathbf{v} = \mathbf{v}\,\frac{1 + r_1 m_{2c}'(0)\Lambda^2 + r_2 m_{3c}'(0)}{(r_1 m_{2c}(0)\Lambda^2 + r_2 m_{3c}(0))^2}\,\mathbf{v}, \tag{F.29}$$

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

By the implicit differentiation of (F.16), we obtain that

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

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

$$\begin{aligned}&\left(\frac{r_2}{a_2^2} - \frac{1}{n}\sum_{i=1}^p \frac{1}{(\sigma_i^2 a_1 + a_2)^2}\right) a_3 - \left(\frac{1}{n}\sum_{i=1}^p \frac{\sigma_i^2}{(\sigma_i^2 a_1 + a_2)^2}\right) a_4 = \frac{1}{n}\sum_{i=1}^p \frac{1}{(\sigma_i^2 a_1 + a_2)^2}, \\ &\left(\frac{r_1}{a_1^2} - \frac{1}{n}\sum_{i=1}^p \frac{\sigma_i^4}{(\sigma_i^2 a_1 + a_2)^2}\right) a_4 - \left(\frac{1}{n}\sum_{i=1}^p \frac{\sigma_i^2}{(\sigma_i^2 a_1 + a_2)^2}\right) a_3 = \frac{1}{n}\sum_{i=1}^p \frac{\sigma_i^2}{(\sigma_i^2 a_1 + a_2)^2}.\end{aligned} \tag{F.30}$$

Then by (F.28) and (F.29), we get

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

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

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

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

$$\max_{i,j} \mathbb{E}|\sqrt{n} z_{ij}^{(\alpha)}|^a = \mathrm{O}(1), \quad \alpha = 1, 2, \tag{F.31}$$

for some fixed $a > 4$. Then (F.26) *holds for $q = n^{2/a - 1/2}$ on an event with probability* $1 - \mathrm{o}(1)$.

Proof of Corollary F.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 $\widetilde{Z}_1$ and $\widetilde{Z}_2$, with entries

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

By the moment conditions (F.31) and a simple union bound, we have

$$\mathbb{P}(\widetilde{Z}_1 = Z_1, \widetilde{Z}_2 = Z_2) = 1 - \mathrm{O}(n^{-a\varepsilon}). \tag{F.32}$$

Using (F.31) and integration by parts, it is easy to verify that

$$|\mathbb{E}\widetilde{z}_{ij}^{(\alpha)}| = \mathrm{O}(n^{-2-\varepsilon}), \quad \mathbb{E}|\widetilde{z}_{ij}^{(\alpha)}|^2 = n^{-1} + \mathrm{O}(n^{-2-\varepsilon}), \quad \alpha = 1, 2, . \tag{F.33}$$

Then we can centralize and rescale $\widetilde{Z}_1$ and $\widetilde{Z}_2$ as $\widehat{Z}_\alpha := (\widetilde{Z}_\alpha - \mathbb{E}\widetilde{Z}_\alpha)/(\mathbb{E}|\widetilde{z}_{11}^{(\alpha)}|^2)^{1/2}$, $\alpha = 1, 2$. Now $\widehat{Z}_1$ and $\widehat{Z}_2$ satisfy the assumptions in Theorem F.7 with $q = n^{-c_a + \varepsilon}$, and (F.26) gives that

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

Then using (F.33) and (F.37) below, we obtain that

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

where we also used the bound $\|\mathbb{E}\widetilde{Z}_\alpha\| = \mathrm{O}(n^{-1-\varepsilon})$ by (F.33). This shows that (F.26) also holds for $G(\widetilde{Z}_1, \widetilde{Z}_2, z)$ with $q = n^{-c_a + \varepsilon}$, and hence concludes the proof by (F.32). □

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

F.3 Proof of Theorem F.7

The main difficulty for the proof of Theorem F.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

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

In this case, the problem is reduced to proving the anisotropic local law for G with $U = \mathrm{Id}$ and $V = \mathrm{Id}$, such that the entries of Y_1 and Y_2 are independent. This can be handled using the standard resolvent methods as in e.g. [21, 37, 55]. To go from the Gaussian case to the general X case, we will adopt a continuous self-consistent comparison argument developed in [22].

For the case $U = \mathrm{Id}$ and $V = \mathrm{Id}$, we need to deal with the following resolvent:

$$G_0(z) := \begin{pmatrix} -z I_{p \times p} & \Lambda Z_1^\top & Z_2^\top \\ Z_1 \Lambda & -I_{n_1 \times n_1} & 0 \\ Z_2 & 0 & -I_{n_2 \times n_2} \end{pmatrix}^{-1}, \quad z \in \mathbb{C}_+, \tag{F.34}$$

and prove the following result.

Proposition F.9. *Suppose Assumption F.1 holds, and Z_1, Z_2 satisfy the bounded support condition* (F.8) *with $q = n^{-1/2}$. Suppose U and V are identity. Then the estimate* (F.26) *holds for $G_0(z)$.*

In Section F.3.1, we collect some a priori estimates and resolvent identities that will be used in the proof of Theorem F.7 and Proposition F.9. Then in Section F.3.2 we give the proof of Proposition F.9, which concludes Theorem F.7 for i.i.d. Gaussian Z_1 and Z_2. Finally, in Section F.3.3, we describe how to extend the result in Theorem F.7 from the Gaussian case to the case with generally distributed entries of Z_1 and Z_2. In the proof, we always denote the spectral parameter by $z = E + \mathrm{i}\eta$.

F.3.1 Basic estimates

The estimates in this section work for general G, that is, we do not require U and V to be identity. First, note that $Z_1^\top Z_1$ (resp. $Z_2^\top Z_2$) is a standard sample covariance matrix, and it is well-known that its nonzero eigenvalues are all inside the support of the Marchenko-Pastur law $[(1-\sqrt{d_1})^2, (1+\sqrt{d_1})^2]$ (resp. $[(1-\sqrt{d_2})^2, (1+\sqrt{d_2})^2]$) with probability $1 - \mathrm{o}(1)$ [50]. In our proof, we shall need a slightly stronger probability bound, which is given by the following lemma. Denote the eigenvalues of $Z_1^\top Z_1$ and $Z_2^\top Z_2$ by $\lambda_1(Z_1^\top Z_1) \geqslant \cdots \geqslant \lambda_p(Z_1^\top Z_1)$ and $\lambda_1(Z_2^\top Z_2) \geqslant \cdots \geqslant \lambda_p(Z_2^\top Z_2)$.

Lemma F.10. *Suppose Assumption F.1 holds, and Z_1, Z_2 satisfy the bounded support condition* (F.8) *for some deterministic parameter $q \equiv q(n)$ satisfying $n^{-1/2} \leqslant q \leqslant n^{-\phi}$ for some (small) constant $\phi > 0$. Then for any constant $\varepsilon > 0$, we have with high probability,*

$$\lambda_1(Z_1^\top Z_1) \leqslant (1+\sqrt{d_1})^2 + \varepsilon, \tag{F.35}$$

and

$$(1-\sqrt{d_2})^2 - \varepsilon \leqslant \lambda_p(Z_2^\top Z_2) \leqslant \lambda_1(Z_2^\top Z_2) \leqslant (1+\sqrt{d_2})^2 + \varepsilon. \tag{F.36}$$

Proof. This lemma essentially follows from [21, Theorem 2.10], although the authors considered the case with $q \prec n^{-1/2}$ only. The results for larger q follows from [56, Lemma 3.12], but only the bounds for the largest eigenvalues are given there in order to avoid the issue with the smallest eigenvalue when d_2 is close to 1. However, under the assumption (F.3), the lower bound for the smallest eigenvalue follows from the same arguments as in [56]. Hence we omit the details. □

With this lemma, we can obtain the following a priori estimate on the resolvent $G(z)$ for $z \in \mathbf{D}$.

Lemma F.11. *Suppose the assumptions of Lemma F.10 holds. Then there exists a constant $C > 0$ such that the following estimates hold uniformly in $z, z' \in \mathbf{D}$ with high probability:*

$$\|G(z)\| \leqslant C, \tag{F.37}$$

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

$$\left|\mathbf{u}^\top \left[G(z) - G(z')\right] \mathbf{v}\right| \leqslant C|z - z'|. \tag{F.38}$$

Proof. As in (F.15), we let $\{\lambda_k\}_{1 \leqslant k \leqslant p}$ be the eigenvalues of $WW^\top$. By Lemma F.10 and the assumption (F.3), we obtain that $\lambda_p \geqslant \lambda_p(Z_2^\top Z_2) \gtrsim 1$, which further implies the estimate that $\inf_{z \in \mathbf{D}} \min_{1 \leqslant k \leqslant p} |\lambda_k - z| \gtrsim 1$. Together with (F.15), we obtain (F.37) and (F.38). □

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

Definition F.12 (Minors)**.** *For any $(p+n) \times (p+n)$ matrix $\mathcal{A}$ and $\mathbb{T} \subseteq \mathcal{I}$, we define the minor $\mathcal{A}^{(\mathbb{T})} := (\mathcal{A}_{\mathfrak{a}\mathfrak{b}} : \mathfrak{a}, \mathfrak{b} \in \mathcal{I} \setminus \mathbb{T})$ as the $(p+n-|\mathbb{T}|) \times (p+n-|\mathbb{T}|)$ matrix obtained by removing all rows and columns indexed by $\mathbb{T}$. Note that we keep the names of indices when defining $\mathcal{A}^{(\mathbb{T})}$, i.e. $(\mathcal{A}^{(\mathbb{T})})_{ab} = \mathcal{A}_{ab}$ for $a, b \notin \mathbb{T}$. Correspondingly, we define the resolvent minor as (recall* (F.13)*)*

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

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 (F.14)*. For convenience, we will adopt the convention that for any minor $\mathcal{A}^{(T)}$ defined as above, $\mathcal{A}_{ab}^{(T)} = 0$ if $a \in \mathbb{T}$ or $b \in \mathbb{T}$. Moreover, we will abbreviate $(\{a\}) \equiv (a)$ and $(\{a, b\}) \equiv (ab)$.*

Lemma F.13. *We have the following resolvent identities.*

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

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

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

$$G_{i\mathfrak{a}} = -G_{ii}\left(WG^{(i)}\right)_{i\mathfrak{a}}, \quad G_{\mu\mathfrak{b}} = -G_{\mu\mu}\left(W^\top G^{(\mu)}\right)_{\mu\mathfrak{b}}. \tag{F.40}$$

(iii) For $\mathfrak{a} \in \mathcal{I}$ and $\mathfrak{b}, \mathrm{fc} \in \mathcal{I} \setminus \{\mathfrak{a}\}$,

$$G^{(\mathfrak{a})}_{\mathfrak{b}\mathfrak{c}} = G_{\mathfrak{b}\mathfrak{c}} - \frac{G_{\mathfrak{b}\mathfrak{a}}G_{\mathfrak{a}\mathfrak{c}}}{G_{\mathfrak{a}\mathfrak{a}}}, \quad \frac{1}{G_{\mathfrak{b}\mathfrak{b}}} = \frac{1}{G^{(\mathfrak{a})}_{\mathfrak{b}\mathfrak{b}}} - \frac{G_{\mathfrak{b}\mathfrak{a}}G_{\mathfrak{a}\mathfrak{b}}}{G_{\mathfrak{b}\mathfrak{b}}G^{(\mathfrak{a})}_{\mathfrak{b}\mathfrak{b}}G_{\mathfrak{a}\mathfrak{a}}}. \tag{F.41}$$

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

The following lemma gives large deviation bounds for bounded supported random variables.

Lemma F.14 (Lemma 3.8 of [57])**.** *Let (x_i), (y_j) be independent families of centered and independent random variables, and (A_i), (B_{ij}) be families of deterministic complex numbers. Suppose the entries x_i, y_j have variances at most n^{-1} and satisfy the bounded support condition (F.8) with $q \leqslant n^{-\phi}$ for some constant $\phi > 0$. Then we have the following bound:*

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

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

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 $\sqrt{n}y_j$ exist in the sense of (B.1)*, then we have stronger bounds*

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

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

F.3.2 Entrywise local law

The main goal of this subsection is to prove the following entrywise local law. The anisotropic local law (F.26) then follows from the entrywise local law combined with a polynomialization method as we will explain later. Recall that in the setting of Proposition F.9, we have $q = n^{-1/2}$ and

$$W = (\Lambda Z_1^\top, Z_2^\top). \tag{F.42}$$

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

$$\max_{\mathfrak{a},\mathfrak{b}\in\mathcal{I}} |(G_0)_{\mathfrak{a}\mathfrak{b}}(z) - \Pi_{\mathfrak{a}\mathfrak{b}}(z)| \prec n^{-1/2}. \tag{F.43}$$

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

Step 1: Large deviations estimates. In this step, we prove some (almost) optimal large deviation estimates on the off-diagonal entries of G, and on the following Z variables. In analogy to [57, Section 3] and [22, Section 5], we introduce the Z variables

$$Z^{(\mathbb{T})}_{\mathfrak{a}} := (1 - \mathbb{E}_{\mathfrak{a}})\big(G^{(\mathbb{T})}_{\mathfrak{a}\mathfrak{a}}\big)^{-1}, \quad \mathfrak{a} \notin \mathbb{T},$$

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

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

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

For simplicity, we introduce the random error $\Lambda_o := \max_{\mathfrak{a} \ne \mathfrak{b}} \left| G_{\mathfrak{a}\mathfrak{a}}^{-1} G_{\mathfrak{a}\mathfrak{b}} \right|$. The following lemma gives the desired large deviations estimates on Λ_o and the Z variables.

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

$$\Lambda_o + \max_{\mathfrak{a} \in \mathcal{I}} |Z_{\mathfrak{a}}| \prec n^{-1/2}. \tag{F.46}$$

Proof. Note that for any $\mathfrak{a} \in \mathcal{I}$, $H^{(\mathfrak{a})}$ and $G^{(\mathfrak{a})}$ also satisfies the assumptions for Lemma F.11. Hence (F.37) and (F.38) also hold for $G^{(\mathfrak{a})}$. Now applying Lemma F.14 to (F.44) and (F.45), and using the a priori bound (F.37), we get that for any $i \in \mathcal{I}_1$,

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

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

$$\sum_{\nu \in \mathcal{I}_2 \cup \mathcal{I}_3} \left| G_{\mu\nu}^{(i)} \right|^2 \leqslant \sum_{\mathfrak{a} \in \mathcal{I}} \left| G_{\mu\mathfrak{a}}^{(i)} \right|^2 = \left[G^{(i)} (G^{(i)})^* \right]_{\mu\mu} = \mathrm{O}(1). \tag{F.47}$$

Similarly, applying Lemma F.14 to Z_μ and Z_ν in (F.45) and using (F.37), we obtain the same bound. we have

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

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

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

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

Note that comibining (F.37) and (F.46), we immediately conclude (F.43) for $\mathfrak{a} \ne \mathfrak{b}$.

Step 2: Self-consistent equations. This is the key step of the proof for Proposition F.15, which derives approximate self-consistent equations safisfised by $m_2(z)$ and $m_3(z)$. More precisely, we will show that $(m_2(z), m_3(z))$ satisfies (F.23) for some small error $|\mathcal{E}_{2,3}| \prec n^{-1/2}$. Then in Step 3 we will apply Lemma F.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

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

Note that by (F.22), we have $|m_{2c} + b_2| \lesssim (\log n)^{-1}$ and $|m_{3c} + b_3| \lesssim (\log n)^{-1}$. Together with (F.16), (F.20) and (F.7), we obtain the following basic estimates

$$|m_{2c}| \sim |m_{3c}| \sim 1, \quad |z + \sigma_i^2 r_1 m_{2c} + r_2 m_{3c}| \sim 1, \quad |1 + \gamma_n m_c| \sim |1 + \gamma_n m_{1c}| \sim 1, \tag{F.50}$$

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 (F.50) into (F.18), we get

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

Then we claim the following result.

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

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

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

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

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

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

where we recall Definition F.12, and

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

By (F.41) we can bound that

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

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

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

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

$$|\varepsilon_i| + |\varepsilon_\mu| \prec n^{-1/2}. \tag{F.57}$$

With (F.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 (F.53), (F.57) and (F.46), we obtain that

$$\mathbf{1}(\Xi) G_{ii} = \mathbf{1}(\Xi)\left[-\frac{1}{z + \sigma_i^2 r_1 m_2 + r_2 m_3} + \mathrm{O}_\prec\left(n^{-1/2}\right)\right]. \tag{F.58}$$

Plugging it into the definitions of m and m_1 in (F.14), we get

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

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

As a byproduct, we obtain from these two estimates that

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

Together with (F.50), we get that

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

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

$$\mathbf{1}(\Xi)\left(G_{\mu\mu} + \frac{1}{1+\gamma_n m_1}\right) = \mathrm{O}_\prec(n^{-1/2}), \quad \mathbf{1}(\Xi)\left(G_{\nu\nu} + \frac{1}{1+\gamma_n m}\right) = \mathrm{O}_\prec(n^{-1/2}). \tag{F.63}$$

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

$$\mathbf{1}(\Xi)\left(m_2 + \frac{1}{1+\gamma_n m_1}\right) = \mathrm{O}_\prec\left(n^{-1/2}\right), \quad \mathbf{1}(\Xi)\left(m_3 + \frac{1}{1+\gamma_n m}\right) = \mathrm{O}_\prec\left(n^{-1/2}\right). \tag{F.64}$$

Finally, plugging (F.59) and (F.60) into (F.64), we conclude (F.52). □

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

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

Once we know (F.65), then by (F.22) and (F.38), we get $\max_{\alpha=2}^3 |m_{\alpha c}(z) - m_{\alpha c}(0)| = \mathrm{O}((\log n)^{-1})$ and $\max_{\alpha=2}^3 |m_\alpha(z) - m_\alpha(0)| = \mathrm{O}((\log n)^{-1})$ with high probability for all $z \in \mathbf{D}$. Together with (F.65), we obtain that

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

and

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

The condition (F.66) shows that Ξ holds with high probability, and the condition (F.67) verifies the condition (F.21) of Lemma F.6. Then applying Lemma F.6 to (F.52), we obtain that

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

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

$$\max_{\mathfrak{a}\in\mathcal{I}} |G_{\mathfrak{a}\mathfrak{a}}(z) - \Pi_{\mathfrak{a}\mathfrak{a}}(z)| \prec n^{-1/2}. \tag{F.69}$$

Together with the off-diagonal estimate in (F.46), we conclude (F.43). □

Now we give the proof of (F.65).

Proof of (F.65). By (F.15), we get

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

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

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

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

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

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

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

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

$$c \leqslant \omega_2 \leqslant 1, \quad c \leqslant \omega_3 \leqslant 1, \quad \text{with high probability.} \tag{F.71}$$

Also one can verify from (F.70) that (ω_2, ω_3) satisfy approximately the same equations as (F.19):

$$r_1\omega_2 + r_2\omega_3 = 1 - \gamma_n + \mathrm{O}_\prec(n^{-1/2}), \quad f(\omega_2) = 1 + \mathrm{O}_\prec(n^{-1/2}). \tag{F.72}$$

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

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

Proof of Proposition F.9. With (F.43), one can use the polynomialization method in [21, Section 5] to get the anisotropic local law (F.26) for G_0 with $q = n^{-1/2}$. The proof is exactly the same, except for some minor differences in notations, so we omit the details. ☐

F.3.3 Anisotropic local law

In this subsection, we finish the proof of Theorem F.7 for a general X satisfying the bounded support condition (F.8) with $q \leqslant n^{-\phi}$ for some constant $\phi > 0$. Proposition F.9 implies that (F.26) holds for 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 satisfying the assumptions in Theorem F.7,

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

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

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

$$\prod_{i \in \mathcal{I}_1} \prod_{\mu \in \mathcal{I}_2 \cup \mathcal{I}_3} \rho_{\mu i}^\theta (\mathrm{d}Z_{\mu i}^\theta). \tag{F.73}$$

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

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

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

We shall prove (F.26) through interpolation matrices Z^θ between Z^0 and Z^1. We have see that (F.26) holds for Z^0 by Proposition F.9. Using (F.73) and fundamental calculus, we get the following basic interpolation formula: for $F : \mathbb{R}^{n\times p} \to \mathbb{C}$,

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

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

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

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

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

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

$$\mathbb{E}\left|G_{\mathbf{uv}}(Z^1, z) - \Pi_{\mathbf{uv}}(z)\right|^p \leqslant (n^\varepsilon q)^p.$$

Together with Markov's inequality, we conclude (F.26). Underlying the proof of (F.75) is an expansion approach, which is very similar to the ones for Lemma 7.10 of [22] and Lemma 6.11 of [37]. So we omit the details.

F.3.4 Proofs of Lemma F.5 and Lemma F.6

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

Proof of Lemma F.5. One can check that the equations in (F.16) are equivalent to the following ones:

$$r_1 m_{2c} = -(1 - \gamma_n) - r_2 m_{3c} - z \left(m^{-1}_{3c} + 1\right), \quad g_z(m_{3c}(z)) = 1, \qquad \text{(F.76)}$$

where

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

We first show that there exists a unique solution $m_{3c}(z)$ to the equation $g_z(m_{3c}(z)) = 1$ under the conditions in (F.21), and the solution satisfies (F.22). Now we abbreviate $\varepsilon(z) := m_{3c}(z) - m_{3c}(0)$, and from (F.76) we obtain that

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

which implies

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

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

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

Then (F.77) defines a mapping $h : \mathbb{C} \to \mathbb{C}$, which maps $\varepsilon^{(k)}$ to $\varepsilon^{(k+1)} = h(\varepsilon^{(k)})$.
With direct calculation, one can get the derivative

$$g'_z(m_{3c}(0)) = -1 - \frac{1}{n}\sum_{i=1}^{p} \frac{\sigma_i^2(1 - \gamma_n) - z\left[1 - \sigma_i^2\left(2m^{-1}_{3c}(0) + 1\right)\right]}{\left[z - \sigma_i^2(1 - \gamma_n) + (1 - \sigma_i^2)r_2 m_{3c}(0) - \sigma_i^2 z\left(m^{-1}_{3c}(0) + 1\right)\right]^2}.$$

Then it is easy to check that there exist constants $\widetilde{c}, \widetilde{C} > 0$ depending only on τ in (F.7) and (F.20) such that

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

and

$$\left|\frac{g_z(m_{3c}(0) + \varepsilon_1) - g_z(m_{3c}(0) + \varepsilon_2) - g'_z(m_{3c}(0))(\varepsilon_1 - \varepsilon_2)}{g'_z(m_{3c}(0))}\right| \leqslant \widetilde{C}|\varepsilon_1 - \varepsilon_2|^2, \qquad \text{(F.79)}$$

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

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

as long as $r \leqslant \delta$ and $|z| \leqslant c_\delta$ for some constant $c_\delta > 0$ depending only on $\widetilde{C}$ and δ. Now it suffices to prove that h restricted to B_r is a contraction, which then implies that $\varepsilon := \lim_{k\to\infty} \varepsilon^{(k)}$ exists and $m_{3c}(0) + \varepsilon$ is a unique solution to the second equation of (F.76) subject to the condition $\|\varepsilon\|_\infty \leqslant r$. From the iteration relation (F.77), using (F.78) one can readily check that

$$\varepsilon^{(k+1)} - \varepsilon^{(k)} = h(\varepsilon^{(k)}) - h(\varepsilon^{(k-1)}) \leqslant \widetilde{C}|\varepsilon^{(k)} - \varepsilon^{(k-1)}|^2. \tag{F.80}$$

Hence as long as r is chosen to be sufficiently small such that $2r\widetilde{C} \leqslant 1/2$, then h is indeed a contraction mapping on B_r, which proves both the existence and uniqueness of the solution $m_{3c}(z) = m_{3c}(0) + \varepsilon$, if we choose c_0 in (F.21) as $c_0 = \min\{c_\delta, r\}$. After obtaining $m_{3c}(z)$, we can then find $m_{2c}(z)$ using the first equation in (F.76).

Note that with (F.79) and $\varepsilon^{(0)} = 0$, we get from (F.77) that $|\varepsilon^{(1)}| \leqslant \widetilde{C}|z|$. With the contraction mapping, we have the bound

$$|\varepsilon| \leqslant \sum_{k=0}^{\infty} |\varepsilon^{(k+1)} - \varepsilon^{(k)}| \leqslant 2\widetilde{C}|z|. \tag{F.81}$$

This gives the bound (F.22) for $m_{3c}(z)$. Using the first equation in (F.76), we immediately obtain the bound $r_1|m_{2c}(z) - m_{2c}(0)| \leqslant C|z|$. This gives (F.22) 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 (F.16) and treat $m_{2c}(z)$ as the solution to the following equation:

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

Then with similar arguments as above between (F.76) and (F.81), we can conclude (F.22) for $m_{2c}(z)$. This concludes the proof of Lemma F.5. □

Proof of Lemma F.6. Under (F.21), we can obtain equation (F.76) approximately up to some small error

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

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

G Missing Details from the Experiments

G.1 Synthetic Settings

In Figure 1 (c), we plot the test error of the target task for $n_2 = 4p$ and n_1 ranging from p to $20p$.

G.2 Image and Text Classification Settings

Note: For text classification tasks, the source task training data size ranges from 500 to 1,500 and target task training data size is 1000; For ChestX-ray14, the training data size is 10,000.

Task similarity. We validate that MTL performs better when the source task is more similar to the target task. We show the result on the sentiment analysis tasks. For a target task, we manually select a similar task and a dissimilar task based on prior knowledge. Figure 2a confirms the result. Recall that Section 3.3 shows that increasing the data size of the source task does not always improve the performance of MTL for the target task. In Figure 2b, we show that for source task MR and target task SST, there is a transition from positive to negative transfer as we increase the data size of the source task. When the source task data size is particularly large compared to the target task, we show that applying the covariance alignment algorithm results in more significant gains. In Figure 2c, we observe that the benefit from aligning task covariances becomes more significant for LSTM and MLP as we increase the number of datapoints of the source task.

[1]

[1]http://nlp.stanford.edu/data/wordvecs/glove.6B.zip

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.

```
Divide (X_1, Y_1) randomly into S batches: (x^(1), y^(1)), ..., (x^(S), y^(S)).
for i = 1, ..., S do
    for j = 1, ..., T do
        Update B, W_1, W_2 using the training data {x^(k), x^(k)}_{k=1}^i and (X_2, Y_2).
    end for
    Let a_i = ĝ(B; W_2) be the validation accuracy.
    if a_i < a_{i-1} or a_i > τ then
        break
    end if
end for
```

(a) Task pair TREC and CR

(b) Task pair MR and SST

Figure 3: The performance of aligning task covariances depends on data size. As the ratio between source task data size and target task data size increases, the performance improvement from aligning task covariances increases.