

Tight Bounds for Multi-Task Learning in High-Dimensional Regression with Covariate and Model Shifts

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1 Introduction

Multi-task learning that is applied on heterogenous data can often result in suboptimal models (or negative transfer in more technical terms). In a previous work [4], we identified three factors that help determine when multi-task learning works, and when it doesn't. In this work, we zoom in to the task covariance part of [4] to further understand when multi-task learning works under covariate and model shifts. By using random matrix theory, we can explain several phenomena that are not explained by the techniques of [4]. These are achieved through tight generalization bounds established in the high-dimensional linear regression setting.

- (i) **Negative transfer:** we establish a fundamental limit that is caused by model shift. Moreover, this cannot be corrected via changing the model capacity or reweighting the tasks.
- (ii) **De-noising effect of MTL:** we show that multi-task transfer has a de-noising effect of reducing the variance of the estimator. When this variance reduction effect is bigger than the bias caused by model shift, we get positive transfer.
- (iii) **Covariate shift affects the rate of transfer:** we further show that covariate shift can control the rate in which transfer occurs.

2 Problem Setup

In the multi-task learning (MTL) problem, we are given the input of k tasks $(X_1, Y_1), (X_2, Y_2), \dots, (X_k, Y_k)$. We use a shared body (module) $B \in \mathbb{R}^{p \times r}$ for all tasks and a separate head (module) $\{A_i \in \mathbb{R}^r\}_{i=1}^k$ for each task. This corresponds to minimizing the following optimization objective.

$$f(B; A_1, \dots, A_k) = \sum_{i=1}^k \|X_i B A_i - Y_i\|^2. \quad (2.1)$$

Note that we consider the natural parameterization without reweighting the tasks above. The shared body B plays an important role because it allows information transfer between different task data. There are two ways to ensure the sharing of information between tasks.

- Adding a regularization over B , e.g. [2, 3].
- Controlling the capacity r of B , e.g. [1, 4]. Moreover, [1] observed that controlling the capacity can outperform the implicit capacity control of adding regularization over B .

Data generation. We shall assume that each task data follows a linear model. For every $1 \leq i \leq k$, we assume that

$$Y_i = X_i \beta_i + \varepsilon_i,$$

where $\beta_i \in \mathbb{R}^p$ is the model parameter for the i -th task. Each row of $X_i \in \mathbb{R}^{n_i \times p}$ is assumed to be drawn i.i.d. from a fixed distribution with covariance matrix Σ_i . We assume that for every row x of X_i , we have

$$\mathbb{E}[xx^\top] = \Sigma_i.$$

We also write $x = \Sigma_i^{1/2} z_i$, where z_i is a random vector with mean 0 and variance 1.

Objectives. We will designate the k -th task as the target. Our goal is to come up with an estimator $\hat{\beta}$ to provide accurate predictions for the target task, provided with the other auxiliary task data. Concretely, we focus on two objectives.

- Estimation error for the target model β_t : we consider their distance

$$e(\hat{\beta}) := \mathbb{E}_{\varepsilon_i, \forall 1 \leq i \leq k} \left[\left\| \hat{\beta} - \beta_t \right\|^2 \right].$$

- Test error for the target task:

$$\begin{aligned} te(\hat{\beta}) &:= \mathbb{E}_{x \sim \Sigma_k} \left[\mathbb{E}_{\varepsilon_i, \forall 1 \leq i \leq k} \left[(x^\top \hat{\beta} - x^\top \beta_t)^2 \right] \right] \\ &= \mathbb{E}_{\varepsilon_i, \forall 1 \leq i \leq k} \left[(\hat{\beta} - \beta_t)^\top \Sigma_k (\hat{\beta} - \beta_t) \right]. \end{aligned}$$

2.1 Hypothesis

Our hypothesis is that the heterogeneity among the multiple tasks can be categorized into two classes, *covariate shift* and *model shift*. We consider two natural questions within each category.

- How does covariate shift affect the rate of information transfer? For example, is it better to have the same covariance matrix or not?
- Under model shift, when do we get positive vs. negative transfer? How does the type of transfer depend on the number of data points, the distance of the task models etc?

2.1.1 Covariate Shift

A natural setting is when the covariance matrices Σ_i are different across tasks, i.e. having different spectrum or singular vectors. This is also known as covariate shift in the literature. **Our hypothesis is that the covariate shift can slow down the convergence of learning the true θ as a function of the number of data points.** A special case of this setting is that the single-task models are the same across all the tasks, i.e. $\beta_i = \beta$, for all $1 \leq i \leq k$.

Since all tasks share the same underlying model β , we use a simplified objective as follows.

$$f(w) = \sum_{i=1}^k \|X_i w - Y_i\|^2. \quad (2.2)$$

Equation (2.2) is simplified from equation (2.1) by setting A_i to be 1 for all tasks.

Proposition 2.1. *Suppose that $n > p$. When there is no model shift, adding the source task data always reduces the estimation error and the test error for the target task, i.e.*

$$e(\hat{\beta}_{s,t}) \leq e(\hat{\beta}_t), \text{ and} \quad (2.3)$$

$$te(\hat{\beta}_{s,t}) \leq te(\hat{\beta}_t) \quad (2.4)$$

Proof. Equation (2.3) is simply because

$$e(\hat{\beta}_{s,t}) = \text{Tr} [(X_1^\top X_1 + X_2^\top X_2)^{-1}] \leq \text{Tr} [(X_1^\top X_1)^{-1}] = e(\hat{\beta}_t).$$

Equation (2.4) follows because

$$\begin{aligned} te(\hat{\beta}_{s,t}) &= \text{Tr} [(X_1^\top X_1 + X_2^\top X_2)^{-1} \Sigma_2] = \text{Tr} \left[\left(\Sigma_2^{-1/2} X_1^\top X_1 \Sigma_2^{-1/2} + \Sigma_2^{-1/2} X_2^\top X_2 \Sigma_2^{-1/2} \right)^{-1} \right] \\ &\leq \text{Tr} \left[\left(\Sigma_2^{-1/2} X_2^\top X_2 \Sigma_2^{-1/2} \right)^{-1} \right] = \text{Tr} [(X_2^\top X_2)^{-1} \Sigma_2] = te(\hat{\beta}_t). \end{aligned}$$

□

2.1.2 Model Shift

In addition to covariate shift, in general the single-task models can also be different across different tasks. **Here the hypothesis is that the optimal B is captured by a low-rank approximation of the single-task models.**

2.2 The High-Dimensional Setting

setup motivation and notations We would like to get insight on how covariate and model shifts affect the rate of transfer. For the case of two tasks, we can get precise rates using random matrix theory. For the sake of clarity, we call task 1 the source task and task 2 the target task, i.e. $\beta_1 = \beta_s$ and $\beta_2 = \beta_t$.

3 Negative Transfer: The Limit Caused by Model Shifts

Next we describe lower bounds that guarantee negative transfer to complement Theorem 4.1.

Theorem 3.1 (Negative transfer under model shift). *In the setting of Theorem 4.1, we have $te(\hat{\beta}_{s,t}) \geq te(\hat{\beta}_t)$ when*

$$\Delta_{var} \leq \left(1 - 4\sqrt{\frac{p}{n_1}} - \frac{2p}{n_1} \right) \Delta_\beta$$

In the special case that $\beta_s - \beta_t$ is i.i.d. with mean 0 and variance d^2 and $\Sigma_1 = \text{Id}$, we can get a tighter lower bound that guarantees negative transfer when

$$\Delta_{var} \leq \left(1 - \sqrt{\frac{p}{n_1}} \right)^4 \Delta_\beta. \quad (3.1)$$

We describe examples based on Theorem 4.1 and Theorem 3.1 to show several conceptual insights.

Example 3.2 (The effect of d , the distance of task models). We consider a simple setting where $\Sigma_1 = \text{Id}$. Suppose that $\beta_s - \beta_t$ is a vector with mean zero and variance d^2 . Hence the task models have distance $d^2 \cdot p$ in expectation.

We first consider $\Sigma_2 = \text{Id}$. In this case, we can simplify Δ_β as follows

$$\Delta_\beta := d^2 \cdot \sum_{i=1}^p \frac{(1 + a_3)\lambda_i^2 + a_4\lambda_i^4}{(a_1\lambda_i^2 + a_2)^2}. \quad (3.2)$$

Now we solve the equations (5.3), (5.4), (4.5), (4.6) to get

$$a_1 = \frac{c_1(c_1 + c_2 - 1)}{(c_1 + c_2)^2}, a_2 = \frac{c_2(c_1 + c_2 - 1)}{(c_1 + c_2)^2}, a_3 = \frac{c_2}{(c_1 + c_2)(c_1 + c_2 - 1)}, a_4 = \frac{c_1}{(c_1 + c_2)(c_1 + c_2 - 1)}. \quad (3.3)$$

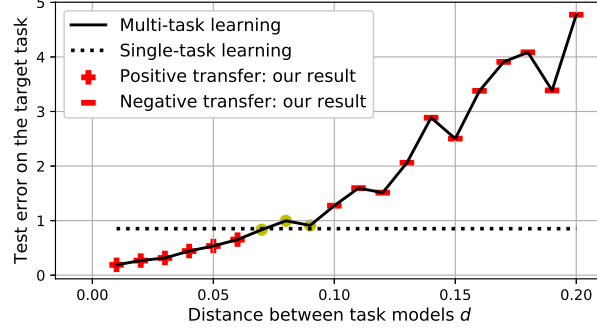


Figure 1: Positive vs negative transfer as a parameter of the task model distances.

Then we obtain

$$\Delta_{\beta} = p \cdot d^2 \cdot \frac{c_1^2(c_1 + c_2)}{(c_1 + c_2 - 1)^3}, \Delta_{\text{var}} = \sigma^2 \cdot \frac{c_1}{(c_2 - 1)(c_1 + c_2 - 1)}. \quad (3.4)$$

We demonstrate our result with a simulation. We consider a setting where $p = 200$, $n_1 = 90p$, $n_2 = 30p$. **Fill in other params.** We fix the target task and vary the source task, by varying the task model distance parameter d . We show that Theorem 4.1 predicts whether we can get positive or negative transfer. Figure 1 shows the result. We obtain the following insight from the simulation.

- Adding the source task has the effect of reducing the variance of the estimator, independent of the model shift.
- Model shift introduces an additional bias term, which scales with d^2 , the distance of the two task models. Hence, the type of transfer is determined by the tradeoff between the bias caused by model shift and the reduction of variance.

4 The De-Noising Effect of Multi-Task Learning

In this case, β_s and β_t are different. From [4], we know that either we need to explicitly restrict the capacity r of B , or implicitly add a regularization on B . **We focus on the former case in this section.** Following [4], we consider the case when $r = 1$ since there are only two tasks.

4.1 The Objective with Shared Weights

We begin by considering the simplified equation (2.2) to solve for the target task. By putting the two tasks together, we get

$$\begin{aligned} \hat{\beta}_{s,t} &= (X_1^\top X_1 + X_2^\top X_2)^{-1} (X_1^\top Y_1 + X_2^\top Y_2) \\ &= (X_1^\top X_1 + X_2^\top X_2)^{-1} ((X_1^\top X_1 \beta_s + X_2^\top X_2 \beta_t) + (X_1^\top \varepsilon_1 + X_2^\top \varepsilon_2)) \\ &= \beta_t + (X_1^\top X_1 + X_2^\top X_2)^{-1} (X_1^\top X_1 (\beta_s - \beta_t) + (X_1^\top \varepsilon_1 + X_2^\top \varepsilon_2)) \end{aligned}$$

Hence

$$e(\hat{\beta}_{s,t}) = \|(X_1^\top X_1 + X_2^\top X_2)^{-1} X_1^\top X_1 (\beta_s - \beta_t)\|^2 + \sigma^2 \text{Tr}[(X_1^\top X_1 + X_2^\top X_2)^{-1}], \text{ and} \quad (4.1)$$

$$te(\hat{\beta}_{s,t}) = \left\| \Sigma_2^{1/2} (X_1^\top X_1 + X_2^\top X_2)^{-1} X_1^\top X_1 (\beta_s - \beta_t) \right\|^2 + \sigma^2 \cdot \text{Tr}[(X_1^\top X_1 + X_2^\top X_2)^{-1} \Sigma_2] \quad (4.2)$$

We can see that because of model shift, i.e. $\beta_s \neq \beta_t$. We can no longer guarantee that $te(\hat{\beta}_{s,t}) \leq te(\hat{\beta}_t)$. The goal of this part is to show conditions under which we get positive vs. negative transfer.

For technical reasons, we will consider the test error. From Lemma 5.5, we know that

$$\text{Tr}[(X_1^\top X_1 + X_2^\top X_2)^{-1} \Sigma_2] = \frac{1}{n_1 + n_2} \cdot \text{Tr} \left[\left(a_1 \Sigma_2^{-1/2} \Sigma_1 \Sigma_2^{-1/2} + a_2 \text{Id} \right)^{-1} \right],$$

where a_1, a_2 are specified in Theorem 5.1. Hence the variance part is reduced by the following amount

$$\Delta_{\text{var}} := \sigma^2 \cdot \left(\frac{p}{n_2 - p} - \frac{1}{n_1 + n_2} \text{Tr} \left[(a_1 M^\top M + a_2 \text{Id})^{-1} \right] \right) \quad (4.3)$$

It remains to consider the increment from the first term in $te(\hat{\beta}_{s,t})$, which is bounded using the following lemma.

Theorem 4.1 (Positive transfer under model shift). *Let a_1, a_2 be the solutions from equations (5.3) and (5.4). Denote by $M := \Sigma_1^{1/2} \Sigma_2^{-1/2}$. We have $te(\hat{\beta}_{s,t}) \leq te(\hat{\beta}_t)$ when*

$$\Delta_{\text{var}} \geq \left(1 + \sqrt{\frac{p}{n_1}} \right)^2 \Delta_\beta, \quad (4.4)$$

where

$$\Delta_\beta := \frac{n_1^2}{(n_1 + n_2)^2} (\beta_s - \beta_t)^\top \Sigma_1^{1/2} M \frac{(1 + a_3) \text{Id} + a_4 M^\top M}{(a_2 + a_1 M^\top M)^2} M^\top \Sigma_1^{1/2} (\beta_s - \beta_t),$$

and a_3, a_4 are the solutions of the following linear equations

$$\left(\frac{n_2}{a_2^2} - \sum_{i=1}^p \frac{1}{(a_2 + \lambda_i^2 a_1)^2} \right) a_3 - \left(\sum_{i=1}^p \frac{\lambda_i^2}{(a_2 + \lambda_i^2 a_1)^2} \right) a_4 = \sum_{i=1}^p \frac{1}{(a_2 + \lambda_i^2 a_1)^2}, \quad (4.5)$$

$$\left(\frac{n_1}{a_1^2} - \sum_{i=1}^p \frac{\lambda_i^4}{(a_2 + \lambda_i^2 a_1)^2} \right) a_4 - \left(\sum_{i=1}^p \frac{\lambda_i^2}{(a_2 + \lambda_i^2 a_1)^2} \right) a_3 = \sum_{i=1}^p \frac{\lambda_i^2}{(a_2 + \lambda_i^2 a_1)^2}. \quad (4.6)$$

Theorem 4.1 shows upper bounds that guarantee positive transfer, which is determined by the change of variance Δ_{var} and a certain model shift bias parameter Δ_β determined by the covariate shift matrix and the model shift.

Example 4.2 (The effect of n_1 , the source task data size).

5 The Effect of Covariate Shift on the Rate of Transfer

As Proposition 2.1 shows, if β_s and β_t are equal, then adding the source task dataset always helps learn the target task. The goal of this section is to understand how covariate shift affects the rate of transfer. **add conceptual msg**

The estimator using the source and target together from minimizing (2.2) is

$$\hat{\beta}_{s,t} = (X_1^\top X_1 + X_2^\top X_2)^{-1} (X_1^\top Y_1 + X_2^\top Y_2)$$

The estimation error of $\hat{\beta}_{s,t}$ is

$$e(\hat{\beta}_{s,t}) = \sigma^2 \cdot \text{Tr}[(X_1^\top X_1 + X_2^\top X_2)^{-1}]. \quad (5.1)$$

The estimation error using the target alone is

$$e(\hat{\beta}_t) = \sigma^2 \cdot \text{Tr}[(X_2^\top X_2)^{-1}]. \quad (5.2)$$

The improvement of estimation error from adding the source task is then given by $e(\hat{\beta}_t) - e(\hat{\beta}_{s,t})$. For the test error on the target task, the improvement from adding the source task is

$$te(\hat{\beta}_t) - te(\hat{\beta}_{s,t}) = \sigma^2 \cdot \text{Tr} \left[((X_2^\top X_2)^{-1} - (X_1^\top X_1 + X_2^\top X_2)^{-1}) \cdot \Sigma_2 \right].$$

We can get a precise result on the improvement of adding the source task data that only depends on the covariance matrices Σ_1, Σ_2 and the number of data points n_1, n_2 . We shall consider the high-dimensional setting such that

$$\gamma_n := \frac{p}{n_1 + n_2} \rightarrow \gamma, \quad c_n := \frac{n_1}{n_1 + n_2} \rightarrow c, \quad \text{as } n_1, n_2 \rightarrow \infty,$$

for some constants $\gamma \in (0, \infty)$ and $c \in (0, 1)$.

Theorem 5.1 (Positive transfer rate under covariate shift). *Let $\lambda_1, \lambda_2, \dots, \lambda_p$ denote the singular values of $\Sigma_1^{1/2} \Sigma_2^{-1/2}$. When there is no model shift, we have that*

$$\begin{aligned} e(\hat{\beta}_{s,t}) &= \sigma^2 \cdot \text{Tr} \left[\frac{1}{(n_1 + n_2)a_1 \Sigma_1 + (n_1 + n_2)a_2 \Sigma_2} \right] \\ te(\hat{\beta}_{s,t}) &= \sigma^2 \cdot \text{Tr} \left[\frac{1}{(n_1 + n_2)a_1 \Sigma_2^{-1/2} \Sigma_1 \Sigma_2^{-1/2} + (n_1 + n_2)a_2 \text{Id}} \right] \end{aligned}$$

where a_1, a_2 are the solutions of the following equations

$$a_1 + a_2 = 1 - \frac{p}{n_1 + n_2} \tag{5.3}$$

$$a_1 + \sum_{i=1}^p \frac{a_1}{(n_1 + n_2)a_1 + (n_1 + n_2)a_2/\lambda_i^2} = \frac{n_1}{n_1 + n_2}. \tag{5.4}$$

redo the following As a remark, we see that Proposition 2.1 follows from Theorem 5.1. The amount of reduction on estimation error and test error for the target task is given as

$$\begin{aligned} e(\hat{\beta}_t) - e(\hat{\beta}_{s,t}) &= \sigma^2 p \cdot \text{Tr} \left[\frac{1}{(n_2 - p)\Sigma_2} - \frac{1}{(n_1 + n_2)a_1 \Sigma_1 + (n_1 + n_2)a_2 \Sigma_2} \right], \\ te(\hat{\beta}_t) - te(\hat{\beta}_{s,t}) &= \sigma^2 p \cdot \text{Tr} \left[\frac{1}{n_2 - p} - \frac{1}{(n_1 + n_2)a_1 \Sigma_2^{-1/2} \Sigma_1 \Sigma_2^{-1/2} + (n_1 + n_2)a_2 \text{Id}} \right]. \end{aligned}$$

Because

$$\begin{aligned} e(\hat{\beta}_{s,t}) &\leq e(\hat{\beta}_t) \Leftrightarrow (n_2 - p)\Sigma_2 \preceq (n_1 + n_2)a_1 \Sigma_1 + (n_1 + n_2)a_2 \Sigma_2 \\ &\Leftrightarrow \mathbf{0} \preceq (n_1 + n_2)a_1 \Sigma_1 + (n_1 - (n_1 + n_2) \cdot a_1)\Sigma_2, \end{aligned}$$

which is true since $a_1 \leq n_1/(n_1 + n_2)$ by equation (5.4). The proof for $te(\hat{\beta}_{s,t}) \leq te(\hat{\beta}_t)$ follows by multiplying $\Sigma_2^{-1/2}$ on both sides of the inequalities above.

Now we apply Theorem 5.1 to show how covariate shift affects the rate of transfer.

Example 5.2 (When $\Sigma_1 = \Sigma_2$). In this case, we have $\lambda_i = 1$ for all $1 \leq i \leq p$. And $a_1 + a_2 = 1 - p/(n_1 + n_2)$. Hence

$$te(\hat{\beta}_{s,t}) = \frac{\sigma^2 p^2}{n_1 + n_2 - p} \quad \text{and} \quad e(\hat{\beta}_{s,t}) = \frac{\sigma^2 p}{n_1 + n_2 - p} \text{Tr} [\Sigma_2^{-1}].$$

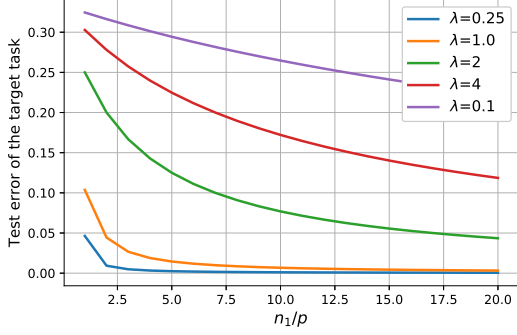


Figure 2: When $\Sigma_1 = \Sigma_2/\lambda$.

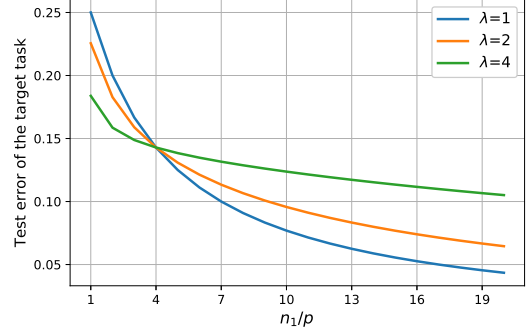


Figure 3: When Σ_1 and Σ_2 are complementary.

Example 5.3 (When $\Sigma_1 = \Sigma_2/\lambda$). In this case, equations (5.3) and (5.4) become

$$a_1 + a_2 = 1 - p/(n_1 + n_2), a_1 + \frac{p}{n_1 + n_2} \cdot \frac{a_1}{a_1 + \lambda^2 a_2} = \frac{n_1}{n_1 + n_2}.$$

By solving these, we can get the test errors (the estimation error behaves similarly). Figure 2 shows how they grow as we increase the number of source task data points. Here $n_2 = 4p$ and n_1 ranges from p to $20p$. We can see that the smaller λ is, the lower the test errors will be.

Example 5.4 (When Σ_1 and Σ_2 are complementary). Here we have that for $\Sigma_1^{-1/2}\Sigma_2^{1/2}$, the first $p/2$ singular values of Σ_1 is λ and the rest is $1/\lambda$. For this case, equations (5.3) and (5.4) become

$$a_1 + a_2 = 1 - \frac{p}{n_1 + n_2}, a_1 + \frac{p}{2(n_1 + n_2)} \cdot \left(\frac{a_1}{a_1 + \lambda^2 a_2} + \frac{a_1}{a_1 + \frac{a_2}{\lambda^2}} \right) = \frac{n_1}{n_1 + n_2}.$$

It's not hard to verify that there is only one valid solution from the above. After solving these, we get the test error for the target task as follows.

$$\frac{p}{2(n_1 + n_2)} \cdot \left(\frac{1}{\frac{a_1}{\lambda^2} + a_2} + \frac{1}{a_1 \lambda^2 + a_2} \right).$$

In Figure 3, we plot the test error of the target task for $n_2 = 4p$ and n_1 ranging from p to $20p$. We observe the following two phases as we increase n_1/p .

- When $n_1 \leq n_2$, having complementary covariance matrices leads to lower test error compared to the case when $\Sigma_1 = \Sigma_2$.
- When $n_1 > n_2$, having complementary covariance matrices leads to higher test error compared to the case when $\Sigma_1 = \Sigma_2$.

To prove Theorem 5.1, we study the spectrum of the random matrix model:

$$Q = \Sigma_1^{1/2} Z_1^T Z_1 \Sigma_1^{1/2} + \Sigma_2^{1/2} Z_2^T Z_2 \Sigma_2^{1/2},$$

where $\Sigma_{1,2}$ are $p \times p$ deterministic covariance matrices, and $X_1 = (x_{ij})_{1 \leq i \leq n_1, 1 \leq j \leq p}$ and $X_2 = (x_{ij})_{n_1+1 \leq i \leq n_1+n_2, 1 \leq j \leq p}$ are $n_1 \times p$ and $n_2 \times p$ random matrices, respectively, where the entries x_{ij} , $1 \leq i \leq n_1 + n_2 \equiv n$, $1 \leq j \leq p$, are real independent random variables satisfying

$$\mathbb{E} z_{ij} = 0, \quad \mathbb{E} |z_{ij}|^2 = n^{-1}. \quad (5.5)$$

For now, we assume that the random variables x_{ij} are i.i.d. Gaussian, but we know that universality holds for generally distributed entries.

Lemma 5.5. *In the setting of Theorem 5.1, we have with high probability $1 - o(1)$,*

$$\text{Tr}((X_1^\top X_1 + X_2^\top X_2)^{-1}) = \frac{1}{n_1 + n_2} \cdot \text{Tr} \left[\frac{1}{a_1 \Sigma_1 + a_2 \Sigma_2} \right] + O \left(\frac{1}{n^{1-\varepsilon}} \right).$$

for any constant $\varepsilon > 0$. In particular, when $n_1 = 0$, we have that $a_1 = 0$ and $a_2 = (n_2 - p)/n_2$, hence

$$\text{Tr}[(X_2^\top X_2)^{-1}] = \frac{1}{n_2 - p} \text{Tr} \left[\frac{1}{\Sigma_2} \right] + O \left(\frac{1}{n_2^{1-\varepsilon}} \right).$$

6 Extensions to the Sparse Setting

One important case is the sparse case, where we assume that the β_i 's are sparse in the sense that each β_i is in a subspace of dimension $k_i \ll p$. In other words,

$$\beta_i = \sum_{j=1}^{k_i} a_j^{(i)} v_j^{(i)},$$

where $\{v_j^{(i)}\}$ is a set of k_i orthonormal vectors. For $X_i = Z_i \Sigma_i^{1/2}$, we have

$$X_i \beta_i = Z_i \Sigma_i^{1/2} \beta_i = Z_i \Sigma_i^{1/2} P_i \beta_i, \quad P_i := \sum_{j=1}^{k_i} v_j^{(i)} (v_j^{(i)})^\top.$$

Then we have

$$\frac{1}{n_i} \mathbb{E} \left[P_i \Sigma_i^{1/2} Z_i^T Z_i \Sigma_i^{1/2} P_i \right] = P_i \Sigma_i P_i.$$

Hence our analysis will be valid with projected covariance matrices $P_i \Sigma_i P_i$. Moreover, due to the sparsity assumption, it is natural to have restricted isometry property:

$$\frac{1}{n_i} P_i \Sigma_i^{1/2} Z_i^T Z_i \Sigma_i^{1/2} P_i \approx P_i \Sigma_i P_i.$$

Finally, for our analysis it is not necessary to assume that β_T is sparse for the target.

References

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7 Proofs of Theorem bla

The proofs of Theorem 4.1 and Theorem 3.1 involve two parts.

Part I: Bounding the bias from model shift. We relate the first term in equation (4.2) to Δ_β .

Proposition 7.1. *In the setting of Theorem 4.1, we have that*

$$\left(1 - 4\sqrt{\frac{p}{n_1}} - 2\frac{p}{n_1}\right) \Delta_\beta \leq \left\| \Sigma_2^{1/2} (X_1^\top X_1 + X_2^\top X_2)^{-1} X_1^\top X_1 (\beta_s - \beta_t) \right\|^2 \leq \left(1 + \sqrt{\frac{p}{n_1}}\right)^4 \Delta_\beta.$$

For the special case when $\Sigma_1 = \text{Id}$ and $\beta_s - \beta_t$ is i.i.d. with mean 0 and variance d^2 , we further have

$$\left(1 - \sqrt{\frac{p}{n_1}}\right)^4 \Delta_\beta \leq \left\| \Sigma_2^{1/2} (X_1^\top X_1 + X_2^\top X_2)^{-1} X_1^\top X_1 (\beta_s - \beta_t) \right\|^2.$$

Proof. The proof follows by applying equation (7.2). Recall that $X_1^\top X_1 = \Sigma_1^{1/2} Z_1^\top Z_1 \Sigma_1^{1/2}$. Denote by $\mathcal{E} = Z_1^\top Z_1 - n_1 \text{Id}$. Let $K = (X_1^\top X_1 + X_2^\top X_2)^{-1}$. Let $\alpha = \left\| \Sigma_2^{1/2} K \Sigma_1 (\beta_s - \beta_t) \right\|^2$. We have

$$\begin{aligned} & \left\| \Sigma_2^{1/2} (X_1^\top X_1 + X_2^\top X_2)^{-1} X_1^\top X_1 (\beta_s - \beta_t) \right\|^2 \\ &= n_1^2 \alpha + 2n_1 (\beta_s - \beta_t)^\top \Sigma_1^{1/2} \mathcal{E} \Sigma_1^{1/2} K \Sigma_2 K \Sigma_1 (\beta_s - \beta_t) + \left\| \Sigma_2^{1/2} K \Sigma_1^{1/2} \mathcal{E} \Sigma_1^{1/2} (\beta_s - \beta_t) \right\|^2 \\ &\leq n_1 \left(n_1^2 + \frac{2n_1}{p} (p + 2\sqrt{n_1 p}) + (p + 2\sqrt{n_1 p})^2 \right) \alpha = n_1^2 \left(1 + \sqrt{\frac{p}{n_1}} \right)^4 \alpha. \end{aligned} \quad (7.1)$$

Here we use the following on the second term in equation (7.1)

$$\begin{aligned} & \left| (\beta_s - \beta_t)^\top \Sigma_1^{1/2} \mathcal{E} \Sigma_1^{1/2} K \Sigma_2 K \Sigma_1 (\beta_s - \beta_t) \right| \\ &= \left| \text{Tr} \left[\mathcal{E} \Sigma_1^{1/2} K \Sigma_2 K \Sigma_1 (\beta_s - \beta_t) (\beta_s - \beta_t)^\top \Sigma_1^{1/2} \right] \right| \\ &\leq \|\mathcal{E}\| \cdot \left\| \Sigma_1^{1/2} K \Sigma_2 K \Sigma_1 (\beta_s - \beta_t) (\beta_s - \beta_t)^\top \Sigma_1^{1/2} \right\|_* \\ &\leq n_1 \left(2\sqrt{\frac{p}{n_1}} + \frac{p}{n_1} \right) \cdot \left\| \Sigma_1^{1/2} K \Sigma_2 K \Sigma_1 (\beta_s - \beta_t) (\beta_s - \beta_t)^\top \Sigma_1^{1/2} \right\|_* \quad (\text{by equation (7.2)}) \\ &= n_1 \left(2\sqrt{\frac{p}{n_1}} + \frac{p}{n_1} \right) \alpha \quad (\text{since the matrix inside is rank 1}) \end{aligned}$$

The third term in equation (7.1) can be bounded similarly.

For the other direction, we simply note that the third term in equation (7.1) is positive. And the second term is bigger than $-2n_1^2 (2\sqrt{\frac{p}{n_1}} + \frac{p}{n_1}) \alpha$ using equation (7.2). \square

Part II: The limit of $\left\| \Sigma_2^{1/2} (X_1^\top X_1 + X_2^\top X_2)^{-1} \Sigma_1 (\beta_s - \beta_t) \right\|^2$ using random matrix theory. We consider the same setting as in previous subsection:

$$X_1^\top X_1 := \Sigma_1^{1/2} Z_1^\top Z_1 \Sigma_1^{1/2}, \quad X_2^\top X_2 = \Sigma_2^{1/2} Z_2^\top Z_2 \Sigma_2^{1/2},$$

where z_{ij} , $1 \leq i \leq n_1 + n_2 \equiv n$, $1 \leq j \leq p$, are real independent random variables satisfying (5.5). For now, we assume that the random variables z_{ij} are i.i.d. Gaussian, but we know that universality holds for generally distributed entries. Assume that p/n_1 is a small number such that $Z_1^\top Z_1$ is roughly an isometry, that is, under (5.5), [If we assume the variances of the entries of \$Z_1\$ are 1, then we have](#)

$$-n_1 \left(2\sqrt{\frac{p}{n_1}} - \frac{p}{n_1} \right) \leq Z_1^\top Z_1 - n_1 \text{Id} \leq n_1 \left(2\sqrt{\frac{p}{n_1}} + \frac{p}{n_1} \right). \quad (7.2)$$

(revise the following proof) It remain to study the following expression

$$\begin{aligned} \frac{1}{X_1^\top X_1 + X_2^\top X_2} \Sigma_2 \frac{1}{X_1^\top X_1 + X_2^\top X_2} &= \Sigma_2^{-1/2} \left(\frac{1}{A^\top Z_1^\top Z_1 A + Z_2^\top Z_2} \right)^2 \Sigma_2^{-1/2} \\ &\stackrel{d}{=} \Sigma_2^{-1/2} V \left(\frac{1}{\Lambda Z_1^\top Z_1 \Lambda + Z_2^\top Z_2} \right)^2 V^\top \Sigma_2^{-1/2}, \end{aligned}$$

where

$$A := \Sigma_1^{1/2} \Sigma_2^{-1/2} = U \Lambda V^\top, \quad \Lambda = \text{diag}(\lambda_1, \dots, \lambda_p). \quad (7.3)$$

Using

$$\left(\frac{1}{\Lambda Z_1^\top Z_1 \Lambda + Z_2^\top Z_2} \right)^2 = \frac{d}{dz} \Big|_{z=0} \frac{1}{\Lambda Z_1^\top Z_1 \Lambda + Z_2^\top Z_2 - z},$$

we need to study the resolvent of

$$G(z) = (\Lambda Z_1^\top Z_1 \Lambda + Z_2^\top Z_2 - z)^{-1}.$$

Its local law can be studied as in previous subsection (be careful we need to switch the roles of Z_1 and Z_2). More precisely, we have that

$$G(z) \approx \text{Diag} \left(\frac{1}{-z(1 + m_3(z) + \lambda_i^2 m_4(z))} \right)_{1 \leq i \leq p} = \frac{1}{-z(1 + m_3(z) + \Lambda^2 m_4(z))}.$$

Here $m_{3,4}(z)$ satisfy the following self-consistent equations

$$\frac{n_2}{n} \frac{1}{m_3} = -z + \frac{1}{n} \sum_{i=1}^p \frac{1}{1 + m_3 + \lambda_i^2 m_4}, \quad \frac{n_1}{n} \frac{1}{m_4} = -z + \frac{1}{n} \sum_{i=1}^p \frac{\lambda_i^2}{1 + m_3 + \lambda_i^2 m_4}. \quad (7.4)$$

Then we calculate the derivatives of $u_3 := z m_3$ and $u_4 := z m_4$ with respect to z :

$$\frac{n_2}{n} \frac{1}{u_3^2} u_3' = \frac{1}{n} \sum_{i=1}^p \frac{1 + u_3' + \lambda_i^2 u_4'}{(z + u_3 + \lambda_i^2 u_4)^2}, \quad \frac{n_1}{n} \frac{1}{u_4^2} u_4' = \frac{1}{n} \sum_{i=1}^p \frac{\lambda_i^2 (1 + u_3' + \lambda_i^2 u_4')}{(z + u_3 + \lambda_i^2 u_4)^2}. \quad (7.5)$$

We can solve the above equations to get u_3' and u_4' . Then we have

$$G^2(z) \approx \frac{1 + u_3'(z) + \Lambda^2 u_4'(z)}{(z + u_3(z) + \Lambda^2 u_4(z))^2}$$

in certain sense.

$$a_3 \rightarrow a_2, \quad a_4 \rightarrow a_1$$

We now simplify the expressions for $z \rightarrow 0$ case. When $z \rightarrow 0$, we shall have

$$u_3(z) = -a_3 + O(z), \quad u_4(z) = -a_4 + O(z), \quad a_3, a_4 > 0.$$

For $z \rightarrow 0$, the equations in (7.4) are reduced to

$$\frac{n_2}{n} \frac{1}{a_2} = 1 + \frac{1}{n} \sum_{i=1}^p \frac{1}{a_2 + \lambda_i^2 a_1}, \quad \frac{n_1}{n} \frac{1}{a_1} = 1 + \frac{1}{n} \sum_{i=1}^p \frac{\lambda_i^2}{a_2 + \lambda_i^2 a_1}. \quad (7.6)$$

It is easy to see that these equations are equivalent to

$$a_1 + a_2 = 1 - \gamma_n, \quad a_1 + \frac{1}{n} \sum_{i=1}^p \frac{a_1}{a_1 + a_2 / \lambda_i^2} = \frac{n_1}{n}. \quad (7.7)$$

The equations in (7.5) reduce to

$$\begin{aligned} \left(\frac{n_2}{n} \frac{1}{a_2^2} - \frac{1}{n} \sum_{i=1}^p \frac{1}{(a_2 + \lambda_i^2 a_1)^2} \right) a_3 - \left(\frac{1}{n} \sum_{i=1}^p \frac{\lambda_i^2}{(a_2 + \lambda_i^2 a_1)^2} \right) a_4 &= \frac{1}{n} \sum_{i=1}^p \frac{1}{(a_2 + \lambda_i^2 a_1)^2}, \\ \left(\frac{n_1}{n} \frac{1}{a_1^2} - \frac{1}{n} \sum_{i=1}^p \frac{\lambda_i^4}{(a_2 + \lambda_i^2 a_1)^2} \right) a_4 - \left(\frac{1}{n} \sum_{i=1}^p \frac{\lambda_i^2}{(a_2 + \lambda_i^2 a_1)^2} \right) a_3 &= \frac{1}{n} \sum_{i=1}^p \frac{\lambda_i^2}{(a_2 + \lambda_i^2 a_1)^2}. \end{aligned} \quad (7.8)$$

where we denote $b_3 := u'_3(0)$ and $b_4 := u'_4(0)$. Thus we have

$$\left(\frac{1}{\Lambda Z_1^\top Z_1 \Lambda + Z_2^\top Z_2} \right)^2 = G^2(0) \approx \frac{1 + b_3 + \Lambda^2 b_4}{(a_3 + \Lambda^2 a_4)^2}.$$

This gives that

$$\begin{aligned} \frac{1}{X_1^\top X_1 + X_2^\top X_2} \Sigma_2 \frac{1}{X_1^\top X_1 + X_2^\top X_2} &= \Sigma_2^{-1/2} V \left(\frac{1}{\Lambda Z_1^\top Z_1 \Lambda + Z_2^\top Z_2} \right)^2 V^\top \Sigma_2^{-1/2} \\ &\approx \Sigma_2^{-1/2} V \frac{1 + b_3 + \Lambda^2 b_4}{(a_3 + \Lambda^2 a_4)^2} V^\top \Sigma_2^{-1/2} = \Sigma_2^{-1/2} \frac{1 + b_3 + b_4 A^\top A}{(a_3 + a_4 A^\top A)^2} \Sigma_2^{-1/2}. \end{aligned}$$

Hence we have

$$\begin{aligned} (\beta_s - \beta_t)^\top X_1^\top X_1 \frac{1}{X_1^\top X_1 + X_2^\top X_2} \Sigma_2 \frac{1}{X_1^\top X_1 + X_2^\top X_2} X_1^\top X_1 (\beta_s - \beta_t) \\ \approx (\beta_s - \beta_t)^\top \Sigma_1 \Sigma_2^{-1/2} \frac{1 + a_3 + a_4 A^\top A}{(a_2 + a_1 A^\top A)^2} \Sigma_2^{-1/2} \Sigma_1 (\beta_s - \beta_t). \end{aligned}$$

Proof of Lemma 5.5.

Proof. (revise the following proof) We assume that $\Sigma_1^{-1/2} \Sigma_2$ has eigendecomposition

$$\Sigma_1^{-1/2} \Sigma_2^{1/2} = O D O^\top, \quad D = \text{diag}(d_1, \dots, d_p). \quad (7.9)$$

Then by the rotational invariance of Gaussian matrices, we have

$$\tilde{Q} \stackrel{d}{=} \Sigma_1^{1/2} O \tilde{Q} O^\top \Sigma_1^{1/2}, \quad \tilde{Q} := X_1^\top X_1 + D X_2^\top X_2 D.$$

Thus we study the spectrum of \tilde{Q} instead. We define $\mathcal{G}(z) := (\tilde{Q} - z)^{-1}$ for $z \in \mathbb{C}_+$. With some random matrix tools, we have that

$$\mathcal{G}(z) \approx \text{Diag} \left(\frac{1}{-z(1 + m_3(z) + d_i^2 m_4(z))} \right)_{1 \leq i \leq p} = \frac{1}{-z(1 + m_3(z) + D^2 m_4(z))}$$

in certain sense. Here $m_{3,4}(z)$ satisfy the following self-consistent equations

$$\frac{n_1}{n} \frac{1}{m_3} = -z + \frac{1}{n} \sum_{i=1}^p \frac{1}{1 + m_3 + d_i^2 m_4}, \quad \frac{n_2}{n} \frac{1}{m_4} = -z + \frac{1}{n} \sum_{i=1}^p \frac{d_i^2}{1 + m_3 + d_i^2 m_4} \quad (7.10)$$

When $z \rightarrow 0$, we shall have

$$m_3(z) = -\frac{a_3}{z} + O(1), \quad m_4(z) = -\frac{a_4}{z} + O(1), \quad a_3, a_4 > 0.$$

Then for $z \rightarrow 0$, the equations in (7.10) are reduced to

$$\frac{n_1}{n} \frac{1}{a_3} = 1 + \frac{1}{n} \sum_{i=1}^p \frac{1}{a_3 + d_i^2 a_4}, \quad \frac{n_2}{n} \frac{1}{a_4} = 1 + \frac{1}{n} \sum_{i=1}^p \frac{d_i^2}{a_3 + d_i^2 a_4}. \quad (7.11)$$

First, it is easy to see that these equations are equivalent to

$$a_3 + a_4 = 1 - \gamma_n, \quad a_3 + \frac{1}{n} \sum_{i=1}^p \frac{a_3}{a_3 + d_i^2 [(1 - \gamma_n) - a_3]} = c_n. \quad (7.12)$$

Furthermore, we have

$$\begin{aligned} \text{Tr}(Q^{-1}) &= \lim_{z \rightarrow 0} \text{Tr} \left[\Sigma_1^{-1/2} O \mathcal{G}(z) O^T \Sigma_1^{-1/2} \right] = \text{Tr} \left[\Sigma_1^{-1/2} O \left(\frac{1}{a_3 + D^2 a_4} \right) O^T \Sigma_1^{-1/2} \right] \\ &= \text{Tr} \left[\Sigma_1^{-1/2} \frac{1}{a_3 + \Sigma_1^{-1} \Sigma_2 a_4} \Sigma_1^{-1/2} \right] = \text{Tr} \left[\frac{1}{a_3 \Sigma_1 + a_4 \Sigma_2} \right]. \end{aligned}$$

□