Estimation of Conditional Mean Operator under the Bandable Covariance Structure

Kwangmin Lee\textsuperscript{1}, Kyoungjae Lee\textsuperscript{2}, and Jaeyong Lee\textsuperscript{1}

\textsuperscript{1}Department of Statistics, Seoul National University
\textsuperscript{2}Department of Statistics, Inha University

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Abstract

We consider high-dimensional multivariate linear regression models, where the joint distribution of covariates and response variables is a multivariate normal distribution with a bandable covariance matrix. The main goal of this paper is to estimate the regression coefficient matrix, which is a function of the bandable covariance matrix. Although the tapering estimator of covariance has the minimax optimal convergence rate for the class of bandable covariances, we show that it has a sub-optimal convergence rate for the regression coefficient; that is, a minimax estimator for the class of bandable covariances may not be a minimax estimator for its functionals. We propose the blockwise tapering estimator of the regression coefficient, which has the minimax optimal convergence rate for the regression coefficient under the bandable covariance assumption. We also propose a Bayesian procedure called the blockwise tapering post-processed posterior of the regression coefficient and show that the proposed Bayesian procedure has the minimax optimal convergence rate for the regression coefficient under the bandable covariance assumption.
We show that the proposed methods outperform the existing methods via numerical studies.

1 Introduction

Consider the multivariate linear regression model

\[ Y_i = CX_i + \epsilon_i, \quad i = 1, \ldots, n, \]

where \( Y_i \in \mathbb{R}^q \) is a response vector, \( X_i \in \mathbb{R}^{p_0} \) is a covariate vector, \( C \in \mathbb{R}^{q \times p_0} \) is a regression coefficient matrix, and \( \epsilon_i \in \mathbb{R}^q, i = 1, 2, \ldots, n, \) are independent and identically distributed error vectors from a \( q \)-dimensional normal distribution with mean zero. The multivariate linear regression model has been used for various fields of applications. For example, Zhao et al. (2018) analyzed atmospheric data using the model to forecast PM2.5 concentration, and Qian et al. (2020) used the model to analyze the genomics data.

For the estimation of the multivariate linear regression coefficient \( C \in \mathbb{R}^{q \times p_0} \), one of the most commonly used approaches is a penalized least square method, which finds the minimizer of the following objective function,

\[ f(C) = \sum_{i=1}^{n} ||Y_i - CX_i||^2_F + P(C), \]

where \( P(C) \) is a penalty term. The penalized least square method penalizes the objective function when the estimate \( C \) deviates from the low dimensional structure which the true coefficient matrix \( C \) is assumed to have, and it is especially useful under high-dimensional settings, where \( p_0 \) and \( q \) can grow to infinity as \( n \to \infty \). Various penalized methods for the multivariate linear regression model have been suggested (Chen and Huang, 2012; Chen et al., 2013; Uematsu et al., 2019).

Employing a covariance estimation method is another approach for the estimation of the regression coefficient. The coefficient matrix \( C \) can be considered as a function of the joint covariance matrix of the covariate vector \( X \in \mathbb{R}^{p_0} \) and the response vector \( Y \in \mathbb{R}^q \). Assume that \( Z = (X^T, Y^T)^T \in \mathbb{R}^{p_0+q} \) follows a joint distribution with a mean vector \( \mu \).
and a covariance matrix $\Sigma$ such that

\[
\begin{align*}
\mu &= \begin{pmatrix} \mu_X \\ \mu_Y \end{pmatrix} \\
\Sigma &= \begin{pmatrix} \Sigma_{XX} & \Sigma_{XY} \\ \Sigma_{YX} & \Sigma_{YY} \end{pmatrix},
\end{align*}
\]

where $\mu_X \in \mathbb{R}^p_0$, $\mu_Y \in \mathbb{R}^q$, $\Sigma_{XX} \in \mathbb{R}^{p_0 \times p_0}$ and $\Sigma_{YY} \in \mathbb{R}^{q \times q}$. Then, we have

\[
(\mu_0, \Psi_0) := (\mu_Y - \Sigma_{YX} \Sigma_{XX}^{-1} \mu_X, \Sigma_{YX} \Sigma_{XX}^{-1}) = \arg\min_{(\mu, \Psi)} \mathbb{E}\{(Y - \mu - \Psi X)(Y - \mu - \Psi X)^T\},
\]

and $\mu_0 + \Psi_0 x$ is the conditional mean of $Y$ given $X = x$ if $Z$ follows the multivariate Gaussian distribution. Note that $\mu_0$ is the zero vector if we assume that $\mu_X$ and $\mu_Y$ are zero vectors. In this case, the coefficient matrix $C$ in the multivariate regression model corresponds to $\Psi_0 = \Sigma_{YX} \Sigma_{XX}^{-1}$, which is a function of the covariance matrix $\Sigma$ and is called the conditional mean operator. Thus, covariance estimators can be used for the estimation of the conditional mean operator.

We need to consider a high-dimensional covariance estimation method when we use a covariance estimator for the multivariate regression model under high-dimensional settings. Suppose $Z_1, Z_2, \ldots, Z_n$ are independent and identically generated from a $p$-dimensional distribution with mean zero and covariance matrix $\Sigma$. We refer to the estimation of covariance $\Sigma$ as high-dimensional covariance estimation when $p$ is assumed to go to infinity as $n \to \infty$. Since traditional covariance estimation methods, such as the sample covariance matrix and the Bayesian method by the inverse-Wishart prior, are not consistent when $p$ is larger than $n$ (Johnstone and Lu, 2009; Lee and Lee, 2018), various structural assumptions on covariance matrices have been used to reduce the number of effective parameters. For example, the banded covariances (Lee et al., 2020), the bandable covariances (Bickel and Levina, 2008), sparse covariances (Cai et al., 2013) and sparse spiked covariances (Cai et al., 2015) have been considered. These structural assumptions can be used in the joint covariance matrix of covariates and response variables when we employ covariance estimation for the multivariate regression under the high-dimensional settings.
In this paper, we consider the multivariate linear regression model, where the covariate vector and the response vector jointly follow a multivariate normal distribution with a bandable covariance matrix. Under the bandable covariance assumption, the farther apart two variables are, the smaller their covariance is. On the frequentist side, Cai and Zhou (2010, 2012) proved that the tapering estimator of covariance has the minimax optimal convergence rates for the class of bandable covariances under the spectral norm, Frobenius norm, and matrix $l_1$ norm. Therefore, a naive approach would be estimating the conditional mean operator based on the tapering estimator of covariance (or other minimax covariance estimators).

Unfortunately, even if a covariance estimator $\hat{\Sigma}$ has the minimax optimal convergence rate for the covariance $\Sigma$, it does not imply that $f(\hat{\Sigma})$ has also the minimax optimal convergence rate for $f(\Sigma)$ where $f$ is a function on the space of covariances. Thus, the estimator for $\Sigma_{YX} \Sigma^{-1}_{XX}$ based on the tapering estimator of covariance may not have the minimax optimal convergence rate. Furthermore, there is no Bayesian method achieving the minimax posterior convergence rate for the class of bandable covariances. Note that Silva and Ghahramani (2009), Khare et al. (2011) and Lee et al. (2020) proposed Bayesian procedures for banded covariances, but the class of bandable covariances considered in this paper is larger than the class of banded covariances.

We investigate the decision-theoretic property of the tapering estimator when the parameter of interest is the conditional mean operator, $\Sigma_{YX} \Sigma^{-1}_{XX}$, instead of the covariance itself. We define the tapering estimator of regression coefficient as the plug-in estimator, the tapering estimator of covariance plugged into the conditional mean operator, and show that the tapering estimator of regression coefficient has a sub-optimal convergence rate for $\Sigma_{YX} \Sigma^{-1}_{XX}$ under the bandable covariance assumption. We propose a minimax optimal estimator for $\Sigma_{YX} \Sigma^{-1}_{XX}$ by modifying the tapering estimator of regression coefficient and call it the blockwise tapering estimator of regression coefficient.

As a Bayesian procedure for the conditional mean operator under the bandable covariance assumption, we propose post-processed posterior method (Lee et al., 2020). A post-processed posterior (Lee et al., 2020) is a posterior constructed by transforming pos-
terior samples from the initial posterior, which is typically a computationally convenient posterior. This idea is especially useful when it is difficult to impose a prior distribution on a restricted parameter space due to an unknown normalizing constant. For a given parameter space $\Theta^*$, suppose that we are interested in restricted parameter space, $\Theta \subset \Theta^*$. A post-processed posterior can be obtained by generating samples from an initial posterior on $\Theta^*$ and post-processing the posterior samples so that the transformed post-processed samples belong to $\Theta$. When the post-processing function is a projection map from $\Theta^*$ to $\Theta$, the method is called the posterior projection method. The posterior projection method has been suggested for various settings including Dunson and Neelon (2003), Gunn and Dunson (2005), Lin and Dunson (2014) and Chakraborty and Ghosal (2020), and was investigated in general aspects by Patra and Dunson (2018). The idea of transforming posterior samples was also used for the inference on covariance or precision matrices in Lee et al. (2020) and Bashir et al. (2018).

We suggest two post-processed posteriors for the conditional mean operator. Both methods use the inverse-Wishart distribution as the initial prior distribution on the unconstrained covariance matrix space and use the tapering function and the blockwise tapering function as the post-processing functions for the conditional mean operator $\Sigma_{YX} \Sigma_{XX}^{-1}$. We present the asymptotic analysis to justify the proposed post-processed posteriors, and show that the post-processed posterior by the blockwise tapering function has the minimax optimal convergence rate.

The rest of the paper is organized as follows. In Section 2, we introduce the blockwise tapering estimator for the inference of the conditional mean operator under the bandable covariance assumption and show that this estimator has the minimax convergence rate. In Section 3, we introduce the post-processed posteriors for the conditional mean operator, and present the posterior convergence rates. Simulation studies and real data analysis are given in Section 4. We conclude this paper with a discussion section. The proofs of theorems that give the upper bound and lower bound of the convergence rate of the blockwise tapering estimator are given in Appendix A, and the proofs of the other theorems and lemma are given in the supplementary material.
2 Blockwise tapering estimator and minimax analysis

2.1 Notation

Let $q$, $k$ and $l$ be positive integers with $l \vee k \leq q$. For a $q \times q$-matrix $\Sigma$ and positive real numbers $\sigma_{ij}$, $1 \leq i, j \leq q$, let $\Sigma = (\sigma_{ij})_{1 \leq i,j \leq q} = (\sigma_{ij})$ when $\sigma_{ij}$ is equal to the $(i,j)$ element of $\Sigma$. We define sub-matrix operators $M_{l}^{(k)} : \mathbb{R}^{q \times q} \mapsto \mathbb{R}^{k^* \times k^*}$, where $k^* = \{(l + k - 1) \wedge q\} - (l \vee 1) + 1$, and $M_{*}^{(k)} : \mathbb{R}^{q \times q} \mapsto \mathbb{R}^{q \times q}$ as

\[ M_{l}^{(k)}(\Sigma) = (\sigma_{ij})_{(l \vee 1) \leq i,j \leq \{(l + k - 1) \wedge q\}} \]

\[ M_{*}^{(k)}(\Sigma) = (\sigma_{ij}[1 \leq i,j \leq \{(l + k - 1) \wedge q\}])_{1 \leq i,j \leq q}, \]

for $\Sigma = (\sigma_{ij})_{1 \leq i,j \leq q}$. Let $\Sigma_{ab,cd}$ be the sub-block matrix of $\Sigma \in \mathbb{R}^{q \times q}$ with $(a, a+1, \ldots, b-1,b)$ rows and $(c, c+1, \ldots, d-1,d)$ columns for positive integers $a,b,c$ and $d$ with $1 \leq a < b \leq q$ and $1 \leq c < d \leq q$. We also let $X_{ab} = (x_{a}, x_{a+1}, \ldots, x_{b-1}, x_{b}) \in \mathbb{R}^{b-a+1}$ for a vector $X = (x_{1}, x_{2}, \ldots, x_{q}) \in \mathbb{R}^{q}$ and positive integers $a$ and $b$ with $1 \leq a < b \leq q$.

For a $q \times q$-matrix $\Sigma = (\sigma_{ij})_{1 \leq i,j \leq q}$ and a positive integer $k$ with $k \leq q$, define the tapering function $T_{k}(\Sigma)$, which was first defined in Cai and Zhou (2010), as

\[ T_{k}(\Sigma) = (w_{ij}^{(k)} \sigma_{ij})_{1 \leq i,j \leq q}, \]

where

\[ w_{ij}^{(k)} = \begin{cases} 1, & \text{when } |i - j| \leq k/2 \\ 2 - \frac{|i - j|}{k/2}, & \text{when } k/2 < |i - j| < k. \\ 0, & \text{otherwise} \end{cases} \]

For any sequences $a_n$ and $b_n$ of positive real numbers, we denote $a_n = o(b_n)$ if $\lim_{n \to \infty} a_n/b_n = 0$, and $a_n = O(b_n)$ if $\limsup_{n \to \infty} a_n/b_n = C$ for a positive constant $C$. We denote $a_n \preceq b_n$ if $a_n \leq Cb_n$ for all sufficiently large $n$ and a positive constant $C$.

Let $||\Sigma|| = ||\Sigma||_2 = \{\lambda_{max}(\Sigma \Sigma^T)\}^{1/2}$ be the spectral norm of a covariance matrix $\Sigma$, where $\lambda_{max}(\Sigma)$ is the maximum eigenvalue of $\Sigma$. Given positive integers $p$ and $p_0$ with
$p_0 < p$, let $A_{XX} = A_{(p_0+1):p,1:p_0}$ and $A_{YX} = A_{(p_0+1):p,1:p_0}$ for a positive $p \times p$-matrix $A$. We also let $\Sigma_{0,XX}$ and $\Sigma_{0,YX}$ denote $(\Sigma_0)_{XX}$ and $(\Sigma_0)_{YX}$, respectively.

### 2.2 Blockwise Tapering Estimator

Let $n$, $p$, and $p_0$ be positive integers with $p_0 < p$. Suppose $Z_1, Z_2, \ldots, Z_n$ are independent and identically distributed from a $p$-variate Gaussian distribution with mean zero and covariance matrix $\Sigma_0$, which is denoted by $N_p(0, \Sigma_0)$, where $Z_i = (X_i^T, Y_i^T)^T$, $X_i \in \mathbb{R}^{p_0}$ and $Y_i \in \mathbb{R}^{p-p_0}$ for $i \in \{1, 2, \ldots, p\}$. When only the first $p_0$ elements of $Z_i$, i.e. $X_i$, are given, the conditional mean vector for the other $p - p_0$ variables is

$$
\Sigma_{0,YX}(\Sigma_{0,XX})^{-1}X_i.
$$

The conditional mean operator $\Sigma_{0,YX}(\Sigma_{0,XX})^{-1}$ in (1) is the estimand we focus on in this paper. We define the transformation $\psi$ from a covariance to the conditional mean operator as

$$
\psi(\Sigma) := \psi(\Sigma; p_0) = \Sigma_{YX}(\Sigma_{XX})^{-1},
$$

for $\Sigma \in C_p$, where $C_p$ is the set of all $p \times p$-dimensional positive definite matrices.

We assume $\Sigma_0$ belongs to a class of bandable covariances, $\mathcal{F}_\alpha$, which is defined as

$$
\mathcal{F}_\alpha := \mathcal{F}_{p,\alpha}(M, M_0, M_1)
$$

$$
= \left\{ \Sigma = (\sigma_{ij})_{1 \leq i,j \leq p} \in C_p : \sum_{(i,j):|i-j|\geq k} |\sigma_{ij}| \leq Mk^{-\alpha}, \forall k \geq 1, \lambda_{\max}(\Sigma) \leq M_0, \lambda_{\min}(\Sigma) \geq M_1 \right\},
$$

for some positive constants $\alpha, M > 0$ and $0 < M_1 < M_0$, where $\lambda_{\min}(\Sigma)$ is the minimum eigenvalue of $\Sigma$. Bickel and Levina (2008) and Cai and Zhou (2010) also considered the same class of bandable covariances except the minimum eigenvalue condition.

A natural estimator for $\psi(\Sigma_0)$ is the plug-in estimator, the tapering estimator of covariance plugged into $\psi$, for the tapering estimator of covariance has the minimax optimal convergence rate for the class of bandable covariances under the spectral norm loss (Cai and Zhou, 2010). For the positive-definiteness is necessary for the covariance estimator,
we modify the tapering estimator of covariance so that it is positive-definite and call it \textit{adjusted tapering estimator of covariance}:

\[
T^{(\epsilon_n)}_k(S_n) := T_k(S_n) + ([\epsilon_n - \lambda_{\min}\{T_k(S_n)\}] \lor 0)I_p,
\]

where \(\epsilon_n > 0\) is the positive-definite adjustment parameter, \(S_n\) is the sample covariance matrix \(\sum_{i=1}^{\mathbf{Z}} \mathbf{Z}_i \mathbf{Z}_i^T/n\), and \(I_p\) is the \(p \times p\) identity matrix. We call the plug-in estimator with adjusted tapering estimator of covariance the \textit{tapering estimator of regression coefficient}, in short \textit{the tapering estimator}.

Since every column vector in the tapering estimator is not the zero vector with probability one, the tapering estimator uses all variables in a given covariate vector when the estimator is used as the regression coefficient. In other words, in the variable selection perspective, all variables are selected when the tapering estimator is used. Note that selecting out negligible covariates can increase the accuracy of a regression estimator, and partial correlations between covariates and responses have been used as a criterion for the variable selection (Li et al., 2017; Bühlmann et al., 2010). We find covariates which have weak partial correlations with the response variables under the bandable covariance assumption by investigating the elements in the inverse matrix of the covariance, called the precision matrix in Theorem 2.1.

**Theorem 2.1.** Suppose \(\Sigma_0 \in \mathcal{F}_{p,\alpha}(M, M_0, M_1)\), and let \(\Sigma_0^{-1} = (w_{ij})\). There exist some positive constants \(C\) and \(\lambda\) depending only on \(M_0\), \(M_1\) and \(M\) such that

\[
\max_j \sum_i \{|w_{ij}| : |i - j| > a k \log k\} \leq C(k^{-a\lambda+1} + k^{-\alpha}),
\]

for all \(a > 0\) and all sufficiently large integer \(k\) with \(p > k \lor (a k \log k)\).

See the supplementary material for the proof. Note Lauritzen (1996) showed that the partial correlation between variable \(i\) and variable \(j\), \(\rho_{ij}\), is

\[
\rho_{ij} = \frac{w_{ij}}{\sqrt{w_{ii}w_{jj}}},
\]

where \(\Sigma_0^{-1} = (w_{ij})\). Since \(|w_{ii}| \geq M_0^{-1}\) for all \(i \in \{1, 2, \ldots, p\}\), each element in response vector \((Z_i)_{p_0+1:p}\) has negligibly weak partial correlations with remote covariates \((Z_i)_j\), i.e.
variables with \(|j - p_0| \) large and \(j \leq p_0\), when \(k\) is sufficiently large by Theorem 2.1. Thus, selecting out these negligible covariates could yield a more accurate estimator for the conditional mean operator.

Based on the above argument, we propose the **blockwise tapering estimator of regression coefficient**, in short the **blockwise tapering estimator**. Let \(Z\) be the set of all integers and 

\[
\lfloor x \rfloor = \max\{z \in Z : z \leq x\}.
\]

For positive real numbers \(a\) and \(\epsilon_n\), and a positive integer \(k\) with \(2\lfloor ak \log k \rfloor \leq p_0\), define the **blockwise tapering estimator** as

\[
\phi(S_n; 2\lfloor ak \log k \rfloor, \epsilon_n) := \phi(S_n; p_0, 2\lfloor ak \log k \rfloor, \epsilon_n)
\]

\[
\quad = T_k(S_n)YX \Lambda(\epsilon_n)\{T_k(S_n)XX; 2\lfloor ak \log k \rfloor\}, \tag{2}
\]

where \(\Lambda(\epsilon_n)(A; b)\) is defined as for a \(p_0 \times p_0\) matrix \(A\)

\[
\Lambda(\epsilon_n)(A; b) = \begin{pmatrix}
O_{(p_0-b) \times (p_0-b)} & O_{(p_0-b) \times b} \\
O_{b \times (p_0-b)} & \{M_{p_0-b+1}^{(b)}(A) + ([\epsilon_n - \lambda_{\min}\{M_{p_0-b+1}^{(b)}(A)\}] \vee 0)I_b\}^{-1}
\end{pmatrix},
\]

where \(O_{c \times d}\) is the \(c \times d\)-zero matrix for positive integers \(c\) and \(d\). Given a covariate vector \(x \in \mathbb{R}^{p_0}\), the blockwise tapering estimator uses only \(x_{(p_0-2\lfloor ak \log k \rfloor+1):p_0}\). Thus, the covariates which have weak partial correlations with response variables are not used.

### 2.3 Minimax Analysis of Blockwise Tapering Estimator

We give the convergence rates of the tapering and blockwise tapering estimators and show that the blockwise tapering estimator has the minimax convergence rate. We use the loss function on \(\mathbb{R}^{(p-p_0) \times p_0}\)

\[
L\{\hat{C}, \psi(\Sigma_0)\} = ||\hat{C} - \psi(\Sigma_0)||_2, \tag{3}
\]

for a pair of parameter \(\psi(\Sigma_0)\) and estimator \(\hat{C}\). The loss function gives the upper bound of the estimation error of \(E(Y \mid X = x)\) given \(x \in \mathbb{R}^{p_0}\), because the definition of the operator norm gives

\[
||\hat{C}x - E(Y \mid X = x)||_2 = ||\{\hat{C} - \psi(\Sigma_0)\}x||_2
\]

\[
\leq L\{\hat{C}, \psi(\Sigma_0)\}||x||_2.
\]
We show that the tapering estimator has a sub-optimal convergence rate under the loss function (3), while the blockwise tapering estimator has the minimax optimal convergence rate.

Theorem 2.2 gives the convergence rate of the tapering estimator. If we set $\epsilon_n$ such that

$$p^{1/2}5^{k/2}n \exp(-\lambda n) \leq \epsilon_n^2 \leq (k + \log p)/n,$$

then the convergence rate is $(k + \log p)/n + k^{-2\alpha}$, which is the same rate as the convergence rate of the tapering estimator of covariance (Cai and Zhou, 2010).

**Theorem 2.2.** Suppose $\Sigma_0 \in \mathcal{F}_{p,\alpha}(M, M_0, M_1)$. Let $k$ be a positive integer with $k < p$. If

$$k \vee \log p = o(n), \epsilon_n = O(1) \text{ and } |k/2| > \{4M/\lambda_{\min}(\Sigma_0)\}^{1/\alpha},$$

then there exist some positive constants $C$ and $\lambda$ depending only on $M$, $M_0$, $M_1$ and $\alpha$ such that

$$E_{\Sigma_0}(||\psi(\Sigma_0) - \psi\{T_k^{(\epsilon_n)}(S_n)\}||^2) \leq C\left\{k^{-2\alpha} + \frac{k + \log p}{n} + \epsilon_n^2 + \frac{p^{1/2}5^{k/2}n \exp(-\lambda n)}{\epsilon_n^2}\right\},$$

for all sufficiently large $n$.

The proof of this theorem is given in the supplementary material.

Next, we show the convergence rate of the blockwise tapering estimator. The blockwise tapering estimator is designed to estimate $\phi(\Sigma_0; 2\lfloor ak \log k \rfloor, 0)$ which approximates $\psi(\Sigma_0)$. Lemma 2.3 gives the approximation error, which is negligible when $k$ is large enough. Based on the approximation error, the convergence rate of the blockwise tapering estimator is given in Theorem 2.4. If we set $\epsilon_n$ such that

$$p^{1/2}5^{k/2}n \exp(-\lambda n) \leq \epsilon_n^2 \leq k/n,$$

then the convergence rate of the blockwise tapering estimator is $k/n + k^{-2(\alpha \wedge (\alpha r - 1))}$.

**Lemma 2.3.** Suppose $\Sigma_0 \in \mathcal{F}_{p,\alpha}(M, M_0, M_1)$. There exist some positive constants $C$ and $\tau$ depending only on $M$, $M_0$ and $M_1$ such that

$$||\psi(\Sigma_0) - T_k(\Sigma_0)_{YX\Lambda(0)}\{T_k(\Sigma_{0,XX}); 2|ak \log k|\}|| \leq C(k^{-\alpha} + k^{-\alpha r + 1}),$$

for all $a > 0$ and all sufficiently large integers $k$ and $p_0$ with $|ak \log k|/2 \geq k$ and $2|ak \log k| < p_0$.

The proof of this lemma is given in the supplementary material.
Theorem 2.4. Suppose $\Sigma_0 \in F_{\rho, \alpha}(M, M_0, M_1)$. If $k \vee \log p = o(n)$, $\lfloor k/2 \rfloor > \{4M/\lambda_{\min}(\Sigma_0)\}^{1/\alpha}$ and $\epsilon_n = O(1)$, then there exist some positive constants $C$, $\lambda$ and $\tau$ depending only on $M$, $M_0$, $M_1$ and $\alpha$ such that

$$E_{\Sigma_0} (||\psi(\Sigma_0) - \phi(S_n; 2\lfloor ak \log k \rfloor, \epsilon_n)||^2) \leq C \left\{ k^{-2(\alpha \wedge (\alpha - 1))} + \frac{k}{n} + \epsilon_n^2 + \frac{p_{1/2}^{1/2} k^{1/2} \exp(-\lambda n)}{\epsilon_n^2} \right\},$$

for all $a > 0$ and all sufficiently large $n$, $k$ and $p_0$ with $\lfloor ak \log k \rfloor / 2 \geq k$ and $p_0 > 2\lfloor ak \log k \rfloor$.

The proof of this theorem is given in Appendix A.1.

Next, we give the lower bound of the minimax risk for the conditional mean operator under the bandable covariance assumption to show that the blockwise tapering estimator is a minimax optimal estimator. Let $\hat{C} = \hat{C}(X_1, X_2, \ldots, X_n)$ be an estimator on $\mathbb{R}^{p-p_0 \times p_0}$. The minimax risk is defined as

$$\inf_{\hat{C}} \sup_{\Sigma_0 \in F_{\alpha}} E ||\psi(\Sigma_0) - \hat{C}||^2.$$ 

Theorem 2.5 gives a lower bound of the minimax risk as $n^{-2\alpha/(2\alpha + 1)}$. If we set $k$, $a$ and $\epsilon_n$ of the blockwise tapering estimator such that $k = n^{1/(2\alpha + 1)}$, $a > (\alpha + 1)/\tau$ and $p_{1/2}^{1/2} \leq k/n$, then the convergence rate is the same as the lower bound asymptotically. Thus, the minimax convergence rate is $n^{-2\alpha/(2\alpha + 1)}$, and the blockwise tapering estimator attains the convergence rate.

Theorem 2.5. There exist some positive constants $C$ and $\gamma$ depending only on $M$, $M_0$, $M_1$ and $\alpha$ such that

$$\inf_{\hat{C}} \sup_{\Sigma_0 \in F_{\alpha}} E ||\psi(\Sigma_0) - \hat{C}||^2 \geq Cn^{-2\alpha/(2\alpha + 1)},$$

for all sufficiently large $n$ and $p_0$ with $p_0 > \gamma n^{1/(2\alpha + 1)}$.

See Appendix A.2 for the proof.
3 Blockwise Tapering Post-Processed Posterior

We propose the Bayesian counterparts of the tapering estimator and the blockwise tapering estimator using the post-processed posterior method. See Lee et al. (2020). The algorithm for the post-processed posteriors consists of the following two steps.

(a) (Initial posterior sampling step) First, we obtain the initial conjugate posterior distribution on the unconstrained parameter space. We take the inverse-Wishart distribution $\text{IW}_p(B_0, \nu_0)$ as the initial prior distribution of which density function is

$$\pi^i(\Sigma) \propto |\Sigma|^{-\nu_0/2} e^{-\text{tr}(\Sigma^{-1}B_0)/2}, \quad \Sigma \in \mathcal{C}_p,$$

where $B_0 \in \mathcal{C}_p$ and $\nu_0 > 2p$. Then, the initial posterior distribution $\pi^i(\Sigma|Z_n)$ is $\text{IW}_p(B_0 + nS_n, \nu_0 + n)$, where $n$ is the number of observations, $S_n = n^{-1} \sum_{i=1}^n Z_iZ_i^T$ and $Z_n = (Z_1, \ldots, Z_n)$. We generate $\Sigma^{(1)}, \Sigma^{(2)}, \ldots, \Sigma^{(N)}$ from the initial posterior distribution.

(b) (Post-processing step) Second, we post-process the samples from the initial posterior distribution with $\psi\{T_k^{(\epsilon_n)}(\cdot)\}$ or $\phi(\cdot; 2\lfloor ak \log k \rfloor, \epsilon_n)$, which are called the tapering function and the blockwise tapering function.

We call the post-processed posteriors obtained from the post-processing functions the tapering post-processed posterior (tapering PPP) and the blockwise tapering post-processed posterior (blockwise tapering PPP).

We use the decision-theoretic framework (Lee and Lee, 2018; Lee et al., 2020) to prove the minimax optimality of the blockwise tapering post-processed posterior. We define P-loss $\mathcal{L}(\cdot, \cdot)$ and P-risk $\mathcal{R}(\cdot, \cdot)$ for the conditional mean operator as

$$\mathcal{L}\{\psi(\Sigma_0), \pi^{pp}(\cdot | Z_n; f)\} := E^\pi_i(||\psi(\Sigma_0) - f(\Sigma)||^2 | Z_n)$$

$$\mathcal{R}\{\psi(\Sigma_0), (\pi^i, f)\} := E_{\Sigma_0}\{E^\pi_i(||\psi(\Sigma_0) - f(\Sigma)||^2 | Z_n)\},$$

where $\pi^{pp}(\cdot | Z_n; f)$ is the post-processed posterior distribution derived from initial prior $\pi^i$ and post-processing function $f$, and $(\pi^i, f)$ is a pair of initial prior $\pi^i$ and post-processing
function $f$. Theorems 3.1 and 3.2 give the P-risk convergence rates of the tapering and the blockwise tapering post-processed posteriors, respectively. The convergence rates are the same as their frequentist counterparts.

**Theorem 3.1.** Suppose $\Sigma_0 \in \mathcal{F}_{p,\alpha}(M, M_0, M_1)$. Let $k$ be a positive integer with $k < p_0$, and let the prior $\pi^i$ of $\Sigma$ be $IW_p(A_n, \nu_n)$ for $A_n \in C_p$ and $\nu_n > 2p$. If $\epsilon_n = O(1)$, $\lfloor k/2 \rfloor > \{4M/\lambda_{\min}(\Sigma_0)\}^{1/\alpha}$ and $k \lor \|A_n\| \lor (\nu_n - 2p) \lor \log p = o(n)$, then there exist positive constants $C$ and $\lambda$ depending only on $M$, $M_0$ and $M_1$ such that

$$E_{\Sigma_0} \{E^{\pi^i}[\|\psi(\Sigma_0) - \psi(T_k^{(\epsilon_n)}(\Sigma))\|^2 | Z_n]\} \leq C \{k^{-2\alpha} + \frac{k + \log p}{n} + \epsilon_n^2 + \frac{p^{1/25} \exp(-\lambda n)}{\epsilon_n^2}\},$$

for all sufficiently large $n$ and $k$.

The proof of this theorem is given in the supplementary material.

**Theorem 3.2.** Suppose $\Sigma_0 \in \mathcal{F}_{p,\alpha}(M, M_0, M_1)$. Let the prior $\pi^i$ of $\Sigma$ be $IW_p(A_n, \nu_n)$ for $A_n \in C_p$ and $\nu_n > 2p$. If $\epsilon_n = O(1)$, $\lfloor k/2 \rfloor > \{4M/\lambda_{\min}(\Sigma_0)\}^{1/\alpha}$ and $k \lor \|A_n\| \lor (\nu_n - 2p) \lor \log p = o(n)$, then there exist positive constants $C$, $\tau$ and $\lambda$ depending only on $M$, $M_0$ and $M_1$ such that

$$E_{\Sigma_0} \{E^{\pi^i}[\|\psi(\Sigma_0) - \phi(\Sigma; 2\lfloor ak \log k \rfloor, \epsilon_n)\|^2 | Z_n]\} \leq C \{k^{-2(\alpha \land (\tau - 1))} + \frac{k}{n} + \epsilon_n^2 + \frac{p^{1/25} \exp(-\lambda n)}{\epsilon_n^2}\},$$

then for all $a > 0$ and all sufficiently large $n$, $k$ and $p_0$ with $\lfloor ak \log k \rfloor / 2 > k$ and $p_0 > 2\lfloor ak \log k \rfloor$.

The proof of this theorem is also given in the supplementary material.

Note that the P-risk minimax lower bound is $n^{-2\alpha/(2\alpha + 1)}$ since the P-risk convergence rate is slower than or equal to the frequentist minimax rate (Lee and Lee, 2018). Thus, if we set $k$, $a$ and $\epsilon_n$ of the blockwise tapering post-processed posterior such that $k = n^{1/(2\alpha + 1)}$, $p^{1/25} \exp(-\lambda n) \leq \epsilon_n^2 \leq k/n$ and $a > (\alpha + 1)/\tau$, then the P-risk convergence rate is the same as the lower bound asymptotically. Thus, the P-risk minimax convergence rate is $n^{-2\alpha/(2\alpha + 1)}$, and the blockwise tapering post-processed posterior attains the convergence rate.
4 Numerical Studies

4.1 Simulation

We compare the blockwise tapering estimator with the tapering estimator using simulation data. We define the true covariance matrix $\Sigma^*_0 \in \mathbb{R}^{p \times p}$ as below. Let $\Sigma^*_0 = (\sigma^*_{0,ij})_{1 \leq i,j \leq p}$, where

$$
\sigma^*_{0,ij} = \begin{cases} 
1, & 1 \leq i = j \leq p \\
\rho|i-j|^{-(\alpha+1)}, & 1 \leq i \neq j \leq p
\end{cases},
$$

and let $\Sigma_0 = \Sigma^*_0 + \{0.5 - \lambda_{\min}(\Sigma^*_0)\}I_p$, which guarantees the minimum eigenvalue of $\Sigma_0$ is bounded away from zero. We set $\rho = 0.6$ and $\alpha = 0.1$ for $\Sigma_0$ and generate data $Z_1, \ldots, Z_n$ from $N_p(0, \Sigma_0)$ independently, where $p \in \{500, 1000\}$ and $n = p/2$. Let $p_0 = 0.8p$ and fix the positive-definite adjustment parameter $\epsilon_n$ as 0.5. We define the error reduction value by choosing the blockwise tapering estimator over the tapering estimator as

$$
d_f(S_n; k, a) = ||\psi\{T_k(\epsilon_n)(S_n)\} - \psi(\Sigma_0)|| - ||\phi(S_n; 2[ak\log k], \epsilon_n) - \psi(\Sigma_0)||.
$$

We repeat generating the simulation data $T$ times, and let $Z_n^{(i)}$ and $S_n^{(i)}$ denote the data and the sample covariance matrix, respectively, in the $i$th repetition for $i \in \{1, 2, \ldots, T\}$. We summarize the error reduction values from the repetitions as t-value

$$
t_f(k, a; T) = \frac{\sum_{i=1}^{T} d_f(S_n^{(i)}; k, a)/T}{[\sum_{i=1}^{T} \{d_f(S_n^{(i)}; k, a) - \sum_{i=1}^{T} d_f(S_n^{(i)}; k, a)/T\}^2/T]^{1/2}},
$$

which is the performance measure for the comparison between the tapering and blockwise tapering estimators. We also compare the blockwise tapering PPP with the tapering PPP for the same simulation data. We define the error reduction value by choosing the blockwise tapering PPP over the tapering estimator as

$$
d_b(Z_n; k, a) = ||\hat{C}^{(TPPP)}(Z_n) - \psi(\Sigma_0)|| - ||\hat{C}^{(bTPPP)} - \psi(\Sigma_0)||,
$$

where $\hat{C}^{(TPPP)}$ and $\hat{C}^{(bTPPP)}$ are the posterior means of the tapering PPP and the blockwise tapering PPP, respectively. We define the t-value for $T$ repetitions as

$$
t_b(k, a; T) = \frac{\sum_{i=1}^{T} d_b(Z_n^{(i)}; k, a)/T}{[\sum_{i=1}^{T} \{d_b(Z_n^{(i)}; k, a) - \sum_{i=1}^{T} d_b(Z_n^{(i)}; k, a)/T\}^2/T]^{1/2}}.
$$
We evaluate $t_f(k, a; 100)$ and $t_b(k, a; 100)$ for $k \in \{2, 3, \ldots, 10\}$ and $a \in \{5, 10, 20\}$. For the post-processed posteriors we generate 1000 posterior samples in each setting. We represent the result of the evaluations in Figure 1. When $p$ is large and $k$ is small, the effects

Figure 1: The evaluated t-values $t_f(k, a; 100)$, the summarized error reductions by choosing the blockwise tapering estimator over the tapering estimator, are represented in the upper plots. The dimension of the covariance $p$ is set to 500 and 1000. As the tuning parameters of the methods, $k \in \{2, 3, \ldots, 10\}$ and $a \in \{5, 10, 20\}$ are used. The evaluated t-values $t_b(k, a; 100)$, the summarized error reductions by choosing the blockwise tapering post-processed posterior over the tapering post-processed posterior, are represented in the lower plots for the same parameters.

of error reductions by the blockwise tapering estimator and the blockwise tapering post-
processed posterior increase. Note that the convergence rates of the tapering estimator and the tapering PPP contain the additional $\log p/n$ term. The effect of the additional term is increased when another term in the convergence rate, $k/n$, is relatively small. Thus, the error reduction is effective when $p$ is large compared to $k$. The figure also shows that the tapering estimator is slightly better otherwise. If $\log p$ is not relatively large, one does not need to abandon the covariates $X_{1:p_0-2|ak \log k}$ by using the blockwise tapering estimator or the blockwise tapering PPP.

Next, we compare the tapering estimator, blockwise tapering estimator, and their Bayesian versions with two other methods: covariance estimation method and multivariate regression method. A covariance estimator can be used for the estimation of the conditional mean operator by applying the transformation (2). We use the banding estimator (Bickel and Levina, 2008), dual maximum likelihood estimator (Kauermann, 1996), and the banding post-processed posterior (Lee et al., 2020) as covariance estimators for comparison. The multivariate regression method is also used for comparison, since the multivariate linear regression coefficient is the conditional mean operator. We adopt the reduced-rank regression (Chen et al., 2013), the sparse reduced-rank regression (Chen and Huang, 2012) and the method of sparse orthogonal factor regression (SOFAR) (Uematsu et al., 2019).

We need to select tuning parameters for the conditional mean operator estimators. Based on the tuning parameter selection process, we divide the estimation methods into three categories: frequentist covariance-based method, post-processed posterior method, and multivariate regression method.

The tapering and blockwise tapering estimators belong to the frequentist covariance-based method, and the process of the tuning parameter selection is as follows. When a covariance estimator is given, the conditional mean operator and the conditional variance are derived, which yield the conditional distribution under the normality assumption. The log-likelihood function of the conditional distribution is used for the leave-one-out cross-validation. Let $\hat{\Sigma}(Z_{n,-i}, \tau)$ be a frequentist covariance estimator based on $Z_{n,-i} = (Z_1, \ldots, Z_{i-1}, Z_{i+1}, \ldots, Z_n)$ given a tuning parameter vector $\tau$. The derived conditional
mean operator is \( \psi \{ \hat{\Sigma}(Z_{n,-i}, \tau) \} \), and the conditional variance is

\[
\nu \{ \hat{\Sigma}(Z_{n,-i}, \tau) \} := \hat{\Sigma}(Z_{n,-i}, \tau)_{YY} - \hat{\Sigma}(Z_{n,-i}, \tau)_{YX} \{ \hat{\Sigma}(Z_{n,-i}, \tau)_{XX} \}^{-1} \hat{\Sigma}(Z_{n,-i}, \tau)_{XY}.
\]

We select \( \tau \) as the minimizer of

\[
\hat{R}^{(f)}(\tau) = \sum_{i=1}^{n} \log p(Y_i \mid \psi \{ \hat{\Sigma}(Z_{n,-i}, \tau) \} X_i, \nu \{ \hat{\Sigma}(Z_{n,-i}, \tau) \}),
\]

where \((X_i^T, Y_i^T)^T = Z_i\) and \(p(x \mid \mu, \Sigma)\) is the density function of the multivariate normal distribution with mean \(\mu\) and covariance \(\Sigma\). Since the conditional variance can not be derived from the blockwise tapering estimator, we use the conditional variance from the tapering estimator in this case.

For the tuning parameter selection of the post-processed posterior methods, we use the Bayesian leave-one-out cross-validation method (Gelman et al., 2014) to the log-likelihood function of the conditional distribution. Let \(\Sigma_1^{(i)}, \Sigma_2^{(i)}, \ldots, \Sigma_S^{(i)}\) be leave-one-out initial posterior samples which are generated from the initial posterior by \(Z_{n,-i}\) for \(i \in \{1, 2, \ldots, n\}\). We select the tuning parameter vector \(\tau\) as the minimizer of

\[
\sum_{i=1}^{n} \log \frac{1}{S} \sum_{s=1}^{S} p(Y_i \mid \psi^*(\Sigma_s^{(i)}; \tau) X_i, \nu^*(\Sigma_s^{(i)}; \tau))\text{,}
\]

where \(\psi^*\) and \(\nu^*\) are post-processing functions for the conditional mean operator and conditional variance given the tuning parameter \(\tau\), respectively. For the post-processing function of the conditional variance \(\nu^*\), the banding PPP uses \(\nu \{ B_k^{(\epsilon_n)}(\Sigma_s^{(i)}) \}\), where \(B_k^{(\epsilon_n)}\) is the positive-definite adjusted banding operator defined as

\[
B_k^{(\epsilon_n)}(\Sigma) = B_k(\Sigma) + (|\epsilon_n - \lambda_{\min}\{B_k(\Sigma)\}| \vee 0)I_p,
\]

and the tapering and blockwise tapering PPPs use \(\nu \{ T_k^{(\epsilon_n)}(\Sigma_s^{(i)}) \}\).

For the multivariate regression method, we use 10-fold cross-validation method as Chen and Huang (2012), Chen et al. (2013) and Uematsu et al. (2019) suggested. Note that all the methods contain the rank parameter in the tuning parameters. While we select the rank from \(\{0, 1, \ldots, 10\}\) for the reduced-rank regression, \(\{1, 2, \ldots, 10\}\) is considered for
the others. Because if the rank is zero, all the three methods coincide, we only consider the Chen et al. (2013)’s method for the zero rank case.

We set $p = 200$, $\rho = 0.6$ and $\alpha = 0.1, 0.3$ for $\Sigma_0$ and generate $Z_1, Z_2, \ldots, Z_n$ from $N_p(0, \Sigma_0)$ independently for $n \in \{100, 200\}$. We repeat generating the simulation data 100 times for each simulation setting. The performance of each method is measured as

$$\frac{1}{100} \sum_{s=1}^{100} ||\psi(\Sigma_0) - \hat{C}_s||,$$

where $\hat{C}_s$ is the point estimator for the conditional mean operator in the $s$th repetition. For the post-processed posterior methods, we use the posterior mean as the point estimator. Table 1 gives the simulation error. The tapering estimator and the blockwise tapering estimator, and their Bayesian counterparts are the best in all settings. The multivariate regression methods, i.e. the reduced-rank regression, sparse reduced-rank regression and sparse orthogonal factor regression, are the worst in all settings. Unlike the other covariance-based methods, the bandable or banded covariance structure is not considered in the multivariate regression methods. It appears that the multivariate regression framework does not perform well under the high-dimensional bandable covariance assumption.

4.2 Application to forecasting traffic speed

We apply the proposed methods to multivariate regression analysis for small area spatio-temporal data, and use this application to forecast traffic speed in Yeoui-daero, a road in Seoul.

Suppose spatio-temporal data are observed in $S$ spatial regions and $T$ times, where $S$ and $T$ are positive integers. Let $X_{s,t}$ be a random variable at $s$th spatial index and $t$th time index, $s = 1, \ldots, S$ and $t = 1, \ldots, T$. We assume

$$E[\{X_{s_1,t_1} - E(X_{s_1,t_1})\} \{X_{s_2,t_2} - E(X_{s_2,t_2})\}]$$

$$\leq r(|t_1 - t_2|), \quad s_1, s_2 \in \{1, \ldots, S\}, t_1, t_2 \in \{1, \ldots, T\},$$

where $r$ is a real-valued function from the non-negative integer space, and is assumed to
be a decreasing function. Rearranging \((X_{s,t})_{s=1,\ldots,S,t=1,\ldots,T}\), we define \(Z \in \mathbb{R}^{TS}\) as
\[
Z = (X_{1,1}, X_{2,1}, \ldots, X_{S,1}, X_{1,2}, X_{2,2}, \ldots, X_{S,T}), \tag{5}
\]
and let \(E(ZZ^T) = \Sigma_0 = (\sigma_{0,ij})\). We show that \(\Sigma_0\) is a bandable covariance, if the decreasing rate of \(r(x)\) is \(x^{-\alpha-1}\). Note that if \(mS \leq |i-j| < (m+1)S\) for \(m \in \{0,1,\ldots,T-1\}\) and \(i,j \in \{1,2,\ldots,TS\}\), then the time index difference between \(Z_i\) and \(Z_j\) is at least \(m\).
This observation and assumption (4) give \(|\sigma_{0,ij}| \leq r(|i-j|/S)|\) and
\[
\sup_j \sum_i \{|\sigma_{0,ij}| : |i-j| \geq k\} \leq \sup_j \sum_i \{|\sigma_{0,ij}| : |i-j| \geq [k/S]S\} \\
\leq \sup_j \sum_{m=[k/S]S}^{T-1} \sum_{i \in I_m^{(j)}} |\sigma_{0,ij}| \\
\leq S \sum_{m=[k/S]S}^{T-1} r(m),
\]
where \(I_m^{(j)} = \{i \in \{1,2,\ldots,p\} : |i-j|/S = m\}\). If the decreasing rate of \(r(x)\) is \(x^{-\alpha-1}\),

Table 1: Spectral norm errors of estimators for the conditional mean operator.

|                      | \(n = 100\) | \(n = 200\) |
|----------------------|-------------|-------------|
| \(\alpha = 0.1\)    |             |             |
| Tapering estimator   | 0.255       | 0.206       |
| Blockwise tapering estimator | 0.255 | 0.206 |
| Banding estimator    | 0.319       | 0.293       |
| Dual maximum likelihood estimator | 0.365 | 0.319 |
| \(\alpha = 0.3\)    |             |             |
| Tapering post-processed posterior | 0.257 | 0.208 |
| Blockwise tapering post-processed posterior | 0.257 | 0.208 |
| Banding post-processed posterior | 0.323 | 0.293 |
| Reduced-rank regression | 0.509 | 0.509 |
| Sparse reduced-rank regression | 3.324 | 3.324 |
| Sparse orthogonal factor regression | 1.823 | 1.679 |
then

$$\sup_j \sum_i \{|\sigma_{0,ij}| : |i - j| \geq k\} \leq Ck^{-\alpha},$$

for some positive constant $C$. Thus, $\Sigma_0$ is a bandable covariance, and the proposed methods for the conditional mean operator under the bandable covariance assumption can be used to predict $X_{1:S,t_0+1:T}$ given $X_{1:S,1:t_0}$.

Based on the rearrangement (5) and the proposed methods for the conditional mean operator under the bandable covariance assumption, we forecast traffic speed in Yeouidadaero using data from TOPIS (Transport Operation & Information Service, 2021). In the traffic speed data in Yeouidadaero, a daily data set consists of observations in 8 spatial indexes and 24-time indexes. Let a daily traffic speed be $(X_{s,t})_{1 \leq s \leq 8, 1 \leq t \leq 24}$, where time index $t$ indicates the time interval from $(t - 1)$ o’clock to $t$ o’clock, and the allocation of the spatial index $s$ is given in Figure 2. We rearrange $(X_{s,t})_{1 \leq s \leq 8, 1 \leq t \leq 24}$ as (5), and apply the proposed estimators to forecast $X_{1:8,18:24}$ given $X_{1:8,1:17}$.

In the data from TOPIS, we use data from January to October in 2020, excluding weekend data sets and missing data sets. We have 172 days observations which are denoted by $Z_1, Z_2, \ldots, Z_{172} \in \mathbb{R}^{192}$. To apply the proposed methods, we use mean-centered observations $\tilde{Z}_1, \tilde{Z}_2, \ldots, \tilde{Z}_{172} \in \mathbb{R}^{192}$. For the performance measure, let the training data be $Z_{\text{train}} = (\tilde{Z}_1, \tilde{Z}_2, \ldots, \tilde{Z}_{86})$, and the test data be $Z_{\text{test}} = (\tilde{Z}_{87}, \tilde{Z}_{88}, \ldots, \tilde{Z}_{172})$. The forecast errors are summarized as

$$\frac{1}{86} \sum_{i=87}^{172} \|\hat{C}(Z_{\text{train}})(\tilde{Z}_i)_{1:p_0} - (\tilde{Z}_i)_{(p_0+1):p}\|_2,$$

where $p_0 = 17 \times 8$ and $\hat{C}(Z_{\text{train}})$ is a point estimator for the conditional mean operator based on $Z_{\text{train}}$. The summarized forecast errors are represented in Table 2, which shows the tapering and blockwise tapering estimators and their Bayesian versions are the best among all methods.
Figure 2: The eight routes in Yeouido and their index allocation.
Table 2: The root mean square errors of forecast results for traffic speed in Yeoui-daero.

| Method                              | Error |
|-------------------------------------|-------|
| Tapering estimator                  | 2.80  |
| Blockwise tapering estimator        | 2.80  |
| Banding estimator                   | 2.85  |
| Dual maximum likelihood estimator   | 3.33  |
| Tapering post-processed posterior   | 2.78  |
| Blockwise tapering post-processed posterior | 2.78 |
| Banding post-processed posterior    | 2.87  |
| Reduced-rank regression             | 3.59  |
| Sparse reduced-rank regression      | 3.39  |
| Sparse orthogonal factor regression | 4.31  |

5 Discussion

We have considered the estimation of the conditional mean operator under the bandable covariance assumption, which is useful for the multivariate linear regression when there is a natural order in the variables. We showed that the plug-in estimator by the tapering estimator of covariance, which is the minimax optimal estimator for the class of bandable covariance, is sub-optimal for the conditional mean operator. This observation implies that when a function of the covariance matrix is to be estimated, the plug-in estimator by a minimax optimal covariance estimator may not be optimal. We have proposed the blockwise tapering estimator and the blockwise tapering post-processed posterior as minimax-optimal estimators for the conditional mean operator under the bandable covariance assumption. We constructed the estimators by modifying the tapering estimator and the tapering post-processed posterior to exclude the covariates which have small partial correlations with the response variables. Using the numerical studies, we also showed that the blockwise tapering estimator and the blockwise tapering post-processed posterior have smaller errors when $p$ is large enough.
A Proofs of main theorems

In this section, we prove Theorems 2.4 and 2.5, which give the convergence rate of the blockwise tapering estimator and the lower bound of the minimax risk, respectively. The proofs of the other theorems and lemma in Sections 2 and 3 are given in the supplementary material.

We give notations for the proofs. Let $||\Sigma||_F = \text{tr}(\Sigma \Sigma^T)$ and $||\Sigma||_r$ be the Frobenius norm and the matrix $r$-norm for a covariance matrix $\Sigma$, respectively. We also let $W_p(B_0, \nu_0)$ be Wishart distribution of which density function is

$$
\pi(\Sigma) \propto ||\Sigma|^{(\nu_0-p-1)/2}e^{-\text{tr}(B_0^{-1}\Sigma)/2}, \quad \Sigma \in \mathcal{C}_p,
$$

where $B_0 \in \mathcal{C}_p$ and $\nu_0 > p - 1$.

A.1 Proof of Theorem 4

In this subsection, we show the convergence rate of the blockwise tapering estimator by proving Theorem 2.4. First, we present Lemmas A.1-A.4 necessary for the proof of Theorem 2.4.

Lemma A.1. Let $p$ and $k$ be positive integers with $k < p$ and suppose $\Sigma_0 \in \mathcal{F}_{p,\alpha}(M, M_0, M_1)$. There exist some positive constants $C_1$ and $C_2$ depending only on $M$, $M_0$ and $M_1$ such that

$$
||\Sigma_0^{-1} - B_k(\Sigma_0)^{-1}||_1 \leq C_1 k^{-\alpha},
$$

$$
||\Sigma_0^{-1} - T_k(\Sigma_0)^{-1}||_1 \leq C_2 (|k/2|)^{-\alpha},
$$

for all sufficiently large $k$.

The proof of this lemma is given in the supplementary material.

Lemma A.2. Let $n$, $k$ and $p$ be positive integers with $k \leq p$ and suppose $\Sigma_0 \in \mathcal{F}_{p,\alpha}(M, M_0, M_1)$. If $c \leq \lambda_{\min}(\Sigma_0)/2$ and $|k/2| > \{4M/\lambda_{\min}(\Sigma_0)\}^{1/\alpha}$, then

$$
P_{\Sigma_0}[\lambda_{\min}(T_k(S_n)) \leq c] \leq 2p5^k \exp(-\lambda n),
$$

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for some positive constant $\lambda$ depending only on $M_0$ and $M_1$.

The proof of this lemma is given in the supplementary material.

**Lemma A.3.** Let $n$, $p$ and $k$ be positive integers with $k \leq p$ and suppose $\Sigma_0 \in \mathcal{F}_{p,\alpha}(M, M_0, M_1)$. If $k \vee \log p = o(n)$ and $\epsilon_n = O(1)$, then there exists some positive constant $C$ depending only on $M_0$ and $M_1$ such that

$$E_{\Sigma_0}(||T_k^{(\epsilon_n)}(S_n) - \Sigma_0||^4) \leq C,$$

for all sufficiently large $n$.

The proof of this lemma is given in the supplementary material.

**Lemma A.4.** Suppose $\Sigma_0 \in \mathcal{F}_{p,\alpha}(M, M_0, M_1)$. Let $q$ and $k$ be positive integers with $k < q \leq p$, and let $(\Sigma_0)_{1:q,1:q}$ and $\{T_k^{(\epsilon_n)}(S_n)\}_{1:q,1:q}$ denoted by $\Sigma_{0,11}$ and $T_k^{(\epsilon_n)}(S_n)_{11}$, respectively. If $k \vee \log p = o(n)$, $[k/2] > \{4M/\lambda_{\min}(\Sigma_0)\}^{1/\alpha}$ and $\epsilon_n = O(1)$, then there exist some positive constants $C$ and $\lambda$ depending only on $M$, $M_0$, $M_1$ and $\alpha$ such that

$$E_{\Sigma_0}(||T_k^{(\epsilon_n)}(S_n)_{11}^{-1} - \Sigma_{0,11}^{-1}||^2) \leq C\left\{\frac{k + \log p}{n} + k^{-2\alpha} + \epsilon_n^2 + \frac{p^{1/2}5^{k/2}\exp(-\lambda n)}{\epsilon_n^2}\right\},$$

for all sufficiently large $n$.

The proof of this lemma is given in the supplementary material.

Now we prove Theorem 2.4.

**Proof of Theorem 2.4.** We have

$$E(||\psi(\Sigma_0) - T_k(S_n)_{YX}\Lambda^{(\epsilon_n)}\{T_k(S_n)_{XX}; 2[ak \log k]\}||^2)$$

$$\leq 2||\psi(\Sigma_0) - T_k(\Sigma_0)_{YX}\Lambda^{(0)}\{T_k(\Sigma_0)_{XX}; 2[ak \log k]\}||^2 \tag{6}$$

$$+4E(||T_k(\Sigma_0)_{YX} - T_k(S_n)_{YX}||^2 ||\Lambda^{(\epsilon_n)}\{T_k(S_n)_{XX}; 2[ak \log k]\}||^2) \tag{7}$$

$$+4||T_k(\Sigma_0)||^2E(||\Lambda^{(0)}\{T_k(\Sigma_0)_{XX}; 2[ak \log k]\} - \Lambda^{(\epsilon_n)}\{T_k(S_n)_{XX}; 2[ak \log k]\}||^2) \tag{8}$$

By Lemma 2.3, there exist some positive constants $C_1$ and $\lambda_1$ depending only on $M$, $M_0$, $M_1$ and $\alpha$ such that

$$\tag{6} \leq C_1 k^{-2(\alpha \wedge (a\lambda_1 - 1))},$$

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for all sufficiently large $k$ with $\lceil ak \log k \rceil / 2 \geq k$ and $p_0 > 2\lceil ak \log k \rceil$.

Next, we show the upper bound of (7). Let $\tilde{M} := M_{p_0 - 2\lceil ak \log k \rceil + 1}$ in this proof. By the definition of $\Lambda^{(\epsilon_n)}$, we have

$$||\Lambda^{(\epsilon_n)} \{T_k(S_n)_{XX}; 2\lceil ak \log k \rceil \}|| = ||T_k^{(\epsilon_n)} [\tilde{M} \{(S_n)_{XX}\}]^{-1}||,$$

and

$$\begin{align*}
(7) & = 4E(||T_k(\Sigma_0)_{YX} - T_k(S_n)_{YX}||^2 ||T_k^{(\epsilon_n)} [\tilde{M} \{(S_n)_{XX}\}]^{-1}||^2) \\
& \leq \frac{4}{\epsilon_n^2} E(||T_k(\Sigma_0)_{YX} - T_k(S_n)_{YX}||^2 I(\lambda_{\min}[\tilde{M} \{(S_n)_{XX}\}] < M_1/2) \\
& + \frac{16}{M_1^2} E(||T_k(\Sigma_0)_{YX} - T_k(S_n)_{YX}||^2) \\
& \leq \frac{4}{\epsilon_n^2} E(||T_k(\Sigma_0) - T_k(S_n)||^4)^{1/2} P\{\lambda_{\min}(S_n) < M_1/2\}^{1/2} \\
& + \frac{16}{M_1^2} E(||T_k(\Sigma_0) - T_k(S_n)||^2) \\
& \leq \frac{4}{\epsilon_n^2} E(2^3 ||\Sigma_0 - T_k(S_n)||^4 + 2^3 M^4 (\lceil k/2 \rceil)^{-4\alpha})^{1/2} P\{\lambda_{\min}(S_n) < M_1/2\}^{1/2} \\
& + \frac{16}{M_1^2} E(2||\Sigma_0 - T_k(S_n)||^2 + 2M^2 (\lceil k/2 \rceil)^{-2\alpha}) \\
& \leq C_2 \left\{ \frac{1}{\epsilon_n^2} p^{1/2} 5^{k/2} \exp(-\lambda_2 n) + \frac{k + \log p}{n} + k^{-2\alpha} \right\},
\end{align*}$$

for some positive constants $C_2$ and $\lambda_2$ depending only on $M$, $M_0$, $M_1$ and $\alpha$. The first inequality holds since

$$\lambda_{\min}(T_k^{(\epsilon_n)}[\tilde{M} \{(S_n)_{XX}\}]) \geq \epsilon_n.$$

The third inequality holds since

$$||T_k(\Sigma_0) - \Sigma_0||_1 \leq ||B_{\lceil k/2 \rceil}(\Sigma_0) - \Sigma_0||_1 \leq M (\lceil k/2 \rceil)^{-\alpha}. \quad (9)$$

The last inequality holds by Lemmas A.2, A.3 and Theorem 2 of Cai and Zhou (2010). For the upper bound of (8), we have that there exists some positive constant $C_3$ depending
only on $M, M_0$ and $M_1$ such that
\[
E(||\Lambda^{(0)}\{T_k(\Sigma_{0,XX}); 2[ak \log k]\} - \Lambda^{(\epsilon_n)}\{T_k(\Sigma_{0,XX}); 2[ak \log k]\}||^2)
\]
\[
= E(||T_k\{\tilde{M}(\Sigma_{0,XX})\}^{-1} - T_k^{(\epsilon_n)}[\tilde{M}\{(S_n)_{XX}\}]^{-1}||^2)
\]
\[
\leq 2E(||\tilde{M}(\Sigma_{0,XX})^{-1} - T_k^{(\epsilon_n)}[\tilde{M}\{(S_n)_{XX}\}]^{-1}||^2)
\]
\[
+ 2||T_k\{\tilde{M}(\Sigma_{0,XX})\}^{-1} - \tilde{M}(\Sigma_{0,XX})^{-1}||^2
\]
\[
\leq 2E(||\tilde{M}(\Sigma_{0,XX})^{-1} - T_k^{(\epsilon_n)}[\tilde{M}\{(S_n)_{XX}\}]^{-1}||^2) + C_3([k/2])^{-2\alpha},
\]
for all sufficiently large $k$. The first equality is satisfied by the definition of $\Lambda^{(0)}$ and $\Lambda^{(\epsilon_n)}$. The last inequality holds by Lemma A.1 since $\tilde{M}(\Sigma_{0,XX}) \in F_{2[ak \log k], \alpha}(M, M_0, M_1)$. We apply Lemma A.4 and obtain that there exist some positive constants $C_4$ and $\lambda_3$ depending only on $M, M_0, M_1$ and $\alpha$ such that
\[
E(||\tilde{M}(\Sigma_{0,XX})^{-1} - T_k^{(\epsilon_n)}[\tilde{M}\{(S_n)_{XX}\}]^{-1}||^2)
\]
\[
\leq C_4\left\{\frac{k + \log(2ak \log k)}{n} + \epsilon_n^2 + ak \log k \exp(-\lambda_1 n)\right\},
\]
for all sufficiently large $n$. Thus, there exists some positive constant $C_5$ depending only on $M, M_0, M_1$ and $\alpha$ such that
\[
(8) \leq C_5\left\{\frac{k + \log(2ak \log k)}{n} + \epsilon_n^2 + ak \log k 5^k \exp(-\lambda_1 n)\right\},
\]
for all sufficiently large $n$ and $k$. Collecting the upper bounds of (6), (7) and (8), we complete the proof.

\[\square\]

**A.2 Proof of Theorem 5**

In this subsection, we prove Theorem 2.5 which gives the lower bound of the minimax risk for the conditional mean operator under the bandable covariance assumption. For probability measures $P_\theta$ and $P_{\theta'}$, we define
\[
||P_\theta - P_{\theta'}||_1 = \int |p_{\theta'} - p_\theta| d\nu
\]
\[
||P_\theta \wedge P_{\theta'}|| = \int p_{\theta'} \wedge p_\theta d\nu,
\]
where \( p_\theta \) and \( p_{\theta'} \) are probability density functions of \( P_\theta \) and \( P_{\theta'} \), respectively, with respect to the reference measure \( \nu \). First, we provide Lemma A.5 which is a reformulation of the proof of Lemma 6 in Cai and Zhou (2010).

**Lemma A.5.** Suppose \( \Sigma \) and \( \Sigma' \) are \( p \times p \)-positive definite matrices. Let \( P_{\Sigma} \) be the joint distribution of \( X_1, X_2, \ldots, X_n \), which are independent and identically generated from \( N_p(0, \Sigma) \). If \( ||\Sigma - \Sigma'||_2(||\Sigma^{-1}||_2 \wedge ||\Sigma'^{-1}||_2) < 1/2 \), then

\[
||P_{\Sigma} - P_{\Sigma'}||_1^2 \leq n(||\Sigma^{-1}||_2 \wedge ||\Sigma'^{-1}||_2)^2 ||\Sigma - \Sigma'||_2^2.
\]

The proof of this lemma is given in the supplementary material.

**Proof of Theorem 2.5.** Let \( C_{p,p_0} = \{ A \in \mathbb{R}^{p \times p} : A_{1:p_0,1:p_0} \in C_{p_0} \} \), and \( (C_{p,p_0})^\chi \) be the space of estimators on \( C_{p,p_0} \), where \( \chi \) is the sample space. Since for an arbitrary \( B \in \mathbb{R}^{(p-p_0) \times p_0} \) there exists \( A_B \in C_{p,p_0} \) such that \( \psi(A_B,p_0) = B \), it suffices to show

\[
\inf_{\hat{A} \in (C_{p,p_0})^\chi} \sup_{\Sigma_0 \in \mathcal{F}_{p,\alpha}} E[||\psi(\Sigma_0; p_0; \hat{A}) - \psi(\hat{A}; p_0)||^2] \geq C n^{-2\alpha/(2\alpha+1)},
\]

for some positive constant \( C \). Let \( d(\hat{\Sigma}, \Sigma_0) = ||\hat{\Sigma}_{XX}^{-1} - \Sigma_0^{-1}||_2 / ||\Sigma_0||_2 \), which is a semimetric on \( C_{p,p_0} \). For a positive integer \( k \) with \( k < p_0/2 \), let \( \Theta = \{0,1\}^k \), and let \( H(\theta, \theta') \) be the Hamming distance on \( \Theta \). We define

\[
\Sigma(\theta) = \bar{M} I_p + \tau \sum_{m=1}^k \theta_mB(m+p_0;k), \ \theta = (\theta_1, \theta_2, \ldots, \theta_k) \in \Theta,
\]

where \( \tau = \{M(2k)^{-\alpha-1}\} \wedge \{(M_0 - \bar{M})/(2k)\} \), \( \bar{M} = (M_0 + M_1)/2 \), \( B(l;k) = (b_{ij})_{1 \leq i,j \leq k} \) and

\[
b_{ij} = I(i = l \text{ and } l - 2k \leq j \leq l - 1, \text{ or } j = l \text{ and } l - 2k \leq i \leq l - 1). \]

Note that \( \Sigma(\theta) \in \mathcal{F}_{p,\alpha}(M, M_0, M_1) \) for all \( \theta \in \Theta \). Thus,

\[
\inf_{\hat{A} \in (C_{p,p_0})^\chi} \sup_{\Sigma_0 \in \mathcal{F}_{p,\alpha}} E[||\psi(\Sigma_0; p_0; \hat{A}) - \psi(\hat{A}; p_0)||^2] \geq \inf_{\hat{A} \in (C_{p,p_0})^\chi} \sup_{\theta \in \Theta} E[||\psi(\Sigma(\theta); p_0) - \psi(\hat{A}; p_0)||^2]
\]

\[
= \inf_{\hat{A} \in (C_{p,p_0})^\chi} \sup_{\theta \in \Theta} E[d^2(\Sigma(\theta); \hat{A})] \tag{10}
\]
By the Assouad lemma (Cai and Zhou, 2010, Lemma 4), we have, for all \( s > 0 \),

\[
\sup_{\theta \in \Theta} 2^s E[d^s \{ \hat{A}, \Sigma(\theta) \} ] \geq \min_{H(\theta, \theta') \geq 1} \frac{d^s \{ \Sigma(\theta), \Sigma(\theta') \} }{H(\theta, \theta')} \min_{H(\theta, \theta') = 1} ||P_\theta \wedge P_{\theta'}||, \tag{11}
\]

where \( P_\theta \) is the joint distribution of \( n \) independent observations from the multivariate normal distribution with mean zero and covariance \( \Sigma(\theta) \).

First, we show the lower bound of \( d^2 \{ \Sigma(\theta), \Sigma(\theta') \} / H(\theta, \theta') \).

For vector \( v = \{ I(p_0 - k < i \leq p_0) \}_{1 \leq i \leq p_0} \) and all \( \theta, \theta' \in \Theta \) with \( \theta \neq \theta' \), we have

\[
d^2 \{ \Sigma(\theta), \Sigma(\theta') \} \geq \frac{||\{\Sigma(\theta)_{YX} - \Sigma(\theta')_{YX}\}(\bar{M}I_{p_0})^{-1}v||^2}{||v||^2} \\
\geq \bar{M}^{-2} \frac{||\{\Sigma(\theta)_{YX} - \Sigma(\theta')_{YX}\}v||^2}{||v||^2} \\
\geq \bar{M}^{-2} H(\theta, \theta') \tau^2 k,
\]

which implies

\[
\min_{H(\theta, \theta') \geq 1} \frac{d^2 \{ \Sigma(\theta), \Sigma(\theta') \} }{H(\theta, \theta')} \geq \bar{M}^{-2} \tau^2 k. \tag{12}
\]

Next, we consider the lower bound of \( \min_{H(\theta, \theta') = 1} ||P_\theta \wedge P_{\theta'}||. \) We assume \( H(\theta, \theta') = 1, 2\tau k < \bar{M}, 2\tau k/(\bar{M} - 2\tau k) < 1/2 \) and \( (\sqrt{2n^{1/2}k^{1/2}})/(\bar{M} - 2\tau k) \leq 1/2 \). We have

\[
||\Sigma(\theta) - \Sigma(\theta')||_2 \leq ||\Sigma(\theta) - \Sigma(\theta')||_1 \\
\leq 2\tau k,
\]

and

\[
||\Sigma(\theta)^{-1}|| = \lambda_{\min} \{\Sigma(\theta)\}^{-1} \\
\leq \frac{1}{\bar{M} - ||\Sigma(\theta) - MI_p||} \\
\leq \frac{1}{\bar{M} - 2\tau^2 k}.
\]
where the first inequality holds by Lemma 4.14 in Lee et al. (2020). Since $2\tau k/(\bar{M} - 2\tau k) < 1/2$, Lemma A.5 gives

$$
\min_{H(\theta, \theta') = 1} ||P_\theta \land P_{\theta'}|| = 1 - \max_{H(\theta, \theta') = 1} ||P_\theta - P_{\theta'}||_{1/2} \\
\geq 1 - \frac{n^{1/2}||\Sigma(\theta) - \Sigma(\theta')||_F}{2(\bar{M} - 2\tau k)} \\
\geq 1 - \frac{\sqrt{2}n^{1/2}k^{1/2}\tau}{\bar{M} - 2\tau k},
$$

where the last inequality holds since $||\Sigma(\theta) - \Sigma(\theta')||_F \leq (8k\tau^2)^{1/2}$. Since $(\sqrt{2}n^{1/2}k^{1/2}\tau)/(\bar{M} - 2\tau k) \leq 1/2$,

$$
\min_{H(\theta, \theta') = 1} ||P_\theta \land P_{\theta'}|| \geq 1/2.
$$

Thus, collecting inequalities (10), (11) and (12), we get

$$
\inf_{\hat{\Sigma}} \max_{\theta \in \{0, 1\}^k} 2^2\mathbb{E}_{\theta d^2}{\hat{\Sigma}, \Sigma(\theta)} \geq ck^{2}\tau^2,
$$

for some positive constant $c$. Since $\tau \leq M(2k)^{-\alpha - 1}$ we obtain the desired minimax lower bound by setting $k = (\gamma n)^{1/(2\alpha + 1)}/2$, where $\gamma = 16M^2/(\bar{M}^2)$.

Finally, we check the assumed conditions on $k$:

$$
2k < p_0 \\
2\tau k < \bar{M} \\
2\tau k/(\bar{M} - 2\tau k) < 1/2 \\
\frac{\sqrt{2}n^{1/2}k^{1/2}\tau}{\bar{M} - 2\tau k} \leq 1/2.
$$

Note $\tau \leq M(2k)^{-\alpha - 1}$ and $k = (\gamma n)^{1/(2\alpha + 1)}/2$. The first condition is satisfied when $(\gamma n)^{1/(2\alpha + 1)} < p_0$. For the other conditions, we have

$$
2\tau k \leq M(\gamma n)^{-\alpha/(2\alpha + 1)} \\
2\tau k/(\bar{M} - 2\tau k) \leq \frac{M(\gamma n)^{-\alpha/(2\alpha + 1)}}{M - M(\gamma n)^{-\alpha/(2\alpha + 1)}} \\
\frac{\sqrt{2}n^{1/2}k^{1/2}\tau}{\bar{M} - 2\tau k} \leq \frac{M/\gamma^{1/2}}{M - M(\gamma n)^{-\alpha/(2\alpha + 1)}}.
$$
The first and second upper bounds of these inequalities can be arbitrary small numbers for all sufficiently large $n$. The last upper bound is smaller than $1/2$ for all sufficiently large $n$ since $\gamma = 16M^2/(\bar{M}^2)$. Thus, the assumed conditions on $k$ are satisfied for all sufficiently large $n$.

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