Uncertainty quantification for iterative algorithms in linear models with application to early stopping

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Abstract: This paper investigates the iterates $\hat{b}^1, \ldots, \hat{b}^T$ obtained from iterative algorithms in highdimensional linear regression problems, in the regime where the feature dimension p is comparable with the sample size n, i.e., $p \simeq n$. The analysis and proposed estimators are applicable to Gradient Descent (GD), proximal GD and their accelerated variants such as Fast Iterative Soft-Thresholding (FISTA). The paper proposes novel estimators for the generalization error of the iterate \hat{b}^t for any fixed iteration t along the trajectory. These estimators are proved to be \sqrt{n} -consistent under Gaussian designs. Applications to early-stopping are provided: when the generalization error of the iterates is a U-shape function of the iteration t, the estimates allow to select from the data an iteration \hat{t} that achieves the smallest generalization error along the trajectory. Additionally, we provide a technique for developing debiasing corrections and valid confidence intervals for the components of the true coefficient vector from the iterate \hat{b}^t at any finite iteration t. Extensive simulations on synthetic data illustrate the theoretical results.

Keywords and phrases: high-dimensional models, risk estimate, Lasso, generalization error.

Contents

1. Introduction

Consider the linear model

$$(1.1) y = Xb^* + \varepsilon,$$

where $\boldsymbol{y} \in \mathbb{R}^n$ is the response vector, $\boldsymbol{X} \in \mathbb{R}^{n \times p}$ is the design matrix with i.i.d. rows with covariance $\boldsymbol{\Sigma} \in \mathbb{R}^{p \times p}$, and $\boldsymbol{\varepsilon} \in \mathbb{R}^n$ is the noise vector with i.i.d. entries from $N(0, \sigma^2)$. To estimate the coefficient vector in the linear model with dimension p larger or comparable to the sample size n, a common strategy is to consider the penalized least-squares estimator

(1.2)
$$\widehat{\boldsymbol{b}} \in \operatorname*{arg\,min}_{\boldsymbol{b} \in \mathbb{R}^p} \frac{1}{2n} \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{b}\|^2 + \rho(\boldsymbol{b}).$$

This estimator could be ordinary least-squares estimate (if $\rho(\mathbf{b}) = 0$), Ridge regression, Lasso (Tibshirani, 1996), Elastic Net (Zou and Hastie, 2005), group Lasso (Yuan and Lin, 2006), nuclear norm penalization (Koltchinskii et al., 2011) or Slope (Bogdan et al., 2015), to name a few convex examples. Concave penalty functions ρ in (1.2) have also been considered, including SCAD (Fan and Li, 2001) and MCP (Zhang, 2010). The properties of the penalized estimator $\hat{\mathbf{b}}$ in (1.2) are now well understood in high-dimensional regimes where the dimension p is larger than n. For instance, optimal L1 and L2 bounds of Lasso estimator $\hat{\mathbf{b}}$ have been studied extensively (Wainwright, 2009; Bickel et al., 2009; Ye and Zhang, 2010; Bayati and Montanari, 2012; Dalalyan et al., 2017; Bellec et al., 2018, among others). Beyond risk bounds, confidence intervals for single entries of \mathbf{b}^* have been developed in Zhang and Zhang (2014b); Javanmard and Montanari (2014); van de Geer et al. (2014a), and more recently in Cai and Guo (2017); Javanmard and Montanari (2018); Bellec and Zhang (2022b). We refer readers to Bühlmann and Van De Geer (2011); van de Geer (2016) for a comprehensive review of such results. In most results cited above, $p \gg n$ and the L2 risk of (1.2) typically converges to 0, i.e., $\hat{\mathbf{b}}$ is consistent. Consistency, on the other hand, is not granted in the regime where dimension and sample size are of the same order, i.e.,

(1.3)
$$p \simeq n$$
, or $\lim(p/n)$ exists and is finite.

In this regime, Bayati and Montanari (2012); Miolane and Montanari (2021) showed that the Lasso L2 risk, under suitable assumptions, converges to a finite positive constant that can be characterized by a system of nonlinear equations. Regime (1.3) will be in force in the present paper. Since the early works (Bayati and Montanari, 2012; El Karoui et al., 2013; Donoho and Montanari, 2016) on this proportional regime, significant progress was made to develop a unified theory explaining the behaviors of M-estimators and penalized estimators when (1.3) holds, see for instance Thrampoulidis et al. (2018); Celentano et al. (2023); Loureiro et al. (2021). Compared with the early debiasing literature (Zhang and Zhang, 2014a; van de Geer et al., 2014a; Javanmard and Montanari, 2014), new debiasing techniques are needed to construct confidence intervals for components of b^* in this regime, in particular with the need to account for the degrees-offreedom of the estimator (1.2) for the debiasing correction (Bellec and Zhang, 2022a; Celentano et al., 2023; Bellec and Zhang, 2023).

1.1. Iterative algorithms

As we have seen, the properties of the estimator \hat{b} in (1.2) are now well understood, both in the classical high-dimensional regime with $p \gg n$ and in the proportional regime (1.3). In practice, an exact minimizer \hat{b} of (1.2) is typically unavailable in closed-form, and numerical approximations are used instead. To solve the minimization problem (1.2) numerically, the practitioner resorts to iterative algorithms developed in the optimization literature to obtain an approximate solution to (1.2).

For smooth objective functions, this includes first-order methods such as Gradient Descent (GD), its accelerated version known as Accelerated Gradient Descent (AGD) (Nesterov, 1983), or its randomized variants (Bottou, 2010). For non-smooth objective functions, the practitioner typically resorts to coordinate descent (Friedman et al., 2010) or iterative algorithms involving the proximal operator of ρ such as Iterative

Soft-Thresholding Algorithm (ISTA) (Daubechies et al., 2004) and its accelerated version Fast Iterative Soft-Thresholding Algorithm (FISTA) (Beck and Teboulle, 2009). Such iterative algorithm starts with an initializer \hat{b}^1 and then iteratively produces iterates \hat{b}^2 , \hat{b}^3 ,... by applying a nonlinear function to a weighted sum of the previous iterate and the gradient of the first term in (1.2) (the smooth part of the objective function) at the previous iterate. For instance, for a convex penalty function ρ in (1.2) the proximal gradient descent algorithm solves (1.2) with the iterations

(1.4)
$$\widehat{\boldsymbol{b}}^{t+1} = \operatorname{prox}\left[\frac{1}{L}\rho\right]\left(\widehat{\boldsymbol{b}}^t + \frac{1}{nL}\boldsymbol{X}^\top (\boldsymbol{y} - \boldsymbol{X}\widehat{\boldsymbol{b}}^t)\right),$$

where the proximal operator is defined as $\operatorname{prox}[\frac{1}{L}\rho](\boldsymbol{v}) = \operatorname{arg\,min}_{\boldsymbol{b}\in\mathbb{R}^p} \|\boldsymbol{b}-\boldsymbol{v}\|^2/2 + \frac{1}{L}\rho(\boldsymbol{b})$ and the scalar L > 0 is usually taken (Beck and Teboulle, 2009) as an upper bound on the Lipschitz constant of the gradient of the first term in the objective function (1.2), i.e., such that $L \geq \|\boldsymbol{X}^\top \boldsymbol{X}/n\|_{\text{op}}$. For the Lasso problem with $\rho(\boldsymbol{b}) = \lambda \|\boldsymbol{b}\|_1$ in (1.2), the iterations (1.4) become the ISTA iterations

(1.5)
$$\widehat{\boldsymbol{b}}^{t+1} = \operatorname{soft}_{\lambda/L} \left(\widehat{\boldsymbol{b}}^t + \frac{1}{nL} \boldsymbol{X}^\top (\boldsymbol{y} - \boldsymbol{X} \widehat{\boldsymbol{b}}^t) \right),$$

where $\operatorname{soft}_{\lambda/L}(\cdot)$ applies the soft-thresholding $u \mapsto \operatorname{sign}(u)(|u| - \lambda/L)_+$ componentwise. For AGD and FISTA, the recursion formula defining \hat{b}^{t+1} involves the iterates $(\hat{b}^t, \hat{b}^{t-1})$ as we will detail in Sections 3.2 and 3.4 below.

More generally, the focus of the present paper is on iterative algorithm of the form

(1.6)
$$\widehat{\boldsymbol{b}}^{t+1} = \boldsymbol{g}_{t+1}(\widehat{\boldsymbol{b}}^t, \widehat{\boldsymbol{b}}^{t-1}, \boldsymbol{v}^t, \boldsymbol{v}^{t-1}), \quad \text{where} \quad \boldsymbol{v}^t = \frac{1}{n} \boldsymbol{X}^\top (\boldsymbol{y} - \boldsymbol{X} \widehat{\boldsymbol{b}}^t)$$

for nonlinear Lipschitz functions g_{t+1} , in order to include accelerated algorithms from the optimization literature that are of the form (1.6), i.e., using the previous two iterations, including AGD (Nesterov, 1983) and FISTA (Beck and Teboulle, 2009). Our theory actually applies to recursions of the form

(1.7)
$$\widehat{\boldsymbol{b}}^{t+1} = \boldsymbol{g}_{t+1}(\widehat{\boldsymbol{b}}^t, \widehat{\boldsymbol{b}}^{t-1}, \dots, \widehat{\boldsymbol{b}}^2, \widehat{\boldsymbol{b}}^1, \ \boldsymbol{v}^t, \boldsymbol{v}^{t-1}, \dots, \boldsymbol{v}^2, \boldsymbol{v}^1)$$

although the typical optimization algorithms mentioned in the previous paragraph only use the previous two iterates, as in (1.6).

These iterative algorithms are typically stopped when a stopping criterion is met. Existing theories in the optimization literature on iterative algorithms examine their convergence properties regarding the training error, specifically how fast (in t) does the objective function at the iterate \hat{b}^t approach the minimal value in (1.2), or how fast does the iterate \hat{b}^t approach an ideal minimizer \hat{b} of (1.2) as $t \to +\infty$. For instance, Beck and Teboulle (2009) showed that FISTA enjoys a faster rate of convergence compared to ISTA.

1.2. Statistical properties of iterates for small t or when convergence fails

If \hat{b}^t converges to \hat{b} as t increases, it is reasonable to expect that the properties of \hat{b} (e.g., risk bounds, or debiased confidence intervals for components of b^*) are also valid for \hat{b}^t provided t is sufficiently large. One motivation of the present paper is the study of iterates $(\hat{b}^t)_{t\geq 1}$ for small values of t, or when convergence of these iterates fail for the optimization problem (1.2). In such cases, because \hat{b}^t and an ideal solution \hat{b} to (1.2) significantly differ from each other, we should not expect that the statistical properties of \hat{b} are inherited by \hat{b}^t . This calls for a statistical analysis of \hat{b}^t itself, rather than ideal minimizers \hat{b} of the optimization problem (1.2). Two concrete situations for which convergence fails are the following.

- The dataset (\mathbf{X}, \mathbf{y}) is so large that a single iteration of the recursion (1.7) is slow and/or computationally costly. Running the iterations (1.7) until convergence $(t \to +\infty)$ is then not realistic. Still, in such situation, the practitioner may only run a few iterations and use \hat{b}^t for a small t (e.g., t = 5 or t = 10) for statistical purposes, including making predictions at new test data points \mathbf{x}_{new} .
- If the optimization problem (1.2) is non-convex, as is the case with SCAD (Fan and Li, 2001) or MCP (Zhang, 2010), convergence of the iterates to a local or global solution to (1.2) is a subtle problem.

Iterative algorithms may converge to a local optima. Specific algorithms have been developed to ensure good statistical properties under suitable assumptions, such as Restricted Eigenvalue conditions (Zhang, 2010; Feng and Zhang, 2019). However, such conditions are often not verifiable in practice (Bandeira et al., 2013). Despite the absence of any convergence guarantees, the algorithm used to solve (1.2) for SCAD or MCP is still implementable, yielding iterates in the form of (1.7). Despite the lack of verifiable conditions to guarantee convergence, at a given t the iterate \hat{b}^t can still be used for downstream tasks, for instance predictions at test data points \boldsymbol{x}_{new} .

In both situations, convergence does not occur and statistical properties of \hat{b}^t at a finite t are expected to significantly departs from those of \hat{b} . Using \hat{b}^t for statistical purposes, instead of waiting for convergence, is also appealing in order to save computational resources. This calls for a statistical theory of \hat{b}^t itself, rather than ideal minimizers \hat{b} of (1.2). The present makes contributions in this direction with two major applications on the properties of the iterate \hat{b}^t at a fixed t: assessing the predictive performance of \hat{b}^t , and constructing debiased confidence intervals for components of b^* based on \hat{b}^t .

1.3. Early stopping

It is important to recognize that the predictive performance of \hat{b}^t does not necessarily improve as t grows. In fact, early-stopped gradient descent has been found to be effective in several machine learning applications, including non-parametric regression in a reproducing kernel Hilbert space (Raskutti et al., 2014), boosting Bühlmann and Yu (2003); Rosset et al. (2004) and ridge regression (Ali et al., 2019), to name a few. The intuition is that early stopping provides a form of regularization that prevents overfitting (see, e.g., Ali et al. (2019) and the references therein). In these settings, the population risk curve versus the iteration number is U-shaped (first decreasing and then increasing); we will observe instances of this phenomenon in Figures 1-5. For practical purposes, the major question in such situations is to infer from the data if early stopping is beneficial, and when to stop the iterations. The practitioner typically wishes to stop the iteration as soon as the population risk starts to increase; this is only possible if an estimator of the population risk of \hat{b}^t is available. Our results below provide such an estimator that can be effectively computed from the data (X, y).

1.4. Contributions

The aforementioned situations motivate studying the properties of the iterates \hat{b}^t at each step t, in particular for smaller values of t where \hat{b}^t is not yet close to the optimizer \hat{b} . Our focus centers on two key questions:

- (Q1) Can we quantify the predictive performance of \hat{b}^t for each t along the trajectory?
- (Q2) Can we use the iterates \hat{b}^t to construct confidence intervals for the entries of b^* , for instance by deriving asymptotic normality results around \hat{b}^t ?

This paper provides affirmative answers to these questions. Our contributions are summarized as follows:

- i) We introduce a reliable method for estimating the generalization error of each iterate b̂^t obtained from widely-used algorithms that solve (1.2). This estimator takes the form 1/n || ∑_{s≤t} ŵ_{s,t}(y Xb̂^s)||², i.e., the mean square error of the weighted average of the residual vector {y Xb̂^s}_{s≤t} with carefully chosen data-driven weights ŵ_{s,t} defined in Theorem 2.1 below. These weights are algorithm-specific and are computed from the data. The theory also allows us to derive estimators for the generalization error of weighted averages of the iterates. For instance, our approach enables the estimation of the generalization error for the average 1/T ∑t=1/b^t. The corresponding theory is presented in Theorem 2.2.
 ii) The proposed estimator of the generalization error serves as a practical proxy for minimizing the true
- ii) The proposed estimator of the generalization error serves as a practical proxy for minimizing the true generalization error. To identify the iteration index t such that \hat{b}^t has the lowest generalization error, one can choose the t that minimizes the estimated generalization error. This approach offers a viable method for pinpointing the optimal stopping point in the algorithm's trajectory. This application is presented in Corollary 2.3.

- iii) We develop a method for constructing valid confidence intervals for the elements of \boldsymbol{b}^* based on a given iteration t and iterate $\hat{\boldsymbol{b}}^t$. Consequently, one needs not wait for the convergence of the algorithm to construct valid confidence intervals for \boldsymbol{b}^* . In cases where early-stopping is beneficial for achieving smaller generalization error, confidence intervals based on the early-stopped iterate $\hat{\boldsymbol{b}}^{\hat{t}}$ (where \hat{t} is chosen by minimizing the estimated risk) are shorter than the confidence interval based on the fully converged minimizer $\hat{\boldsymbol{b}}$. The theory on asymptotic normality and confidence intervals is provided in Theorem 2.4.
- iv) The proposed method is applicable to a broad spectrum of regression techniques and algorithms. We provide detailed expressions of the weights $\hat{w}_{s,t}$ for several popular algorithms in Section 3. It offers a practical solution for determining the optimal stopping iteration of the algorithm to enjoy the smallest generalization error as a function of t along the trajectory. Extensive simulation studies on synthetic data corroborate our theoretical findings. These studies demonstrate the efficiency of our proposed risk estimator for \hat{b}^t , and confirm the validity of the asymptotic normality results for the entries of b^* derived from \hat{b}^t . The simulations are presented and discussed in of Section 3.

1.5. Related literature

For regression problems in the proportional regime (1.3), the most extensively studied iterative algorithm is Approximate Message Passing (AMP) (Donoho et al., 2009; Bayati and Montanari, 2011, 2012). In the current framework, AMP can be formulated as $\hat{b}^{t+1} = \eta_{t+1}(\hat{b}^t + \sum_{s \leq t} w_{t,s}^{AMP} v^s)$, where $w_{t,s}^{AMP}$ are specific scalar weights. These weights ensure that at each step, the input of η_{t+1} is approximately normally distributed. This construction enables tracking the evolution of the error of \hat{b}^t as a function of t using a simple recursion, referred to as state evolution. AMP has found numerous applications, including for instance in high-dimensional statistics (Bayati and Montanari, 2012; Celentano and Montanari, 2022), spiked models/low-rank matrix denoising (Montanari and Venkataramanan, 2021, and references therein) or sampling (El Alaoui et al., 2022). A proof of the state evolution for non-separable η_t is given in Berthier et al. (2020). The focus of the present is to study algorithms from the optimization literature such as proximal gradient (1.4), AGD or ISTA/FISTA that do not use the special AMP weights.

Celentano et al. (2020); Montanari and Wu (2022) exhibit fundamental limits for the performance of iterations that encompass (1.7). These works show that iterates can be viewed as a Lipschitz function g_* of some AMP algorithm. They characterize the fundamental lower bound obtained by taking the infimum over all g_* and corresponding AMP algorithms, and show that the lower bound is attained by a specific AMP algorithm, termed Bayes-AMP. Our goal in this paper is different: to develop a data-driven estimate of the error of the iterates \hat{b}^t .

Still in the proportional regime, Chandrasekher et al. (2022, 2023); Lou et al. (2024) consider iterations that, in order to compute the (t + 1)-th iterate, use a fresh random batch $(\boldsymbol{x}_i^{t+1}, \boldsymbol{y}_i^{t+1})_{i \in N^{t+1}}$ independent of all the past (here, the past refers to $\hat{\boldsymbol{b}}^t, \hat{\boldsymbol{b}}^{t-1}, ... \hat{\boldsymbol{b}}^1$ as well as the random samples used to compute these). These works characterize the evolution of the iterates' performance (measured by mean square error, or inner product with the ground truth) by a sequence of deterministic scalars defined by simple recursions, and they show that the iterates' performance is close to the deterministic scalars. If samples are reused across iterations, as in the present paper, it is still possible to characterize deterministic equivalents of the performance of the iterates in some cases (see Celentano et al. (2021) for continuous-time iterates, Gerbelot et al. (2022) for discrete-time ones). The deterministic equivalents of the iterates' performance are necessarily more complex than in the fresh random batch setting. This complexity is captured by limiting Gaussian processes indexed by $t \in [T]$ (Celentano et al., 2021; Gerbelot et al., 2022).

For optimization of the least-squares problem, with $\rho(\cdot) = 0$ in (1.2), Ali et al. (2020, 2019); Sheng and Ali (2022) (among others) study equivalences between early stopping and L2 regularization: stopping the iterations of GD or AGD at a fixed t implicitly performs shrinkage of a similar nature to Ridge regression. For gradient descent iterations solving this least-squares problem, Patil et al. (2024) develops estimates of the generalization error of the iterates using leave-one-out cross-validation, and show consistency of these leave-one-out estimates along the GD trajectory. While leave-one-out estimates are close to the goal of the present paper, i.e., to develop estimates of the generalization error along the trajectory of the algorithm, they are not computationally practical without further modifications since they require to running n algorithms in parallel to obtain the leave-one-out estimate.

Outside of the proportional regime (1.3), Luo et al. (2023) develop an efficient approximation of leave-oneout cross validation for iterates $\hat{\boldsymbol{b}}^t$ solving empirical risk minimization problems with additive regularization. The normalized Hessian of the objective function is assumed to be Lipschitz and non-singular at the iterates, which precludes settings of interest for the present paper with p > n and non-smooth penalty in (1.2). For uncertainty quantification of the iterates, Hoppe et al. (2023) extends the classical debiased lasso estimator (Zhang and Zhang, 2014a; Javanmard and Montanari, 2014; van de Geer et al., 2014b) to the iterates of a variant of ISTA. The asymptotic normality in Hoppe et al. (2023) requires a bound on the size of the supports of $\hat{\boldsymbol{b}}^t$ and \boldsymbol{b}^* , as well as $\|\hat{\boldsymbol{b}}^t - \boldsymbol{b}^*\|$ to vanish as $n \to \infty$. This is not the case in the regime (1.3) of interest here where p and n are of the same order. The present paper departs from this analysis of a variant ISTA on several fronts. First, our analysis is grounded in a more general iteration formula (see (1.6) and (1.7)), which encompasses a broader spectrum of algorithms. Second, our results establish asymptotic normality of $\hat{\boldsymbol{b}}^t$ for any t, and do not require $\|\hat{\boldsymbol{b}}^t - \boldsymbol{b}^*\|$ to vanish as $n \to \infty$. In contrast to these studies, the present paper introduces new estimator of the generalization error of algorithm iterates that solve the regression problem (1.2) for p > n and with non-smooth penalty functions. Additionally, we propose a method to construct confidence intervals for the entries of \boldsymbol{b}^* by debiasing the iterate $\hat{\boldsymbol{b}}^t$.

1.6. Notation

Regular variables like a, b, \dots refer to scalars, bold lowercase letters such as a, b, \dots represent vectors, and bold uppercase letters like A, B, \dots indicate matrices. For an integer $n \ge 1$, we use the notation $[n] = \{1, \dots, n\}$. The vectors $e_i \in \mathbb{R}^n, e_j \in \mathbb{R}^p, e_t \in \mathbb{R}^T$ denote the canonical basis vector of the corresponding index. For clarity, we always use implicit index i to loop or sum over [n], index j to loop over [p], and indices t, t', s to loop over [T]. For a real vector $\boldsymbol{a} \in \mathbb{R}^p$, $\|\boldsymbol{a}\|$ denotes its Euclidean norm. For a matrix \boldsymbol{A} , $\|\boldsymbol{A}\|_{\mathrm{F}}$, $\|\boldsymbol{A}\|_{\mathrm{op}}$, $\|\boldsymbol{A}\|_{*}$ denote its Frobenius, operator and nuclear norm, respectively. For a matrix A, we denote its maximum and minimum singular values by $\sigma_{\max}(\mathbf{A})$ and $\sigma_{\min}(\mathbf{A})$, respectively. If \mathbf{A} is symmetric, $\lambda_{\max}(\mathbf{A})$ and $\lambda_{\min}(\mathbf{A})$ are its maximum and minimum eigenvalues. Let $A \otimes B$ be the Kronecker product of matrices A and B. Let $\mathbf{1}_n$ denote the all-ones vector in \mathbb{R}^n , and \mathbf{I}_n denote the identity matrix of size n. For an event E, $\mathbb{I}(E)$ denotes the indicator function of E. It takes the value 1 if the event E occurs and 0 otherwise. Let $N(\mu, \sigma^2)$ denote the Gaussian distribution with mean μ and variance σ^2 , and $N_k(\mu, \Sigma)$ denote the k-dimensional Gaussian distribution with mean μ and covariance matrix Σ . For a random sequence ξ_n , we write $\xi_n = O_P(a_n)$ if ξ_n/a_n is stochastically bounded, and \xrightarrow{p} for convergence in probability and \xrightarrow{d} for convergence in distribution. We reserve the letters c and C to denote generic constants. Additionally, we use $C(\zeta, T, \gamma, \kappa)$ to denote a positive constant that depends only on ζ, T, γ, κ . The exact values of these constants may vary from place to place.

2. Main results

Throughout the paper, given iterates $\hat{b}^1, ..., \hat{b}^t, ..., define v^t \in \mathbb{R}^p$ by

(2.1)
$$\boldsymbol{v}^t = n^{-1} \boldsymbol{X}^\top (\boldsymbol{y} - \boldsymbol{X} \widehat{\boldsymbol{b}}^t) \qquad \text{for } t \ge 1.$$

2.1. Iterates and derivatives

Our first task is to establish some notation (namely, matrices $\mathcal{J}, \mathcal{D} \in \mathbb{R}^{pT \times pT}$) that will be used to construct the proposed estimators. As a warm-up, we will first introduce this notation for proximal gradient descent (Section 2.1.1) and iterates constructed from the two previous ones (Section 2.1.2). Notation for the general form (1.7) will be given in Section 2.1.3.

2.1.1. Proximal gradient descent

Consider the proximal gradient descent iterates (1.4). With this notation and starting with $\hat{b}^1 = 0$, the proximal gradient descent (1.4) iterations can be rewritten as

(2.2)
$$\widehat{\boldsymbol{b}}^{t} = \boldsymbol{g}_{t}(\widehat{\boldsymbol{b}}^{t-1}, \boldsymbol{v}^{t-1}), \quad \text{where } \boldsymbol{g}_{t}(\boldsymbol{b}^{t}, \boldsymbol{v}^{t}) = \text{prox}[\frac{1}{L}\rho](\boldsymbol{b}^{t} + \frac{1}{L}\boldsymbol{v}^{t}).$$

The Jacobian of the function g_t is a matrix of size $p \times 2p$ and can be partitioned into the two $p \times p$ blocks

(2.3)
$$\boldsymbol{J}_{t,t-1} = \frac{\partial \boldsymbol{g}_t}{\partial \boldsymbol{b}^{t-1}} (\widehat{\boldsymbol{b}}^{t-1}, \boldsymbol{v}^{t-1}), \quad \boldsymbol{D}_{t,t-1} = \frac{\partial \boldsymbol{g}_t}{\partial \boldsymbol{v}^{t-1}} (\widehat{\boldsymbol{b}}^{t-1}, \boldsymbol{v}^{t-1}).$$

Next, define $\mathcal{J} \in \mathbb{R}^{pT \times pT}$ and $\mathcal{D} \in \mathbb{R}^{pT \times pT}$ with $T \times T$ blocks of size $p \times p$ as follows

$$(2.4) \qquad \mathcal{J} = \begin{bmatrix} \mathbf{0} & \mathbf{0} & \cdots & \cdots & \mathbf{0} \\ J_{2,1} & \mathbf{0} & \ddots & \cdots & \ddots & \vdots \\ \mathbf{0} & J_{3,2} & \mathbf{0} & \ddots & \cdots & \vdots \\ \mathbf{0} & \mathbf{0} & J_{4,3} & \mathbf{0} & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \mathbf{0} \\ \mathbf{0} & \cdots & \mathbf{0} & \mathbf{0} & J_{T,T-1} & \mathbf{0} \end{bmatrix}, \ \mathcal{D} = \begin{bmatrix} \mathbf{0} & \mathbf{0} & \cdots & \cdots & \mathbf{0} \\ D_{2,1} & \mathbf{0} & \ddots & \cdots & \cdots & \vdots \\ \mathbf{0} & D_{3,2} & \mathbf{0} & \ddots & \cdots & \vdots \\ \mathbf{0} & \mathbf{0} & D_{4,3} & \mathbf{0} & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \mathbf{0} \\ \mathbf{0} & \cdots & \mathbf{0} & \mathbf{0} & D_{T,T-1} & \mathbf{0} \end{bmatrix}.$$

Each **0** block in the above \mathcal{J}, \mathcal{D} is the zero matrix of size $p \times p$. For iterations depending not only on \hat{b}^{t-1}, v^{t-1} but also on previous iterates, the lower triangular blocks of \mathcal{D}, \mathcal{J} will be filled with the corresponding non-zero blocks of the Jacobian of g_t , as shown in the next subsections.

2.1.2. Combining two previous iterates

To incorporate more general algorithms beyond proximal gradient descent, we consider the iteration formula:

(2.5)
$$\widehat{\boldsymbol{b}}^t = \boldsymbol{g}_t(\widehat{\boldsymbol{b}}^{t-1}, \widehat{\boldsymbol{b}}^{t-2}, \boldsymbol{v}^{t-1}, \boldsymbol{v}^{t-2}) \qquad \text{for } t \ge 2$$

Here, \hat{b}^1 serves as an initial vector, and we set $\hat{b}^0 = v^0 = \mathbf{0}_p$. The iteration functions $g_t(\cdot) : \mathbb{R}^{4p} \to \mathbb{R}^p$ are determined by user-specified algorithms. We include \hat{b}^{t-2} and v^{t-2} into the argument of (2.5) to encompass optimization algorithms that update iterates by considering information from the two preceding steps. This general formulation accommodates popular algorithms such as Nesterov's accelerated gradient (AGD) method (Nesterov, 1983, 2003) and the Fast Iterative Shrinkage-Thresholding Algorithm (FISTA) (Beck and Teboulle, 2009). We provide detailed expressions of g_t for several important algorithms in Section 3.

For algorithms with iteration function g_t in (2.5) depending on the previous two iterates, the Jacobian of g_t at a point where g_t is differentiable is a matrix of size $\mathbb{R}^{p \times 4p}$. This Jacobian matrix in $\mathbb{R}^{p \times 4p}$ is naturally partitioned into the four $p \times p$ blocks:

(2.6)
$$\boldsymbol{J}_{t,t-1} = \frac{\partial \boldsymbol{g}_t}{\partial \boldsymbol{b}^{t-1}} (\hat{\boldsymbol{b}}^{t-1}, \hat{\boldsymbol{b}}^{t-2}, \boldsymbol{v}^{t-1}, \boldsymbol{v}^{t-2}), \quad \boldsymbol{D}_{t,t-1} = \frac{\partial \boldsymbol{g}_t}{\partial \boldsymbol{v}^{t-1}} (\hat{\boldsymbol{b}}^{t-1}, \hat{\boldsymbol{b}}^{t-2}, \boldsymbol{v}^{t-1}, \boldsymbol{v}^{t-2}), \\ \boldsymbol{J}_{t,t-2} = \frac{\partial \boldsymbol{g}_t}{\partial \boldsymbol{b}^{t-2}} (\hat{\boldsymbol{b}}^{t-1}, \hat{\boldsymbol{b}}^{t-2}, \boldsymbol{v}^{t-1}, \boldsymbol{v}^{t-2}), \quad \boldsymbol{D}_{t,t-2} = \frac{\partial \boldsymbol{g}_t}{\partial \boldsymbol{v}^{t-2}} (\hat{\boldsymbol{b}}^{t-1}, \hat{\boldsymbol{b}}^{t-2}, \boldsymbol{v}^{t-1}, \boldsymbol{v}^{t-2}).$$

We further define larger matrices $\mathcal{J}, \mathcal{D} \in \mathbb{R}^{pT \times pT}$ by setting the (t, t') block of \mathcal{J} as $J_{t,t'}$ and that of \mathcal{D} as $D_{t,t'}$ for all $t, t' \in [T]$ for all t, t' corresponding to matrices in (2.6), with zeros everywhere else:

$$(2.7) \quad \mathcal{J} = \begin{bmatrix} \mathbf{0} & \mathbf{0} & \cdots & \cdots & \mathbf{0} \\ \mathbf{J}_{2,1} & \mathbf{0} & \ddots & \cdots & \mathbf{0} \\ \mathbf{J}_{3,1} & \mathbf{J}_{3,2} & \mathbf{0} & \ddots & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{J}_{4,2} & \mathbf{J}_{4,3} & \mathbf{0} & \ddots & \mathbf{0} \\ \mathbf{0} & \cdots & \mathbf{0} & \mathbf{J}_{T,T-2} & \mathbf{J}_{T,T-1} & \mathbf{0} \end{bmatrix}, \quad \mathcal{D} = \begin{bmatrix} \mathbf{0} & \mathbf{0} & \cdots & \cdots & \mathbf{0} \\ \mathbf{D}_{2,1} & \mathbf{0} & \ddots & \cdots & \mathbf{0} \\ \mathbf{D}_{3,1} & \mathbf{D}_{3,2} & \mathbf{0} & \ddots & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{D}_{4,2} & \mathbf{D}_{4,3} & \mathbf{0} & \ddots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{D}_{T,T-2} & \mathbf{J}_{T,T-1} & \mathbf{0} \end{bmatrix},$$

An equivalent definition of \mathcal{J}, \mathcal{D} using Kronecker products is

$$\mathcal{J} = \sum_{t=2}^{T} \sum_{s=t-2}^{t-1} (\boldsymbol{e}_t \boldsymbol{e}_s^{\top}) \otimes \boldsymbol{J}_{t,s}, \qquad \mathcal{D} = \sum_{t=2}^{T} \sum_{s=t-2}^{t-1} (\boldsymbol{e}_t \boldsymbol{e}_s^{\top}) \otimes \boldsymbol{D}_{t,s},$$

where e_t, e_s are the *t*-th and *s*-th canonical basis vectors in \mathbb{R}^T .

2.1.3. General form: combining all previous iterates

More generally, our theory applies to iterations that depend on all previous iterates, i.e., iterates of the form

(2.8)
$$\widehat{\boldsymbol{b}}^t = \boldsymbol{g}_t(\widehat{\boldsymbol{b}}^{t-1}, \widehat{\boldsymbol{b}}^{t-2}, \dots, \widehat{\boldsymbol{b}}^2, \widehat{\boldsymbol{b}}^1, \ \boldsymbol{v}^{t-1}, \dots, \boldsymbol{v}^2, \boldsymbol{v}^1)$$

with $\boldsymbol{v}^s = \hat{\boldsymbol{b}}^s = \boldsymbol{0}_p$ for all $s \leq 0$ by convention. With the more general iterations (2.8) depending on all previous iterates, the Jacobian of \boldsymbol{g}_t in (2.8) is now a matrix in $\mathbb{R}^{p \times 2p(t-1)}$ partitioned into blocks

(2.9)
$$\boldsymbol{J}_{t,s} = \frac{\partial \boldsymbol{g}_t}{\partial \boldsymbol{b}^s} \Big(\widehat{\boldsymbol{b}}^{t-1}, ..., \widehat{\boldsymbol{b}}^1, \boldsymbol{v}^{t-1}, ..., \boldsymbol{v}^1 \Big), \quad \boldsymbol{D}_{t,s} = \frac{\partial \boldsymbol{g}_t}{\partial \boldsymbol{v}^s} \Big(\widehat{\boldsymbol{b}}^{t-1}, ..., \widehat{\boldsymbol{b}}^1, \boldsymbol{v}^{t-1}, ..., \boldsymbol{v}^1 \Big)$$

for all s = 1, ..., t - 1. The large matrices $\mathcal{J}, \mathcal{D} \in \mathbb{R}^{pT \times pT}$ are then defined as

(2.10)
$$\mathcal{J} = \sum_{t=2}^{T} \sum_{s=1}^{t-1} (\boldsymbol{e}_t \boldsymbol{e}_s^{\top}) \otimes \boldsymbol{J}_{t,s}, \qquad \mathcal{D} = \sum_{t=2}^{T} \sum_{s=1}^{t-1} (\boldsymbol{e}_t \boldsymbol{e}_s^{\top}) \otimes \boldsymbol{D}_{t,s}$$

This generalizes (2.7) when \hat{b}^t depends on all previous iterates. The matrices \mathcal{J} and \mathcal{D} are always lower triangular block matrices, as in (2.7).

2.2. Lipschitz assumption and the chain rule

Throughout, we assume the following.

Assumption 2.1. The algorithm starts with $\hat{b}^1 = 0$. The iteration function g_t in (2.8) is ζ -Lipschitz and satisfies $g_t(0) = 0$.

The notation in (2.6) and (2.9) naturally arises from the application of the chain rule in the recursive computation of derivatives for the iterates (2.5) and (2.8). While assuming that g_t is Lipschitz (Assumption 2.1) implies that the iterates are differentiable almost everywhere with respect to (X, y) by Rademacher's theorem (a locally Lipschitz function of (y, X) is differentiable almost everywhere), the chain rule may fail for composition of multivariate Lipschitz functions. This technical issue is clearly apparent with the example

(2.11)
$$\phi^*(u,v) = (u,u), \quad \phi^{**}(u,v) = \max(u,v), \quad \phi^{**} \circ \phi^*(u,v) = u.$$

Although $\frac{\partial}{\partial u}(\phi^{**} \circ \phi^*)(u, v) = 1$ clearly holds, the chain rule is undefined because ϕ^{**} is not differentiable at $\phi^*(u, v)$ for all $(u, v) \in \mathbb{R}^2$. A fix to this issue for the composition of locally Lipschitz functions is given in Corollary 3.2 of Ambrosio and Dal Maso (1990): the chain rule for for the composition of two Lipschitz functions $g : \mathbb{R}^k \to \mathbb{R}^q, u : \mathbb{R}^q \to \mathbb{R}^p$ holds almost surely in the modified form $\nabla(g \circ u)(x) = \nabla(g|_{T^u_x})\nabla u(x)$ where $g|_{T^u_x}$ is the restriction of g to the affine space defined in (Ambrosio and Dal Maso, 1990, Corollary 3.2). Thus, in order to leverage the chain rule in our proofs, we will assume that the matrices in (2.6) or (2.9) are all modified, if necessary, in order to grant the chain rule as given in (Ambrosio and Dal Maso, 1990, Corollary 3.2). In many practical examples, the Lipschitz (but not-necessarily differentiable everywhere) nonlinear function used to recursively obtain the iterates is separable, i.e., $g^{sep} : \mathbb{R}^p \to \mathbb{R}^p$ of the form

$$g^{sep}(\boldsymbol{x})_j = g_j(x_j)$$
 for all $\boldsymbol{x} \in \mathbb{R}^p, j \in [p]$ for some functions $g_j : \mathbb{R} \to \mathbb{R}$.

This is the case for the soft-thresholding in (1.5) as well as its variants, FISTA and LQA, detailed in Sections 3.4 and 3.5. In this case by (Ziemer, 1989, Theorem 2.1.11), the chain rule holds almost everywhere for the composition of Lipschitz functions of the form $g_j \circ h$ for $h : \mathbb{R}^k \to \mathbb{R}$ and $g_j : \mathbb{R} \to \mathbb{R}$. Consequently, the usual (unmodified) chain rule is granted almost everywhere for compositions of Lipschitz functions that are either separable or everywhere differentiable.

2.3. Memory matrix

Equipped with the above notation in (2.9) and (2.10), we now introduce the memory matrix. The memory matrix is a key ingredient in the construction of our estimator of the prediction error of the iterate \hat{b}^t obtained from the iterations (2.5) or (2.8).

Definition 2.1. For iterates $\{\hat{b}^1, \hat{b}^2, ..., \hat{b}^T\}$ obtained from the iteration (2.8), with \mathcal{D}, \mathcal{J} defined in (2.10), define the memory matrix $\hat{\mathbf{A}} \in \mathbb{R}^{T \times T}$ as

(2.12)
$$\widehat{\mathbf{A}} = \frac{1}{n} \sum_{i=1}^{n} \left(\mathbf{I}_{T} \otimes (\mathbf{e}_{i}^{\top} \mathbf{X}) \right) \left(\mathbf{I}_{pT} + \mathcal{D}(\mathbf{I}_{T} \otimes \frac{\mathbf{X}^{\top} \mathbf{X}}{n}) - \mathcal{J} \right)^{-1} \mathcal{D}\left(\mathbf{I}_{T} \otimes (\mathbf{X}^{\top} \mathbf{e}_{i}) \right)$$

where $e_i \in \mathbb{R}^n$ is the *i*-th canonical basis vector.

By definition, the memory matrix $\widehat{\mathbf{A}}$ only depends on the data (\mathbf{X}, \mathbf{y}) , the iterates $\widehat{\mathbf{b}}^t$, the vectors \mathbf{v}^t in (2.1), and the derivative matrices in (2.9) evaluated at $(\widehat{\mathbf{b}}^{t-1}, ..., \widehat{\mathbf{b}}^1, \mathbf{v}^{t-1}, ..., \mathbf{v}^1)$. The specific computation of $\widehat{\mathbf{A}}$ thus depends on the iteration function \mathbf{g}_t through the derivative matrices in (2.9) that appear as blocks of \mathcal{D} and \mathcal{J} . The matrix $\widehat{\mathbf{A}}$ will differ significantly for different choices of nonlinear functions \mathbf{g}_t . For the same nonlinear functions \mathbf{g}_t , the matrix $\widehat{\mathbf{A}}$ will also be different for different realizations of the data (\mathbf{X}, \mathbf{y}) , although we observe in practice that the entries of $\widehat{\mathbf{A}}$ concentrate and have small variance with respect to the randomness of (\mathbf{X}, \mathbf{y}) .

In Section 3, we provide detailed expressions of \mathcal{J} and \mathcal{D} for several important algorithms in the optimization literature. While definition (2.12) involves the inverse of a matrix of size $\mathbb{R}^{pT \times pT}$, due to its specific structure, computation of $\widehat{\mathbf{A}}$ requires much fewer resources that performing a matrix inversion or solving a linear system in $\mathbb{R}^{pT \times pT}$. We provide efficient methods to compute $\widehat{\mathbf{A}}$ row by row in Section 4.

An equivalent definition of the matrix $\widehat{\mathbf{A}}$ is to consider the matrix

(2.13)
$$\frac{1}{n} \Big(\boldsymbol{I}_T \otimes \boldsymbol{X} \Big) \Big(\boldsymbol{I}_{pT} + \mathcal{D}(\boldsymbol{I}_T \otimes \frac{\boldsymbol{X}^{\top} \boldsymbol{X}}{n}) - \mathcal{J} \Big)^{-1} \mathcal{D} \Big(\boldsymbol{I}_T \otimes (\boldsymbol{X}^{\top}) \Big)$$

in $\mathbb{R}^{nT \times nT}$ as a matrix by block, with $T \times T$ blocks of size $n \times n$. The matrix $\widehat{\mathbf{A}} \in \mathbb{R}^{T \times T}$ is then obtained by taking the trace of each $n \times n$ block.

Since \mathcal{D} and \mathcal{J} are lower triangular matrices with diagonal blocks equal to $\mathbf{0}_{p \times p}$, both $\mathbf{I}_{pT} + \mathcal{D}(\mathbf{I}_T \otimes \mathbf{X}^\top \mathbf{X}/n) - \mathcal{J}$ and its inverse are lower triangular with diagonal blocks equal to \mathbf{I}_p . Consequently, (2.13) is block lower triangular with diagonal blocks equal to $\mathbf{0}_{n \times n}$. By taking the trace of each $n \times n$ block in (2.13), we see that $\hat{\mathbf{A}} \in \mathbb{R}^{T \times T}$ is lower triangular with zero diagonal entries. It thus always holds that the matrix $\mathbf{I}_T - \hat{\mathbf{A}}/n$ is a lower triangular with all diagonal entries equal to 1, invertible, with $(\mathbf{I}_T - \hat{\mathbf{A}}/n)^{-1}$ also lower triangular with all diagonal entries equal to 1. The matrix

$$(\boldsymbol{I}_T - \widehat{\mathbf{A}}/n)^{-1}$$

plays a critical role in our estimator of the generalization error of each iteration \hat{b}^t in Theorems 2.1 and 2.2 below.

2.4. Probabilistic assumptions and proportional regime

Our main theorems below hold under the following assumptions.

Assumption 2.2. The design matrix \boldsymbol{X} has i.i.d. rows from $\mathsf{N}_p(\mathbf{0}, \boldsymbol{\Sigma})$ for some positive definite matrix $\boldsymbol{\Sigma}$ satisfying $0 < \lambda_{\min}(\boldsymbol{\Sigma}) \le 1 \le \lambda_{\max}(\boldsymbol{\Sigma})$ and $\|\boldsymbol{\Sigma}\|_{\mathrm{op}} \|\boldsymbol{\Sigma}^{-1}\|_{\mathrm{op}} \le \kappa$.

Assumption 2.3. The noise ε is independent of X and has i.i.d. entries from $N(0, \sigma^2)$.

Assumption 2.4. The sample size n and predictor dimension p satisfy $p/n \leq \gamma$ for a constant $\gamma \in (0, \infty)$.

Recall that ζ is the Lipschitz constant in Assumption 2.1. In the results below, $(\zeta, T, \gamma, \kappa)$ can be thought of as constant problem parameters as $n, p \to +\infty$; our upper bounds involve constants $C(\zeta, T, \gamma, \kappa)$ that only depend on these four quantities.

2.5. Estimation of the generalization error of iterates

We are interested in quantifying the performance of each iterate \hat{b}^t . We assess the performance of the iterate \hat{b}^t using the out-of-sample prediction error (also referred to as prediction risk or generalization error)

(2.14)
$$r_t \stackrel{\text{def}}{=} \mathbb{E}\Big[\left(y_{new} - \boldsymbol{x}_{new}^\top \widehat{\boldsymbol{b}}^t \right)^2 | (\boldsymbol{X}, \boldsymbol{y}) \Big] = \| \boldsymbol{\Sigma}^{1/2} (\widehat{\boldsymbol{b}}^t - \boldsymbol{b}^*) \|^2 + \sigma^2,$$

where $(\boldsymbol{x}_{new}, y_{new})$ is a new test sample that has the same distribution as (\boldsymbol{x}_1, y_1) , the first row of $(\boldsymbol{X}, \boldsymbol{y})$. Since $\hat{\boldsymbol{b}}^t$ is measurable with respect to $(\boldsymbol{X}, \boldsymbol{y})$, the last equality above follows from Assumptions 2.2 and 2.3. Note that $(\boldsymbol{x}_{new}, y_{new})$ is only used as a mathematical device to define r_t in (2.14); we do not assume that independent test samples are available. Our first result concerns the estimation of prediction risk r_t for each iterate $\hat{\boldsymbol{b}}^t$.

Theorem 2.1 (Estimation of prediction risk). Let Assumptions 2.1 to 2.4 be fulfilled. For each $t \in [T]$, define the estimate \hat{r}_t of r_t by

(2.15)
$$\hat{r}_t = \frac{1}{n} \Big\| \sum_{s=1}^t \hat{w}_{t,s} \big(\boldsymbol{y} - \boldsymbol{X} \widehat{\boldsymbol{b}}^s \big) \Big\|^2,$$

where $\hat{w}_{t,s} = \boldsymbol{e}_t^\top (\boldsymbol{I}_T - \widehat{\mathbf{A}}/n)^{-1} \boldsymbol{e}_s$. We have for any $t \in [T]$,

(2.16)
$$\mathbb{E}\left|\hat{r}_t - r_t\right| \le n^{-\frac{1}{2}} \operatorname{var}(y_1) C(\zeta, T, \gamma, \kappa).$$

Here $\operatorname{var}(y_1) = \|\mathbf{\Sigma}^{1/2} \mathbf{b}^*\|^2 + \sigma^2$, and $C(\zeta, T, \gamma, \kappa)$ is a constant depending only on ζ, T, γ, κ .

Theorem 2.1 establishes that \hat{r}_t is \sqrt{n} -consistent when $\operatorname{var}(y_1), \zeta, T, \gamma, \kappa$ are constant as $n, p \to +\infty$. The risk estimate \hat{r}_t for \hat{b}^t is determined by both the current residual vector $\boldsymbol{y} - \boldsymbol{X}\hat{\boldsymbol{b}}^t$ and all preceding residual vectors $\{\boldsymbol{y} - \boldsymbol{X}\hat{\boldsymbol{b}}^s\}_{s=1,\dots,t-1}$ through the weighted sum inside the mean squared norm in (2.15). These weights $(\hat{w}_{t,1},\dots,\hat{w}_{t,t})$ are the first t entries of the t-th row of the matrix $(\boldsymbol{I}_T - \hat{\boldsymbol{A}}/n)^{-1}$. The proof of Theorem 2.1 is given in Appendix G.

By construction of the matrices $\widehat{\mathbf{A}}$ and $(\mathbf{I}_T - \widehat{\mathbf{A}}/n)^{-1}$, the definition of these weights are not influenced by the total number of iterations T (e.g., the weights $(\widehat{w}_{s,t})_{s \leq t}$ for any $t \leq T$ are the same if the total number of iterations is T or any T' > T). In other words, opting for a larger T simply enlarges the dimensions of the matrix $\widehat{\mathbf{A}}$ and the inverse matrix $(\mathbf{I}_T - \widehat{\mathbf{A}}/n)^{-1}$, yet the first t entries in the t-th row of $(\mathbf{I}_T - \widehat{\mathbf{A}}/n)^{-1}$ remain unchanged. The necessity of a total number of iteration, T, is arguably artificial; an equivalent presentation would increase the size of $\widehat{\mathbf{A}}$ and $(\mathbf{I}_T - \widehat{\mathbf{A}}/n)^{-1}$ by one row and one column at every new iteration. We opted for a fixed total number of iterations T with matrices $\widehat{\mathbf{A}}$ and $(\mathbf{I}_T - \widehat{\mathbf{A}}/n)^{-1}$ having fixed size $T \times T$ for clarity, to avoid dealing with matrices changing in size.

Remark 2.1 (Risk of initialization). For t = 1, $\hat{w}_{t,s} = \mathbb{I}(s = 1)$ since $(\mathbf{I}_T - \widehat{\mathbf{A}}/n)^{-1}$ is lower triangular with diagonal entries all equal to 1. As a sanity check, we obtain $\hat{r}_1 = n^{-1} ||\mathbf{y} - \mathbf{X}\widehat{\mathbf{b}}^1||^2$ from (2.15), which is an unbiased estimate of the prediction error of the initialization $\widehat{\mathbf{b}}^1$ since $\widehat{\mathbf{b}}^1$ is independent of (\mathbf{X}, \mathbf{y}) .

Besides the individual iterate \hat{b}^t , one might also consider the estimate \bar{b} defined as the average of m consecutive iterates starting from \hat{b}^{t_0} , i.e., $\bar{b} = \frac{1}{m} \sum_{t=t_0}^{t_0+m-1} \hat{b}^t$. The prediction risk of the estimate \bar{b} is then

$$\sigma^{2} + \|\boldsymbol{\Sigma}^{1/2}(\bar{\boldsymbol{b}} - \boldsymbol{b}^{*})\|^{2} = \frac{1}{m^{2}} \sum_{t=t_{0}}^{t_{0}+m-1} \sum_{t'=t_{0}}^{t_{0}+m-1} \left[\sigma^{2} + (\hat{\boldsymbol{b}}^{t} - \boldsymbol{b}^{*})^{\top} \boldsymbol{\Sigma}(\hat{\boldsymbol{b}}^{t'} - \boldsymbol{b}^{*})\right],$$

simply by expanding the square. Estimation of the generalization error of \bar{b} is thus possible provided that we can estimate the terms

(2.17)
$$r_{tt'} \stackrel{\text{\tiny def}}{=} \sigma^2 + (\widehat{\boldsymbol{b}}^t - \boldsymbol{b}^*)^\top \boldsymbol{\Sigma} (\widehat{\boldsymbol{b}}^{t'} - \boldsymbol{b}^*)$$

for each t, t' inside the double sum. The following result derives a \sqrt{n} -consistent estimate of $r_{tt'}$, using the same weights as in Theorem 2.1.

Theorem 2.2 (Proof is given in Appendix F). Let Assumptions 2.1 to 2.4 be fulfilled. For two integers $t, t' \leq T$ define the estimate of $r_{tt'}$ as

(2.18)
$$\hat{r}_{tt'} = \frac{1}{n} \left(\sum_{s=1}^{t} \hat{w}_{t,s} \left(\boldsymbol{y} - \boldsymbol{X} \widehat{\boldsymbol{b}}^{s} \right) \right)^{\top} \left(\sum_{s'=1}^{t'} \hat{w}_{t',s'} \left(\boldsymbol{y} - \boldsymbol{X} \widehat{\boldsymbol{b}}^{s'} \right) \right),$$

where $\hat{w}_{a,b} = \boldsymbol{e}_a^{\top} (\boldsymbol{I}_T - \widehat{\mathbf{A}}/n)^{-1} \boldsymbol{e}_b$ for all $a, b \in [T]$ as in Theorem 2.1. Then

$$\mathbb{E}|\hat{r}_{tt'} - r_{tt'}| + \operatorname{var}(r_{tt'})^{1/2} \le n^{-\frac{1}{2}} C(\zeta, T, \gamma, \kappa) \operatorname{var}(y_1).$$

2.6. An oracle inequality for early stopping

Since Theorem 2.1 provides upper bounds of the form $\mathbb{E}|\hat{r}_t - r_t| \leq n^{-1/2}C(\zeta, T, \gamma, \kappa)\operatorname{var}(y_1)$. A straightforward application of Markov's inequality yields the following.

Corollary 2.3 (Proof is given in Appendix H). Let Assumptions 2.1 to 2.4 be fulfilled. Select an iteration $\hat{t} \in [T]$ by minimizing (2.15), that is, $\hat{t} = \arg\min_{t \in [T]} \|\sum_{s \leq t} \hat{w}_{t,s}(\boldsymbol{y} - \boldsymbol{X} \hat{\boldsymbol{b}}^s)\|^2/n$. Then for any constant $c \in (0, 1/2)$,

$$\mathbb{P}\Big(\|\boldsymbol{\Sigma}^{1/2}(\widehat{\boldsymbol{b}}^{\widehat{t}}-\boldsymbol{b}^*)\|^2 \leq \min_{s\in[T]}\|\boldsymbol{\Sigma}^{1/2}(\widehat{\boldsymbol{b}}^s-\boldsymbol{b}^*)\|^2 + \frac{\operatorname{var}(y_1)}{n^{1/2-c}}\Big) \geq 1 - \frac{C(\zeta,\gamma,T,\kappa)}{n^c} \to 1$$

This means that after running T iterations, we can pick the iteration \hat{t} that minimizes the criterion (2.15), and this choice achieves the smallest prediction error among the first T iterates up to a negligible error term. This is appealing for the settings illustrated in Figures 1 to 5 where the generalization error of the iterates \hat{b}^t is first decreasing in t up to some t_* , before increasing for $t \ge t_*$. The above selection of \hat{t} guarantees that the risk of \hat{b}^t is close to that of \hat{b}^{t_*} .

Given K_n candidate sequences of nonlinear functions, say $(\boldsymbol{g}_t^k)_{t \in [T]}$ for each $k \in [K_n]$, a similar argument using Markov's inequality yields

$$\|\boldsymbol{\Sigma}^{1/2}(\hat{\boldsymbol{b}}^{\hat{t}} - \boldsymbol{b}^{*})\|^{2} \leq \min_{k \in [K_{n}]} \min_{s \in [T]} \|\boldsymbol{\Sigma}^{1/2}(\hat{\boldsymbol{b}}^{s} - \boldsymbol{b}^{*})\|^{2} + \operatorname{var}(y_{1})o_{P}(1)$$

if $(\zeta, \gamma, T, \kappa)$ are constants as $n, p \to +\infty$ and $K_n = o(\sqrt{n})$.

2.7. Alternative weights and covariance-adaptive weights

The proofs of Theorems 2.1 and 2.2 reveal that if $\Sigma = I_p$, the weights $\hat{w}_{t,s}$ in (2.15) and (2.18) can be replaced with the alternative weights

$$\begin{split} \check{w}_{t,s} &= \mathbb{I}\{t=s\} + \frac{1}{n} \operatorname{Tr} \Big[(\boldsymbol{e}_t^\top \otimes \boldsymbol{I}_p) \big(\boldsymbol{I}_{pT} + \mathcal{D} (\boldsymbol{I}_T \otimes \frac{\boldsymbol{X}^\top \boldsymbol{X}}{n}) - \mathcal{J} \big)^{-1} \mathcal{D} (\boldsymbol{e}_s \otimes \boldsymbol{I}_p) \Big] \\ &= \mathbb{I}\{t=s\} + \frac{1}{n} \sum_{j=1}^p (\boldsymbol{e}_t^\top \otimes \boldsymbol{e}_j^\top) \big(\boldsymbol{I}_{pT} + \mathcal{D} (\boldsymbol{I}_T \otimes \frac{\boldsymbol{X}^\top \boldsymbol{X}}{n}) - \mathcal{J} \big)^{-1} \mathcal{D} (\boldsymbol{e}_s \otimes \boldsymbol{e}_j) \end{split}$$
(for $\boldsymbol{\Sigma} = \boldsymbol{I}_p$).

Indeed, these alternative weights $\tilde{w}_{t,s}$ are the (t,s) entries of the matrix $I_T + \hat{C}/n$ in the proof of Theorem 2.2 with $\hat{C} \in \mathbb{R}^{T \times T}$ defined in (F.2). These weights satisfy

(2.19)
$$\mathbb{E}\left[\sum_{s=1}^{T} \frac{1}{n} \left\| \sum_{s=1}^{t} (\hat{w}_{t,s} - \check{w}_{t,s}) (\boldsymbol{y} - \boldsymbol{X} \widehat{\boldsymbol{b}}^{s}) \right\|^{2} \right] \le C(\zeta, T, \gamma) n^{-1/2}, \quad \text{when } \boldsymbol{\Sigma} = \boldsymbol{I}_{p},$$

by (F.10) in the appendix. This means that $\hat{w}_{t,s}$ and $\check{w}_{t,s}$ can be used interchangeably as weights for $(\boldsymbol{y} - \boldsymbol{X}\hat{\boldsymbol{b}}^s)_{s \leq T}$ in the definition of \hat{r}_t when $\boldsymbol{\Sigma} = \boldsymbol{I}_p$.

This interchangeability is lost as soon as $\Sigma \neq I_p$. In this case, the alternative weights $\check{w}_{t,s}$ have expression

(2.20)
$$\check{w}_{t,s} = \mathbb{I}\{t=s\} + \frac{1}{n} \operatorname{Tr} \left[(\boldsymbol{e}_t^\top \otimes \boldsymbol{\Sigma}^{1/2}) \left(\boldsymbol{I}_{pT} + \mathcal{D}(\boldsymbol{I}_T \otimes \frac{\boldsymbol{X}^\top \boldsymbol{X}}{n}) - \mathcal{J} \right)^{-1} \mathcal{D}(\boldsymbol{e}_s \otimes \boldsymbol{\Sigma}^{1/2}) \right]$$

using the correspondence (D.6). The alternative weights $\tilde{w}_{t,s}$ thus require the knowledge of Σ . This is the main reason we presented the main results using the weights $\hat{w}_{t,s}$ and the memory matrix $\widehat{\mathbf{A}}$: The expressions of $\hat{w}_{t,s}$ and $\widehat{\mathbf{A}}$ do not require prior knowledge of Σ or estimating Σ from the data. The weights $\hat{w}_{t,s}$ are thus preferable, and more broadly applicable than $\tilde{w}_{t,s}$. This duality between two interchangeable scalar adjustments, one requiring the knowledge of Σ and one not requiring it, was already observed in regularized M-estimation (Bellec and Shen, 2022, Section 5).

2.8. Iterative debiased estimation

This subsection focuses on asymptotic normality and statistical inference for the entries of b^* using iterate \hat{b}^t . The next theorem shows that the following debiased estimate,

(2.21)
$$\widehat{\boldsymbol{b}}_{j}^{t,\text{debias}} := \underbrace{\widehat{\boldsymbol{b}}_{j}^{t}}_{\text{iterate}} + \underbrace{n^{-1} \sum_{s=1}^{t} \widehat{w}_{t,s} (\boldsymbol{y} - \boldsymbol{X} \widehat{\boldsymbol{b}}^{s})^{\top} \boldsymbol{X} \boldsymbol{\Sigma}^{-1} \boldsymbol{e}_{j}}_{\text{bias correction}},$$

is approximately normally distributed and centered at \boldsymbol{b}_j^* . Above, the observable weights $\hat{w}_{t,s}$ are the same as in Theorem 2.1. The approximate normality below is quantified using the 2-Wasserstein distance between probability distributions in \mathbb{R}^T , defined as $W_2(\mu,\nu) = \inf_{(\boldsymbol{u},\boldsymbol{w})} \mathbb{E}[\|\boldsymbol{u}-\boldsymbol{v}\|^2]^{1/2}$ where the infimum is taken over all couplings $(\boldsymbol{u},\boldsymbol{w})$ of the two probability measures (μ,ν) . We refer to (Villani et al., 2009, Definition 6.8) for several characterizations of convergence with respect to W_2 .

The following result is understood asymptotically as $n, p \to +\infty$. Implicitly, we assume that a sequence of regression problems (1.1) is given, together with nonlinear functions g_t in (2.8). It is implicit that n serves as the index of the sequence, and $p = p^{(n)}, \mathbf{b}^{*(n)}, \mathbf{g}_t^{(n)}$ all implicitly depend on n and may change values as n increases, as long as Assumptions 2.1 to 2.4 are fulfilled for every n. The constants $(T, \zeta, \gamma, \kappa, \sigma^2)$ do not depend on n.

Theorem 2.4. Let Assumptions 2.1 to 2.4 be fulfilled and assume that both T and $\operatorname{var}(y_1)$ are bounded from above by a fixed constant as $n, p \to +\infty$. Then there exists a random vector ζ_i in \mathbb{R}^T with

(2.22)
$$\max_{j \in [p]} W_2 \Big(\mathsf{Law}(\boldsymbol{\zeta}_j), \ \mathsf{N}\Big(\mathbf{0}_T, \big(\mathbb{E}[r_{tt'}]\big)_{(t,t') \in [T] \times [T]} \Big) \Big) \to 0$$

such that for each $t \in [T]$,

(2.23)
$$\sum_{j=1}^{p} \mathbb{E}\left[\left(\sqrt{\frac{n}{\|\boldsymbol{\Sigma}^{-1/2}\boldsymbol{e}_{j}\|^{2}}}\left(\boldsymbol{\widehat{b}}_{j}^{t,\text{debias}}-\boldsymbol{b}_{j}^{*}\right)-\boldsymbol{\zeta}_{jt}\right)^{2}\right] \leq C(\boldsymbol{\zeta},T,\kappa,\gamma) \operatorname{var}(y_{1}).$$

The proof of Theorem 2.4 is given in Appendix I. If $var(y_1)$ stays bounded as $n, p \to +\infty$, the sum over p entries in the left-hand side of (2.23) stays bounded, and at most a constant number of entries may not converge to 0. This is made precise in the following corollary.

Corollary 2.5. Let Assumptions 2.1 to 2.4 be fulfilled and assume that T, $var(y_1)$ are bounded from above by a fixed constant as $n, p \to +\infty$. Let $a_p \to +\infty$ be a slowly increasing sequence (e.g., $a_p = \log p$). There exists a subset $J_{n,p}$ of size at least $p - a_p$ such that

(2.24)
$$\max_{j\in J_{n,p}} W_2\left(\sqrt{\frac{n}{\|\boldsymbol{\Sigma}^{-1/2}\boldsymbol{e}_j\|^2}} \left(\widehat{\boldsymbol{b}}_j^{t,\text{debias}} - \boldsymbol{b}_j^*\right), \quad \mathsf{N}(0,\mathbb{E}[r_t])\right) \to 0.$$

The proof of Corollary 2.5 is given in Appendix J. Convergence in 2-Wasserstein distance implies convergence in distributions (Villani et al., 2009, Def. 6.8 and Theorem 6.9). If $\operatorname{var}(y_1)/\sigma^2$ is bounded as $n, p \to +\infty$, Theorem 2.2 further shows that \hat{r}_t consistently estimates $\mathbb{E}[r_t]$, so that by Slutsky's theorem and (2.24), the z-score

(2.25)
$$\frac{\sqrt{n}(\hat{\boldsymbol{b}}_{j}^{t,\text{debias}} - \boldsymbol{b}_{j}^{*})}{\|\boldsymbol{\Sigma}^{-1/2}\boldsymbol{e}_{j}\|\sqrt{\hat{r}_{t}}}$$

converge to N(0, 1) in distributions uniformly over $j \in J_{n,p}$. For those overwhelming majority of components $j \in J_{n,p}$, Theorem 2.2 and Corollary 2.5 thus provide the $1 - \alpha$ confidence interval for b_i^* :

$$\Big[\widehat{\boldsymbol{b}}_{j}^{t,\text{debias}} - z_{\alpha/2}\sqrt{\frac{\hat{r}_{t}}{n}(\boldsymbol{\Sigma}^{-1})_{jj}}, \quad \widehat{\boldsymbol{b}}^{t,\text{debias}} + z_{\alpha/2}\sqrt{\frac{\hat{r}_{t}}{n}(\boldsymbol{\Sigma}^{-1})_{jj}}\Big],$$

where $z_{\alpha/2}$ is the standard normal quantile defined by $\mathbb{P}(|\mathsf{N}(0,1)| \ge z_{\alpha/2}) = \alpha$.

Asymptotic normality "on average" over coordinates, or only over a large subsets of coordinates, is typical in asymptotic normality results in the proportional regime, see for instance Bayati and Montanari (2012); Sur and Candès (2019); Lei et al. (2018); Berthier et al. (2020); Celentano et al. (2023); Bellec and Zhang (2023). Studying the remaining coordinates ($j \notin J_{n,p}$ above) remains a challenge, and in some situations the remaining coordinates exhibit a "variance spike" where the standard deviation estimate in (2.24) is incorrect and the asymptotic variance of (2.25) is bounded away from 1 (Bellec and Zhang, 2023, Section 3.7).

One application of Corollary 2.5 is early rejection in hypothesis testing. In order to perform a hypothesis test of the form

(2.26)
$$H_{0j}: \boldsymbol{b}_j^* = 0 \qquad \text{against} \qquad H_{1j}: \boldsymbol{b}_j^* \neq 0,$$

for the *j*-th component of the true regression vector \mathbf{b}^* in (1.1). Since the asymptotic normality of the zscore (2.25) is maintained throughout the iterations, one may perform early tests, without waiting for the convergence of $\hat{\mathbf{b}}^t$: reject H_{0j} at the *t*-th iteration if the z-score under H_{0j} is larger than the two-sided quantile of the normal distribution. We may for instance perform this test at $t = 10, 10^2, 10^3$ with an appropriate Bonferroni multiple testing correction. While the estimates \hat{r}_t in (2.15) and $\hat{r}_{tt'}$ in (2.18) do not require the knowledge of the covariance matrix Σ , the construction of the debiased estimate (2.21) requires the knowledge of $\Sigma^{-1} e_j$ or an estimate of it. If unlabeled samples $(\mathbf{x}_i)_{i=n+1,...,N}$ are available for instance, $\Sigma^{-1} e_j$ can be estimated by regressing the *j*-th column onto the others. We emphasize that the knowledge of $\Sigma^{-1} e_j$ is only used in the construction of debiased estimate (2.21), and that the estimate \hat{r}_t of the generalization error is readily usable without any knowledge of Σ .

3. Concrete examples

In this section, we present the analysis of a few popular algorithms aimed at solving minimization problems of the form (1.2), including the least-squares problem, Lasso and MCP. For the five algorithms present in the five subsections below, we present explicit expressions for iteration functions g_t as well as for the corresponding derivative matrices \mathcal{D}, \mathcal{J} and the memory matrix $\hat{\mathbf{A}}$. For each algorithm, these expressions are then used to compute the risk estimate \hat{r}_t in (2.15) and the z-score in (2.25). To illustrate our theoretical results, we conduct extensive simulation studies comparing the proposed risk estimator \hat{r}_t with the actual risk r_t at each iteration t and constructing normal quantile-quantile plots for z-score defined in (2.25) compared to the standard normal distribution. We start this section with the simulation settings.

Simulation setup. We consider three distinct scenarios based on the relationship between the sample size and feature dimension, denoted as (n, p), to generate datasets from the linear model (1.1). These scenarios are:

• Over-parametrized regime: (n, p) = (1200, 1500), in which the number of features surpasses the number of samples.

- Equal-parametrized regime: (n, p) = (1200, 1200), characterized by an equal number of samples and features.
- Under-parametrized regime: (n, p) = (1200, 500), where the number of samples exceeds the number of features.

For each scenario, the design matrix X is generated from a multivariate normal distribution with zero mean and a covariance matrix $\Sigma = (\Sigma_{jk})_{j,k \in [p]}$, where $\Sigma_{jk} = 0.5^{|j-k|}$. The noise vector ε follows the standard normal distribution, namely, $\sigma^2 = 1$. The coefficient vector b^* is chosen with p/20 nonzero entries, set to a constant value such that the signal-to-noise ratio $\|\Sigma^{1/2}b^*\|^2/\sigma^2$ equals 5. For each algorithm in the following subsections, the initial vector is set to $\hat{b}^1 = 0$, and the algorithm runs for T = 500 iterations, except for GD, where T = 3000 is necessary to achieve convergence. For each iterate $(\hat{b}^t)_{t \in [T]}$, we compute both the actual risk r_t following (2.14) and our proposed risk estimator \hat{r}_t as per (2.15), along with the proposed z-score defined in (2.25) with j = 1 (i.e., the first coordinate). Each simulation is replicated 100 times. We present the simulation results for (n, p) = (1200, 1500) for each algorithm in the subsequent subsections, and leave the other (n, p) pair scenarios to Appendix A since their results are very similar to (n, p) = (1200, 1500). Each simulation we tried confirmed the accuracy of the estimated risk \hat{r}_t for estimating r_t as well as the closeness of the z-scores (2.25) to the standard normal distribution.

3.1. Gradient descent

Consider estimating b^* by minimizing the squared loss function $f(b) = \frac{1}{2n} || y - Xb ||^2$. The gradient descent (GD) method finds the minimizer of f(b) by iterations

$$\widehat{\boldsymbol{b}}^{t} = \widehat{\boldsymbol{b}}^{t-1} - \eta \nabla \boldsymbol{f}(\widehat{\boldsymbol{b}}^{t-1}) = \widehat{\boldsymbol{b}}^{t-1} + \frac{\eta}{n} \boldsymbol{X}^{\top} (\boldsymbol{y} - \boldsymbol{X}\widehat{\boldsymbol{b}}^{t-1}),$$

with an initialization $\hat{b}^1 \in \mathbb{R}^p$. Since the function f is an L-smooth with $L = \|X\|_{op}^2/n$, one can take fixed step size $\eta = \frac{1}{L}$. Using the definition $v^t = \frac{1}{n} X^\top (y - X \hat{b}^t)$, the iteration of GD can be written as

(3.1)
$$\widehat{\boldsymbol{b}}^{t} = \boldsymbol{g}_{t}(\widehat{\boldsymbol{b}}^{t-1}, \boldsymbol{v}^{t-1}) = \widehat{\boldsymbol{b}}^{t-1} + \eta \boldsymbol{v}^{t-1} \text{ for } t \ge 2.$$

Therefore, the function g_t is Lipschitz continuous, and the matrices in (2.3) are given by

$$(3.2) J_{t,t-1} = I_p, \quad D_{t,t-1} = \eta I_p.$$

Hence, for GD with iteration (3.1), the expressions of \mathcal{J} and \mathcal{D} in (2.7) become

$$\mathcal{J} = \begin{bmatrix} \mathbf{0} & \mathbf{0} & \cdots & \cdots & \mathbf{0} \\ \mathbf{I}_p & \mathbf{0} & \ddots & \vdots \\ \mathbf{0} & \mathbf{I}_p & \mathbf{0} & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \mathbf{0} \\ \mathbf{0} & \cdots & \mathbf{0} & \mathbf{I}_p & \mathbf{0} \end{bmatrix} = \mathbf{L} \otimes \mathbf{I}_p, \qquad \mathcal{D} = \eta \mathcal{J} = \eta (\mathbf{L} \otimes \mathbf{I}_p),$$

where $\boldsymbol{L} \in \mathbb{R}^{T \times T}$ is the strictly lower triangular matrix $\boldsymbol{L} = \sum_{t=2}^{T} \boldsymbol{e}_t \boldsymbol{e}_{t-1}^{\top}$. Now we proceed to derive the expression for each entry of $\widehat{\mathbf{A}}$ in (2.12) for GD. First, note that $\mathcal{D} = \eta \mathcal{J}$, so that

$$\mathcal{J} - \mathcal{D}(\boldsymbol{I}_T \otimes \frac{\boldsymbol{X}^{\top} \boldsymbol{X}}{n}) = \boldsymbol{L} \otimes (\boldsymbol{I}_p - \eta \boldsymbol{X}^{\top} \boldsymbol{X}/n).$$

Since L is strictly lower triangular, the above display is also lower triangular. With $\Gamma = I_p - \frac{\eta \mathbf{X}^\top \mathbf{X}}{n}$, we have

$$\left(I_{pT} + \mathcal{D}(I_T \otimes \frac{\mathbf{X}^{\top} \mathbf{X}}{n}) - \mathcal{J}\right)^{-1} = \left(I_{pT} - (\mathbf{L} \otimes \mathbf{\Gamma})\right)^{-1} = \sum_{k=0}^{\infty} (\mathbf{L} \otimes \mathbf{\Gamma})^k = \sum_{k=0}^{T-1} \mathbf{L}^k \otimes \mathbf{\Gamma}^k$$

thanks to $(\mathbf{L} \otimes \mathbf{\Gamma})^k = \mathbf{L}^k \otimes \mathbf{\Gamma}^k$ by the mixed-product property and since $\mathbf{L}^k = \mathbf{0}$ for $k \ge T$. In this case, by the definition (2.12) of $\widehat{\mathbf{A}}$, we get

$$\widehat{\mathbf{A}} = \sum_{k=0}^{T-1} \boldsymbol{L}^{k+1} \operatorname{Tr} \left[\frac{\eta}{n} \boldsymbol{X} \boldsymbol{\Gamma}^{k} \boldsymbol{X}^{\top} \right] = \sum_{k=0}^{T-1} \boldsymbol{L}^{k+1} \operatorname{Tr} \left[(\boldsymbol{I}_{p} - \boldsymbol{\Gamma}) \boldsymbol{\Gamma}^{k} \right] = \sum_{k=0}^{T-2} \boldsymbol{L}^{k+1} \operatorname{Tr} \left[(\boldsymbol{I}_{p} - \boldsymbol{\Gamma}) \boldsymbol{\Gamma}^{k} \right].$$

More visually, since each incremental power of L moves the diagonal one step towards the bottom left, we have

$$\widehat{\mathbf{A}} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ \operatorname{Tr}(\boldsymbol{I}_p - \boldsymbol{\Gamma}) & 0 & 0 & 0 \\ \operatorname{Tr}((\boldsymbol{I}_p - \boldsymbol{\Gamma})\boldsymbol{\Gamma}) & \operatorname{Tr}(\boldsymbol{I}_p - \boldsymbol{\Gamma}) & 0 & 0 & 0 \\ \vdots & \ddots & \ddots & \ddots & 0 \\ \operatorname{Tr}((\boldsymbol{I}_p - \boldsymbol{\Gamma})\boldsymbol{\Gamma}^{T-2}) & \dots & \operatorname{Tr}((\boldsymbol{I}_p - \boldsymbol{\Gamma})\boldsymbol{\Gamma}) & \operatorname{Tr}(\boldsymbol{I}_p - \boldsymbol{\Gamma}) & 0 \end{bmatrix}$$

The above simplifications are specific to GD and will typically not be possible for examples involving nonlinear transformations such as soft-thresholding. Computation of $\widehat{\mathbf{A}}$ is straightforward once the eigenvalues of Γ is computed.

Remark 3.1. A closely related estimator to the GD iterates (3.1) is the minimum ℓ_2 norm least-squares estimator, is defined as

(3.3)
$$\widetilde{\boldsymbol{b}} = \arg\min\left\{\|\boldsymbol{b}\| : \boldsymbol{b} \text{ minimizes } \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{b}\|^2\right\}.$$

For n > p, $\tilde{\boldsymbol{b}} = (\boldsymbol{X}^{\top}\boldsymbol{X})^{-1}\boldsymbol{X}^{\top}\boldsymbol{y}$, and for $n \leq p$, $\tilde{\boldsymbol{b}} = \boldsymbol{X}^{\top}(\boldsymbol{X}\boldsymbol{X}^{\top})^{-1}\boldsymbol{y}$. It is equivalent to write $\tilde{\boldsymbol{b}} = (\boldsymbol{X}^{\top}\boldsymbol{X})^{\dagger}\boldsymbol{X}^{\top}\boldsymbol{y}$ where \dagger denotes the Moore-Penrose inverse. The GD iterates $\hat{\boldsymbol{b}}^{t}$ in (3.1) converge to the minnorm least-squares solution $\tilde{\boldsymbol{b}}$ as $t \to \infty$ (Hastie et al., 2022, Proposition 1). We observe this phenomenon in the simulations below where the risk of $\tilde{\boldsymbol{b}}$ is represented by an horizontal green curve.

Simulation results. Define $r_{\infty} := \|\mathbf{\Sigma}^{1/2}(\hat{\mathbf{b}}^{\infty} - \mathbf{b}^*)\| + \sigma^2$, where $\hat{\mathbf{b}}^{\infty} := \lim_{t \to \infty} \hat{\mathbf{b}}^t$ is the min-norm least-squares estimator (3.3), and has closed-form expression $\hat{\mathbf{b}}^{\infty} = \tilde{\mathbf{b}} = (\mathbf{X}^{\top}\mathbf{X})^{\dagger}\mathbf{X}^{\top}\mathbf{y}$. At each iteration $t \in [T]$, we calculate and present the average estimated risk \hat{r}_t , the actual risk r_t , and the limiting risk r_{∞} over 100 repetitions, including 2-standard error bars, in Figure 1a. We also provide the quantile-quantile (Q-Q) plot of the z-score (2.25) at different iterations in Figure 1b.



Fig 1: Risk curves and qq-plots of z-score of GD for (n, p) = (1200, 1500).

Figure 1a shows a strong alignment between our risk estimate \hat{r}_t and the actual risk r_t . Notably, both the risk and the estimated risk reach their minimum at iteration 8, suggesting that \hat{b}^8 yields the lowest outof-sample prediction risk. This observation indicates that it is beneficial to terminate the algorithm as early as iteration 8, rather than continuing with additional iterations, because the risk will blow up quickly after iteration 8. As t increases, we observe from Figure 1a that \hat{r}_t converges to r_{∞} , indicating the effectiveness of our risk estimator for large t. Furthermore, Figure 1b reveals that the quantiles closely match the 45-degree line (shown in red). This alignment supports the conclusion that the z-score (2.25) closely approximates a standard normal distribution.

3.2. Nesterov's accelerated gradient descent (AGD)

The Nesterov's accelerated gradient method (Nesterov, 1983) is a remarkable extension of the gradient descent by utilizing the momentum from previous iterates. It is well known that AGD enjoys quadratic convergence rates, which is faster than the linear convergence rate of the gradient descent. To describe the iteration of AGD, define the sequence of scalars

(3.4)
$$a_0 = 0, \quad a_t = \frac{1 + \sqrt{1 + 4a_{t-1}^2}}{2}, \quad w_t = \frac{1 - a_t}{a_{t+1}} \quad \text{for all } t \ge 1.$$

From some initialization $\widehat{b}^1 \in \mathbb{R}^p$, AGD iterates are defined as the weighted sum

(3.5)
$$\widehat{\boldsymbol{b}}^{t} = (1 - w_{t-1})(\widehat{\boldsymbol{b}}^{t-1} + \eta \boldsymbol{v}^{t-1}) + w_{t-1}(\widehat{\boldsymbol{b}}^{t-2} + \eta \boldsymbol{v}^{t-2}), \quad \text{for all } t \ge 2.$$

Hence, the Jacobian matrices defined in (2.6) are given by

$$\mathbf{J}_{t,t-1} = (1 - w_{t-1})\mathbf{I}_p, \qquad \mathbf{D}_{t,t-1} = \eta(1 - w_{t-1})\mathbf{I}_p, \\
 \mathbf{J}_{t,t-2} = w_{t-1}\mathbf{I}_p, \qquad \mathbf{D}_{t,t-2} = \eta w_{t-1}\mathbf{I}_p.$$

It follows that the expressions of \mathcal{J} and \mathcal{D} in (2.7) become

$$\mathcal{J} = \begin{bmatrix} \mathbf{0} & \mathbf{0} & \cdots & \cdots & \cdots & \mathbf{0} \\ (1 - w_1) \mathbf{I}_p & \mathbf{0} & \ddots & \cdots & \cdots & \vdots \\ w_2 \mathbf{I}_p & (1 - w_2) \mathbf{I}_p & \mathbf{0} & \ddots & \cdots & \vdots \\ \mathbf{0} & w_3 \mathbf{I}_p & (1 - w_3) \mathbf{I}_p & \mathbf{0} & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \mathbf{0} \\ \mathbf{0} & \cdots & \mathbf{0} & w_{T-1} \mathbf{I}_p & (1 - w_{T-1}) \mathbf{I}_p & \mathbf{0} \end{bmatrix}, \quad \mathcal{D} = \eta \mathcal{J}.$$

Remark 3.2. By Proposition 1 in Hastie et al. (2022), the AGD iterate \hat{b}^t in (3.5) also converges to the min-norm least-squares estimator \tilde{b} as $t \to \infty$.

Simulation results. Similar to the plots for gradient descent, we provide results for AGD applied to the least-squares problem. The risk curves are shown in Figure 2a and Q-Q plots of the z-score (2.25) in Figure 2b. The simulation results for AGD are similar to those for GD. Figure 2a clearly shows that the risk estimate \hat{r}_t closely matches the actual risk r_t . In addition, the risk curve suggests stopping the algorithm early at iteration 8 as the estimated risk increases quickly after iteration 8. Both r_t and \hat{r}_t converge to r_{∞} as t increases. Figure 2b again confirms that the z-scores (2.25) are close to a standard normal distribution.



Fig 2: Risk curves and qq-plots of z-score of AGD for (n, p) = (1200, 1500).

3.3. Iterative Shrinkage-Thresholding Algorithm (ISTA)

For regression problems with high-dimensional features, penalized regression are useful to achieve sparse solutions. Consider the Lasso regression

(3.6)
$$\widehat{\boldsymbol{b}} \in \operatorname*{arg\,min}_{\boldsymbol{b} \in \mathbb{R}^p} \frac{1}{2n} \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{b}\|^2 + \lambda \|\boldsymbol{b}\|_1$$

This objective function of the above optimization has two parts, one is the squared loss, the other is an ℓ_1 penalty. ISTA (Daubechies et al., 2004) is a simple algorithm to solve (3.6) by imposing a soft-thresholding

nonlinearity at each iteration. Concretely, let $\operatorname{soft}_{\theta} : \mathbb{R}^p \to \mathbb{R}^p$ denote the elementwise soft-thresholding operator, i.e. $\operatorname{soft}_{\theta}(\boldsymbol{b})_j = (|\boldsymbol{b}_j - \theta|)_+ \operatorname{sgn}(\boldsymbol{b}_j)$. ISTA can be viewed as the proximal gradient descent in Section 2.1.1, and its iteration function \boldsymbol{g}_t is given by

(3.7)
$$\widehat{\boldsymbol{b}}^t = \boldsymbol{g}_t(\widehat{\boldsymbol{b}}^{t-1}, \boldsymbol{v}^{t-1}) = \operatorname{soft}_{\lambda/L}(\widehat{\boldsymbol{b}}^{t-1} + L^{-1}\boldsymbol{v}^{t-1}).$$

The function g_t is Lipschitz continuous since the soft-thresholding is 1-Lipschitz. Let $S^t = \{j \in [p] : |\hat{b}_j^t + L^{-1}v_j^t| > \lambda/L\}$. For ISTA, the expressions of $J_{t,t-1}$ and $D_{t,t-1}$ in (2.3) are the diagonal matrices

$$\boldsymbol{J}_{t,t-1} = \sum_{j \in S^{t-1}} \boldsymbol{e}_{j} \boldsymbol{e}_{j}^{\top} = \text{diag}\Big(\big(\mathbb{I}\{j \in S^{t-1}\} \big)_{j \in [p]} \Big), \qquad \boldsymbol{D}_{t,t-1} = L^{-1} \boldsymbol{J}_{t,t-1}.$$

Substituting the above into (2.4) gives the expressions of \mathcal{J} and \mathcal{D} for ISTA.

Simulation results. We apply ISTA to solve the Lasso regression (3.6) with two regularization parameters $\lambda \in \{0.01, 0.1\}$. The ISTA iterates converge to the Lasso estimator (3.6) (see, e.g., Beck and Teboulle (2009)). We compute the Lasso using the Python module sklearn.linear_model.Lasso and use this Lasso estimator to evaluate the limiting risk r_{∞} . Figure 3a showcases the risk estimator \hat{r}_t and actual risk r_t for each iteration t using ISTA. Furthermore, Figure 3b displays the Q-Q plots of the z-score (2.25) for ISTA. Again, the estimated risk curve closely aligns with the actual risk curve for both values of λ , and the corresponding z-scores closely approximate the standard normal distribution.



Fig 3: Risk curves and qq-plots of z-score of ISTA for (n, p) = (1200, 1500).

3.4. Fast Iterative Shrinkage-Thresholding Algorithm (FISTA)

Similar to the extension from GD to AGD, FISTA (Beck and Teboulle, 2009) is an accelerated version of ISTA, incorporating momentum with the weights (3.4). One advantage of FISTA is that it enjoys faster convergence rate than ISTA (Beck and Teboulle, 2009). Using the same definitions of a_t, w_t in (3.4), FISTA iterates the following steps with some initialization $\hat{b}^1 \in \mathbb{R}^p$:

$$\hat{\boldsymbol{b}}^{t} = \boldsymbol{g}_{t}(\hat{\boldsymbol{b}}^{t-1}, \hat{\boldsymbol{b}}^{t-2}, \boldsymbol{v}^{t-1}, \boldsymbol{v}^{t-2}) = (1 - w_{t-1}) \operatorname{soft}_{\lambda/L}(\hat{\boldsymbol{b}}^{t-1} + L^{-1}\boldsymbol{v}^{t-1}) + w_{t-1} \operatorname{soft}_{\lambda/L}(\hat{\boldsymbol{b}}^{t-2} + L^{-1}\boldsymbol{v}^{t-2}) \text{ for } t \ge 2.$$

Using $S^t = \{j \in [p] : |\hat{b}_j^t + L^{-1} v_j^t| > \lambda/L\}$, the matrices in (2.6) are the diagonal matrices

$$\mathbf{J}_{t,t-1} = (1 - w_{t-1}) \sum_{j \in S^{t-1}} \mathbf{e}_j \mathbf{e}_j^\top, \qquad \mathbf{D}_{t,t-1} = \frac{1}{L} \mathbf{J}_{t,t-1}, \\
 \mathbf{J}_{t,t-2} = w_{t-1} \sum_{j \in S^{t-2}} \mathbf{e}_j \mathbf{e}_j^\top, \qquad \mathbf{D}_{t,t-2} = \frac{1}{L} \mathbf{J}_{t,t-2}.$$

We obtain the expressions of \mathcal{D} and \mathcal{J} for FISTA by substituting the above into (2.7). Similarly to the simulation results for ISTA, we present the risk curves and Q-Q plots of the z-score (2.25) for FISTA in Figure 4.



Fig 4: Risk curves and qq-plots of z-score of FISTA for (n, p) = (1200, 1500).

3.5. Local quadratic approximation in non-convex penalized regression

In this subsection, we consider the folded-concave penalized least-squares,

(3.8)
$$\min_{\boldsymbol{b}\in\mathbb{R}^p}\frac{1}{2n}\|\boldsymbol{y}-\boldsymbol{X}\boldsymbol{b}\|^2 + \sum_{j=1}^p \rho(|\boldsymbol{b}_j|),$$

where $\rho : \mathbb{R}_+ \to \mathbb{R}$ is a concave penalty function. This encompasses SCAD (Fan and Li, 2001) and MCP (Zhang, 2010). For simulations, we set $\rho(\cdot)$ to be the MCP penalty with two positive tuning parameters (λ, τ) , defined as

(3.9)
$$\rho(x;\lambda,\tau) = \begin{cases} \lambda x - \frac{1}{2\tau} x^2 & \text{if } x \le \tau \lambda \\ \frac{1}{2}\tau \lambda^2 & \text{if } x > \tau \lambda \end{cases}.$$

For simplicity, we will omit the parameters (λ, τ) in the notation, using $\rho(x)$ instead of $\rho(x; \lambda, \tau)$. Consequently, the derivative of ρ becomes $\rho'(x) = (\lambda - x/\tau)\mathbb{I}(x \leq \tau\lambda)$. As $\tau \to \infty$, $\rho(x)$ becomes λx , and the optimization problem (3.8) then coincides with the Lasso (3.6).

In order to solve the non-convex penalized regression (3.8), we consider the local isotropic quadratic approximation (LQA) to the least-squares loss $f(\mathbf{b}) := \frac{1}{2n} \|\mathbf{y} - \mathbf{X}\mathbf{b}\|^2$ at a vector $\hat{\mathbf{b}}^{t-1}$, namely

(3.10)
$$f(\boldsymbol{b}) \approx f(\widehat{\boldsymbol{b}}^{t-1}) + (\boldsymbol{b} - \widehat{\boldsymbol{b}}^{t-1})^{\top} \nabla f(\widehat{\boldsymbol{b}}^{t-1}) + (L/2) \|\boldsymbol{b} - \widehat{\boldsymbol{b}}^{t-1}\|^2,$$

where $\nabla f(\hat{\boldsymbol{b}}^{t-1})$ is the gradient of f evaluated at $\hat{\boldsymbol{b}}^{t-1}$, and $L = n^{-1} \|\boldsymbol{X}\|_{\text{op}}^2$ as in previous sections. Applying the above quadratic approximation (3.10) to the least-squares in (3.8) and ignoring the constant term yields the optimization problem

(3.11)
$$\widehat{\boldsymbol{b}}^{t} = \operatorname*{arg\,min}_{\boldsymbol{b}\in\mathbb{R}^{p}} \frac{1}{2} \|\boldsymbol{b} - (\widehat{\boldsymbol{b}}^{t-1} + (nL)^{-1}\boldsymbol{X}^{\top}(\boldsymbol{y} - \boldsymbol{X}\widehat{\boldsymbol{b}}^{t-1}))\|^{2} + \frac{1}{L}\sum_{j=1}^{p} \rho(|\boldsymbol{b}_{j}|).$$

Let \hat{b}_j^t and v_j^t be the *j*-th entry of \hat{b}^t and v^t , respectively. For $\tau \ge 1/L$, the optimization problem (3.11) admits the closed-form solution

(3.12)
$$\widehat{\boldsymbol{b}}_{j}^{t} = \begin{cases} \operatorname{soft}_{\lambda/L} \left(\widehat{\boldsymbol{b}}_{j}^{t-1} + \frac{1}{L} \boldsymbol{v}_{j}^{t-1} \right) (1 - \frac{1}{\tau L})^{-1} & \text{if } |\widehat{\boldsymbol{b}}_{j}^{t-1} + \frac{1}{L} \boldsymbol{v}_{j}^{t-1}| \leq \tau \lambda, \\ \widehat{\boldsymbol{b}}_{j}^{t-1} + \frac{1}{L} \boldsymbol{v}_{j}^{t-1} & \text{otherwise.} \end{cases}$$

In this case, $J_{t,t-1}$ and $D_{t,t-1}$ in (2.3) are the diagonal matrices

$$\boldsymbol{J}_{t,t-1} = \sum_{j=1}^{p} \boldsymbol{e}_{j} \boldsymbol{e}_{j}^{\top} \left[(1 - \frac{1}{\tau L})^{-1} \mathbb{I}\left(|\widehat{\boldsymbol{b}}_{j}^{t-1} + \frac{1}{L} \boldsymbol{v}_{j}^{t-1}| \in [\lambda/L, \tau\lambda] \right) + \mathbb{I}\left(|\widehat{\boldsymbol{b}}_{j}^{t-1} + \frac{1}{L} \boldsymbol{v}_{j}^{t-1}| > \tau\lambda \right) \right]$$

and $D_{t,t-1} = \frac{1}{L} J_{t,t-1}$.

Remark 3.3. If $\tau = \infty$, the MCP function reduces to $\sum_{j=1}^{p} \rho(|\mathbf{b}_j|) = \lambda \|\mathbf{b}\|_1$, so MCP is the same as the Lasso. In this case, the LQA iterations (3.12) become $\hat{\mathbf{b}}^t = \operatorname{soft}_{\lambda/L}(\hat{\mathbf{b}}^{t-1} + \frac{1}{L}\mathbf{v}^{t-1})$, which is the same as ISTA iterations (3.7) in Section 3.3.

Simulation results. For the MCP penalty function (3.9), we consider $\lambda \in \{0.1, 0.2\}$ and $\tau = 3$. We display the curves for the risk estimator \hat{r}_t and the actual risk r_t for each iteration t in Figure 5a. Additionally, the Q-Q plots of the z-score (2.25) are given in Figure 5b. Figure 5a shows that the estimated risk accurately estimates the true risk. The z-scores (2.25) closely approximate the standard normal distribution. Similar to observations in the aforementioned algorithms, LQA reaches its lowest risk level at around iteration 10. This suggests that early stopping could be beneficial for LQA for certain tuning parameters to improve generalization performance. When comparing the lowest points on the risk curves for LQA with other algorithms (GD, AGD, ISTA, and FISTA), LQA achieves the lower risk among the tested algorithms at the given tuning parameters. Figure 5b provides empirical support for the established asymptotic normality of the debiased LQA iterates in Theorem 2.4.



Fig 5: Risk curves and qq-plots of z-score of LQA for (n, p) = (1200, 1500).

4. Efficient computation of the memory matrix

Recall that the memory matrix $\widehat{\mathbf{A}}$ is crucial in the formulae of proposed risk estimator \hat{r}_t in (2.15) and debiased estimator $\widehat{\mathbf{b}}_j^{t,\text{debias}}$ in (2.21). We have provided specific expressions of $\widehat{\mathbf{A}}$ for various algorithms in Section 3. In this section, we provide an efficient way to compute the memory matrix $\widehat{\mathbf{A}}$ in (2.12) for algorithms with the general iterations (2.8).

4.1. Iteratively computing rows of A

Recall the definition of $\widehat{\mathbf{A}}$ in (2.12) is

$$\widehat{\mathbf{A}} = \frac{1}{n} \sum_{i=1}^{n} \big(\boldsymbol{I}_T \otimes (\boldsymbol{e}_i^{\top} \boldsymbol{X}) \big) \Big(\boldsymbol{I}_{pT} + \mathcal{D}(\boldsymbol{I}_T \otimes \frac{\boldsymbol{X}^{\top} \boldsymbol{X}}{n}) - \mathcal{J} \Big)^{-1} \mathcal{D} \big(\boldsymbol{I}_T \otimes (\boldsymbol{X}^{\top} \boldsymbol{e}_i) \big).$$

The first apparent computational hurdle lies in inverting the large matrix $I_{pT} + \mathcal{D}(I_T \otimes \frac{X^{\top}X}{n}) - \mathcal{J}$ of size $pT \times pT$. We now provide an efficient way to compute the memory matrix $\hat{\mathbf{A}}$ without explicitly inverting this large matrix. Recall that \mathcal{D} and \mathcal{J} are $T \times T$ block lower triangular matrices given in (2.7) or (2.10), where each block is of size $p \times p$. It follows that $\mathcal{J} - \mathcal{D}(I_T \otimes \frac{X^{\top}X}{n})$ is also a $T \times T$ block lower triangular matrix with zero diagonal blocks. Let $M_t \in \mathbb{R}^{p \times (pT)}$ be the *t*-th block row of \mathcal{D} . Consider the linear system with unknowns $R_1 \in \mathbb{R}^{p \times pT}, \ldots, R_T \in \mathbb{R}^{p \times pT}$ given by

which can be rewritten with $P_{t,s} = J_{t,s} - D_{t,s} X^{\top} X/n$ as

(4.1)
$$\begin{bmatrix} \boldsymbol{I}_{p} & \boldsymbol{0}_{p \times p} & \cdots & \cdots & \boldsymbol{0}_{p \times p} \\ -\boldsymbol{P}_{2,1} & \boldsymbol{I}_{p} & \boldsymbol{0}_{p \times p} & & \vdots \\ -\boldsymbol{P}_{3,1} & -\boldsymbol{P}_{3,2} & \boldsymbol{I}_{p} & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \boldsymbol{0}_{p \times p} \\ -\boldsymbol{P}_{T,1} & & \cdots & -\boldsymbol{P}_{T,T-1} & \boldsymbol{I}_{p} \end{bmatrix} \begin{bmatrix} \boldsymbol{R}_{1} \\ \boldsymbol{R}_{2} \\ \vdots \\ \boldsymbol{R}_{T-1} \\ \boldsymbol{R}_{T} \end{bmatrix} = \begin{bmatrix} \boldsymbol{M}_{1} \\ \boldsymbol{M}_{2} \\ \vdots \\ \boldsymbol{M}_{T-1} \\ \boldsymbol{M}_{T} \end{bmatrix} = \mathcal{D}.$$

The left-most matrix being lower-triangular with identity diagonal blocks, forward substitution provides the unique solution: starting with $\mathbf{R}_1 = \mathbf{M}_1$ we obtain directly $\mathbf{R}_2 = \mathbf{M}_2 + \mathbf{P}_{2,1}\mathbf{R}_1$, and more generally for all $t \ge 1$,

(4.2)
$$\boldsymbol{R}_{t} = \boldsymbol{M}_{t} + \sum_{s=1}^{t-1} \boldsymbol{P}_{t,s} \boldsymbol{R}_{s} = \sum_{s=1}^{t-1} \boldsymbol{e}_{s}^{\top} \otimes \boldsymbol{D}_{t,s} + \sum_{s=1}^{t-1} \boldsymbol{P}_{t,s} \boldsymbol{R}_{s},$$

where the second equality follows from the observation that \mathcal{D} is block lower triangular with *t*-th row block $M_t = \sum_{s=1}^{t-1} e_s^\top \otimes D_{t,s}$. Given $(\mathbf{R}_s)_{s \leq t-1}$, compute \mathbf{R}_t according to (4.2) and set

(4.3)
$$\widehat{\mathbf{A}}_{t,t'} = \frac{1}{n} \operatorname{Tr} \left[\boldsymbol{X} \boldsymbol{R}_t (\boldsymbol{e}_{t'} \otimes \boldsymbol{X}^\top) \right] \quad \text{for } t' < t, \quad \widehat{\mathbf{A}}_{t,t'} = 0 \quad \text{for } t' \ge t.$$

If only one or two blocks $P_{t,s}$ per row are nonzero as in (2.7), which is satisfied for all examples of Section 3, the recursion (4.2) simplifies in this case to

(4.4)
$$\boldsymbol{R}_{t} = \sum_{s=t-2}^{t-1} \boldsymbol{e}_{s}^{\top} \otimes \boldsymbol{D}_{t,s} + \sum_{s=t-2}^{t-1} \left(\boldsymbol{J}_{t,s} - \boldsymbol{D}_{t,s} \frac{\boldsymbol{X}^{\top} \boldsymbol{X}}{n} \right) \boldsymbol{R}_{s},$$

followed by (4.3). Notably, we may compute each \mathbf{R}_t recursively while only keeping in memory \mathbf{R}_{t-1} and \mathbf{R}_{t-2} , both of size $p \times (pT)$, at each step.

4.2. Hutchinson's trace approximation

The above computation of $\hat{\mathbf{A}}$ using (4.3) can still be prohibitive, as it requires storing in memory matrices $\mathbf{R}_t, \mathbf{R}_{t-1}$ of size at most $p \times (pT)$ at each step, and perform matrix-matrix products with dimensions $p \times p$ and $p \times (pT)$ in (4.4). We now describe an efficient way to approximate the entries of $\hat{\mathbf{A}}$ while avoiding to store intermediate matrices of size $p \times (pT)$. Let $m \ge 1$ be a small constant integer; in simulations we have noticed that m = 1, 2 or 3 already gives accurate estimates. We propose to approximate the trace (4.3) for the (t, s)-th entry of $\hat{\mathbf{A}}$ using Hutchinson's trace approximation (Hutchinson, 1990)

$$\operatorname{Tr}(\boldsymbol{M}) \approx \operatorname{Tr}(\boldsymbol{W}^{\top}\boldsymbol{M}\boldsymbol{W})$$

for any matrix $\boldsymbol{M} \in \mathbb{R}^{n \times n}$, where $\boldsymbol{W} \in \mathbb{R}^{n \times m}$ is a random matrix with i.i.d. entries uniformly distributed in $\{\frac{1}{\sqrt{m}}, \frac{-1}{\sqrt{m}}\}$. The Hanson-Wright inequality ensures that the above approximation holds with high-probability when $\|\boldsymbol{M}\|_{\mathrm{F}}$ is negligible compared to $\mathrm{Tr}(\boldsymbol{M})$. Using this approximation, the computation of the trace of a matrix of size $n \times n$ is reduced to that of a matrix of size $m \times m$.

In our case, we need to approximate the trace in (4.3) using Hutchinson's approximation. To this end, let $\boldsymbol{W} \in \mathbb{R}^{n \times m}$ be a random matrix with i.i.d. entries uniformly distributed in $\{\frac{1}{\sqrt{m}}, \frac{-1}{\sqrt{m}}\}$ independently of everything else. The matrix \boldsymbol{W} is only sampled once, and fixed throughout the following computation. Instead of computing recursively \boldsymbol{R}_t in (4.2), we compute $\bar{\boldsymbol{R}}_t = \boldsymbol{R}_t(\boldsymbol{I}_T \otimes (\boldsymbol{X}^{\top} \boldsymbol{W}))$ iteratively from (4.2) with the recursion

(4.5)
$$\bar{\boldsymbol{R}}_{t} = \sum_{s=1}^{t-1} \boldsymbol{e}_{s}^{\top} \otimes (\boldsymbol{D}_{t,s} \boldsymbol{X}^{\top} \boldsymbol{W}) + \sum_{s=1}^{t-1} \left(\boldsymbol{J}_{t,s} - \boldsymbol{D}_{t,s} \frac{\boldsymbol{X}^{\top} \boldsymbol{X}}{n} \right) \bar{\boldsymbol{R}}_{s}.$$

Once $\bar{\mathbf{R}}_t$ is available, we compute the Hutchinson's approximation for each entry of the *t*-th row of $\hat{\mathbf{A}}$ in (4.3) by

$$\widehat{\mathbf{A}}_{t,t'}^{H} = \frac{1}{n} \operatorname{Tr} \Big[\boldsymbol{W}^{\top} \boldsymbol{X} \bar{\boldsymbol{R}}_{t} (\boldsymbol{e}_{t'} \otimes \boldsymbol{I}_{m}) \Big]$$

for t' < t and 0 for $t' \ge t$. For AGD and FISTA or any iterative algorithm with \mathcal{D}, \mathcal{J} given by (2.7), $\mathbf{D}_{t,s}$ and $\mathbf{J}_{t,s}$ are 0 except for s = t - 1 and s = t - 2. In this case the sums in the recursion for \mathbf{R}_t in (4.2) and $\bar{\mathbf{R}}_t$ in (4.5) are reduced to $\sum_{s=t-2}^{t-1}$ with only two terms. For ISTA and GD, $\mathbf{D}_{t,s}$ and $\mathbf{J}_{t,s}$ are 0 except for s = t - 1 so the sum is reduced to only one term at s = t - 1. In this case, the recursion (4.5) only uses mT matrix-vector products with matrix dimensions smaller than max $\{n, p, T\}$. In particular, if $mT \ll \min\{n, p\}$, it is never needed to perform a matrix-matrix multiplication with two matrices with both dimensions of order n or p. In terms of memory footprint, in the case (2.7), only the last two $\bar{\mathbf{R}}_{t-1}$ and $\bar{\mathbf{R}}_{t-2}$ are needed to compute $\bar{\mathbf{R}}_t$. This is the same cost as storing a matrix of size $p \times (2mT)$, which is negligible compared to storing $\mathbf{X} \in \mathbb{R}^{n \times p}$ as long as $mT \ll n$.

Finally, remark that $\bar{\mathbf{R}}_t$ is 0 except in its first t-1 column blocks, so that only these first t-1 columns blocks need to be stored and computed in the recursion (4.5). More precisely, let $\mathbf{V}_{t,t'} \stackrel{\text{def}}{=} \mathbf{R}_t(\mathbf{e}_{t'} \otimes \mathbf{X}^{\top} \mathbf{W}) \in \mathbb{R}^{p \times m}$ for $t' \leq t-1$ to be t' column block of $\bar{\mathbf{R}}_t$. Then Hutchinson's approximation equals

(4.6)
$$\widehat{\mathbf{A}}_{t,t'}^{H} = \frac{1}{n} \operatorname{Tr}[\mathbf{W}^{\top} \mathbf{X} \mathbf{V}_{t,t'}].$$

At step t, in order to compute $V_t \stackrel{\text{def}}{=} [V_{t,1}, ..., V_{t,t-1}] \in \mathbb{R}^{p \times m(t-1)}$ in the case (2.7) satisfied by all examples of Section 3, we have the recursion formula

$$\boldsymbol{V}_t = \boldsymbol{P}_{t,t-2} \begin{bmatrix} \boldsymbol{V}_{t-2}, \ \boldsymbol{0}_p, \boldsymbol{0}_p \end{bmatrix} + \boldsymbol{P}_{t,t-1} \begin{bmatrix} \boldsymbol{V}_{t-1}, \ \boldsymbol{0}_p \end{bmatrix} + \begin{bmatrix} \boldsymbol{0}_{p \times m(t-3)}, \ \boldsymbol{D}_{t,t-2} \boldsymbol{X}^\top \boldsymbol{W}, \ \boldsymbol{D}_{t,t-1} \boldsymbol{X}^\top \boldsymbol{W} \end{bmatrix},$$

where $P_{t,s} = J_{t,s} - D_{t,s} X^{\top} X/n$ as above. In the case of ISTA and FISTA where the nonlinear functions use the soft-thresholding operator, these approximations let us compute the iterations (1.6) and the memory matrix (2.12) with problem dimensions n = 25,000; p = 40,000; T = 30 on a laptop with 32GB of RAM within four minutes.

5. Discussion

This paper introduces a novel procedure to estimate the out-of-sample prediction error for iterates of gradient descent type algorithms, in the context of high-dimensional regression. As illustrated in Section 3, this riskestimation procedure is applicable to a wide range of algorithms commonly used in optimization, including gradient descent, Nesterov's accelerated gradient descent, iterative shrinkage-thresholding algorithm (Beck and Teboulle, 2009), and local quadratic approximation. The proposed procedure do not require the knowledge of the design covariance Σ or of the noise level σ^2 . The estimates allow the statistician to leverage the benefits of early stopping, by selecting an early iteration $\hat{t} \in [T]$ that minimizes the generalization error among the first T iterations up to negligible error (Corollary 2.3). We have further established the asymptotic normality of the entries of the iterates after a debiasing correction, which can be used to construct confidence intervals for the *j*-th of the ground-truth b^* when $\Sigma^{-1}e_j$ is known or can be estimated (Theorem 2.4). Extensive numerical simulations in Section 3 demonstrate that the proposed estimate is accurate, and that the z-scores defining the confidence intervals are approximately standard normal.

Here we highlight several directions for further exploration. A first avenue for future research is to improve the dependence of the bounds on the number T of iterations. Currently, upper bounds in Theorem 2.2 and other main results involve constants that worst than exponential in T, while we observe in simulations that the risk estimate is still accurate over the whole trajectory for $T \gg \log n$. Another direction of interest is to generalize the estimates of the present paper beyond the square loss in (1.2), for instance with the Huber or least-absolute deviation loss in robust regression, or the logistic loss in classification problems. Another generalization concerns randomized versions of GD such as stochastic gradient descent. Finally, our proofs rely crucially on the Gaussianity of the design, and it would be of interest to extend the validity of the estimates proposed here to different design distributions. Recent progress has been made in this direction (Montanari and Saeed, 2022; Hu and Lu, 2022; Han and Shen, 2023; Pesce et al., 2023; Dudeja et al., 2023) regarding the universality of the training and generalization error of minimizers such as (1.2). An extra challenge presented here is that the validity of \hat{r}_t for estimating r_t requires not only universality of the training and generalization error, but also universality the weights $\hat{w}_{t,s}$.

Supplementary Material

Supplement A

This supplement contains additional numerical results and proofs.

Supplement B

This supplement contains the code and instruction to produce the numerical results.

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Appendices

Appendix A: Additional simulation results

In this section, we provide more simulation results for the other two scenarios (n, p) = (1200, 500) and (n, p) = (1200, 1200), which are similar to the results for (n, p) = (1200, 1500) presented in Section 3.

A.1. Under parametrization: (n, p) = (1200, 500)

A.1.1. GD and AGD

For GD and AGD applied to solve least-squares problem, when (n, p) = (1200, 500), we know that the iterate \hat{b}^t converges to the ordinary least-squares estimate $(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$ as $t \to \infty$. Thus we are able to compute the limiting risk r_{∞} for GD and AGD. We present the simulation results for GD and AGD in Figure 6 and Figure 7, respectively.



Fig 6: Risk curves and qq-plots of z-score of GD for (n, p) = (1200, 500).



Fig 7: Risk curves and qq-plots of z-score of AGD for (n, p) = (1200, 500).

A.1.2. ISTA and FISTA

We present the simulation results for ISTA and FISTA in Figure 8 and Figure 9, respectively.



Fig 8: Risk curves and qq-plots of z-score of ISTA for (n, p) = (1200, 500).



Fig 9: Risk curves and qq-plots of z-score of FISTA for (n, p) = (1200, 500).

A.1.3. LQA

We present the simulation results for LQA in Figure 10.



Fig 10: Risk curves and qq-plots of z-score of LQA for (n, p) = (1200, 500).

A.2. Equal parametrization: (n, p) = (1200, 1200)

In this section, we present the simulation results for the equal parametrization scenario (n, p) = (1200, 1200).

A.2.1. GD and AGD

For GD and AGD, we know that the iterates converge to the min-norm least-squares estimator (3.3) as $t \to \infty$ (Hastie et al., 2022, Proposition 1). Under n = p = 1200, we know that the risk of the min-norm least-squares estimator is infinite (Hastie et al., 2022), i.e., $r_{\infty} = +\infty$. So here we do not plot the horizontal line for r_{∞} .

We present the simulation results for GD and AGD in Figure 11 and Figure 12, respectively.



Fig 11: Risk curves and qq-plots of z-score of GD for (n, p) = (1200, 1200).



Fig 13: Risk curves and qq-plots of z-score of ISTA for (n, p) = (1200, 1200).



Fig 12: Risk curves and qq-plots of z-score of AGD for (n, p) = (1200, 1200).

A.2.2. ISTA and FISTA

We present the simulation results for ISTA and FISTA in Figure 13 and Figure 14, respectively.



Fig 14: Risk curves and qq-plots of z-score of FISTA for (n, p) = (1200, 1200).

A.2.3. LQA

We present the simulation results for LQA in Figure 15.

Appendix B: Preliminary

B.1. Notation

Notation and definitions that will be used in the rest of the paper are given here. Regular variables like a, b, \ldots refer to scalars, bold lowercase letters such as a, b, \ldots represent vectors, and bold uppercase letters like A, B, \ldots indicate matrices. Let $[n] = \{1, 2, \ldots, n\}$ for all $n \in \mathbb{N}$. The vectors $e_i \in \mathbb{R}^n, e_j \in \mathbb{R}^p, e_t \in \mathbb{R}^T$ denote the canonical basis vector of the corresponding index. For a real vector $a \in \mathbb{R}^p$, $\|a\|$ denotes its Euclidean norm. For any matrix A, A^{\dagger} is its Moore–Penrose inverse; $\|A\|_{\mathrm{F}}$, $\|A\|_{\mathrm{op}}$, $\|A\|_*$ denote its Frobenius, operator and nuclear norm, respectively. Let $A \otimes B$ be the Kronecker product of A and B. For A symmetric, $\phi_{\min}(A)$ and $\phi_{\max}(A)$ denote its smallest and largest eigenvalues, respectively. Let $\mathbf{1}_n$ denote the all-ones vector in \mathbb{R}^n , and I_n denote the identity matrix of size n. For a mapping $\mathbb{R}^p \to \mathbb{R}^n : \mathbf{x} \mapsto \mathbf{f}(\mathbf{x})$, we denote its Jacobian by $\frac{\partial \mathbf{f}(\mathbf{x})}{\partial \mathbf{x}} \in \mathbb{R}^{n \times p}$, i.e., $(\frac{\partial \mathbf{f}(\mathbf{x})}{\partial \mathbf{x}})_{i,j} \stackrel{\text{def}}{=} \frac{\partial \mathbf{f}_i(\mathbf{x})}{\partial \mathbf{x}_j}$ for all $i \in [n], j \in [p]$. For a random sequence ξ_n , we write $\xi_n = O_P(a_n)$ if ξ_n/a_n is stochastically bounded. For two scalars $a, b, a \vee b$ denotes the maximum of a and b. Let $\mathbb{I}(\Omega)$ denote the indicator function of event Ω . It takes the value 1 if the event Ω occurs and 0 otherwise.

Let C represent an absolute constant. Additionally, we use $C(\zeta, \gamma)$ to denote a positive constant that only depends on τ and γ . Similarly, we extend this notation to $C(\zeta, \gamma, \kappa, \ldots)$, representing positive constants dependent only on τ , γ , κ , and so forth. The exact value of these constants may vary from place to place. We write $a \leq b$ if $a \leq Cb$ for some absolute constant C.

Let $N(\mu, \sigma^2)$ denote the univariate Gaussian distribution with mean μ and variance σ^2 , and $N_k(\mu, \Sigma)$ denote the k-dimensional Gaussian distribution with mean μ and covariance matrix Σ .

In this paper, we adopt the convention use of the expectation and conditional expectation. For a random variable X, the expressions $\mathbb{E}X$, $\mathbb{E}(X)$, and $\mathbb{E}[X]$ all refer to the expectation of X. Similarly, $\mathbb{E}X^2$, $\mathbb{E}(X^2)$, and $\mathbb{E}[X^2]$ mean that we first square the random variable X and then compute its expectation. In contrast,



Fig 15: Risk curves and qq-plots of z-score of LQA for (n, p) = (1200, 1200).

expressions like $\mathbb{E}(X)^2$ and $\mathbb{E}[X]^2$ denote a different operation; here, we first calculate the expectation of X and then square the result. This convention extends consistently to other power operations and conditional expectations throughout the paper.

B.2. Review of Kronecker product

In this section, we review the definitions and properties of the Kronecker product. Let A be an $m \times n$ matrix, and B be a $p \times q$ matrix. The Kronecker product of A and B, denoted by $A \otimes B$, is defined as:

$$oldsymbol{A}\otimesoldsymbol{B}=egin{bmatrix} a_{11}oldsymbol{B}&\cdots&a_{1n}oldsymbol{B}\ dots&\ddots&dots\ a_{m1}oldsymbol{B}&\cdots&a_{mn}oldsymbol{B}\end{bmatrix},$$

where a_{ij} represents the entry in the *i*-th row and *j*-th column of matrix **A**. Below we list a few properties of the Kronecker product that will be useful in our proofs.

(i) The mixed-product property: If **A**, **B**, **C** and **D** are matrices of such size that the matrix products **AC** and **BD** make sense, then

(B.1)
$$(\boldsymbol{A} \otimes \boldsymbol{B})(\boldsymbol{C} \otimes \boldsymbol{D}) = (\boldsymbol{A}\boldsymbol{C}) \otimes (\boldsymbol{B}\boldsymbol{D}) \in \mathbb{R}^{mp \times nq}.$$

(ii) Inverse property:

(B.2)
$$(\boldsymbol{A} \otimes \boldsymbol{B})^{-1} = \boldsymbol{A}^{-1} \otimes \boldsymbol{B}^{-1} \text{ and } (\boldsymbol{A} \otimes \boldsymbol{B})^{\dagger} = \boldsymbol{A}^{\dagger} \otimes \boldsymbol{B}^{\dagger},$$

where A^{\dagger} means the Moore-Penrose inverse of A.

(iii) Trace property:

(B.3)
$$\operatorname{Tr}(\boldsymbol{A} \otimes \boldsymbol{B}) = \operatorname{Tr}(\boldsymbol{A}) \operatorname{Tr}(\boldsymbol{B})$$

(iv) Norm property:

(B.4)
$$\|\boldsymbol{A} \otimes \boldsymbol{B}\|_{\text{op}} = \|\boldsymbol{A}\|_{\text{op}} \|\boldsymbol{B}\|_{\text{op}} \text{ and } \|\boldsymbol{A} \otimes \boldsymbol{B}\|_{\text{F}} = \|\boldsymbol{A}\|_{\text{F}} \|\boldsymbol{B}\|_{\text{F}}$$

(v) Relationship with vectorization operator: If the matrix product ABC makes sense, then

(B.5)
$$\operatorname{vec}(ABC) = (C^{\top} \otimes A) \operatorname{vec}(B),$$

where $\mathbf{vec}(\cdot)$ is the vectorization operator such that $\mathbf{vec}(B)$ is the vector obtained by stacking vertically the columns of B on top of one another.

Appendix C: Derivative formula

In this section, we provide the derivative formulas for the iteration function g_t in (2.5). These derivative formulas will be important ingredient in the proof of the main results in the next sections. Recall $\hat{b}^1, \hat{b}^2, \ldots, \hat{b}^T$ represent the first T iterates of an algorithm using the iteration function g_t in (2.8), and $v^t = \frac{1}{n} X^{\top} (y - X \hat{b}^t)$ as in (2.1). The error matrix and residual matrix for the first T iterates $\hat{b}^1, \hat{b}^2, \ldots, \hat{b}^T$ are defined as

(C.1)
$$\boldsymbol{H} = [\hat{\boldsymbol{b}}^1 - \boldsymbol{b}^*, \dots, \hat{\boldsymbol{b}}^T - \boldsymbol{b}^*] \in \mathbb{R}^{p \times T}, \quad \boldsymbol{F} = [\boldsymbol{y} - \boldsymbol{X}\hat{\boldsymbol{b}}^1, \dots, \boldsymbol{y} - \boldsymbol{X}\hat{\boldsymbol{b}}^T] \in \mathbb{R}^{n \times T}.$$

We also define $\widehat{B} = [\widehat{b}^1, \ldots, \widehat{b}^T]$ is a matrix of size $p \times T$, $B^* = [b^*, \ldots, b^*]$, $E = [\varepsilon, \ldots, \varepsilon]$ and $Y = [y, \ldots, y]$ are matrices formed by repeating the vectors b^* , ε , and y column-wise T times. Therefore, we have $H = \widehat{B} - B^*$, and $F = Y - X\widehat{B}$. Recall also the matrices $D_{t,s}, J_{t,s}$ in (2.9) and the large matrices $\mathcal{D}, \mathcal{J} \in \mathbb{R}^{pT \times pT}$ in (2.10).

Lemma C.1 (Derivative of iterates). For $(\hat{b}^1, ..., \hat{b}^T)$ in (2.8), for almost every (X, ε) ,

(C.2)
$$\frac{\partial \hat{\boldsymbol{b}}^t}{\partial x_{ij}} = n^{-1} (\boldsymbol{e}_t^\top \otimes \boldsymbol{I}_p) \mathcal{M}^{-1} \mathcal{D} \Big[\Big((\boldsymbol{F}^\top \boldsymbol{e}_i) \otimes \boldsymbol{e}_j \Big) - \Big((\boldsymbol{H}^\top \boldsymbol{e}_j) \otimes (\boldsymbol{X}^\top \boldsymbol{e}_i) \Big) \Big]$$

(C.3)
$$\frac{\partial \boldsymbol{b}^t}{\partial \epsilon_l} = n^{-1} (\boldsymbol{e}_t^\top \otimes \boldsymbol{I}_p) \mathcal{M}^{-1} \mathcal{D} (\boldsymbol{1}_T \otimes \boldsymbol{X}^\top \boldsymbol{e}_l),$$

where $\boldsymbol{e}_i, \boldsymbol{e}_l \in \mathbb{R}^n, \boldsymbol{e}_j \in \mathbb{R}^p, \boldsymbol{e}_t \in \mathbb{R}^T$ and $\mathcal{M} = \boldsymbol{I}_{pT} + \mathcal{D}(\boldsymbol{I}_T \otimes \frac{\boldsymbol{X}^\top \boldsymbol{X}}{n}) - \mathcal{J}.$

The derivative results in Lemma C.1 directly imply the following by the product rule.

Corollary C.2 (Derivative of residuals). Let F_{lt} be the (l,t)-th entry of \mathbf{F} , i.e., $F_{lt} = \mathbf{e}_l^\top \mathbf{F} \mathbf{e}_t$. Under the conditions of Lemma C.1, for each $i, l \in [n], j \in [p], t \in [T]$, we have

(C.4)
$$\frac{\partial F_{lt}}{\partial x_{ij}} = D_{ij}^{lt} + \Delta_{ij}^{lt} \quad and \quad \frac{\partial F \boldsymbol{e}_t}{\partial \epsilon_i} = \boldsymbol{e}_i - n^{-1} (\boldsymbol{e}_t^\top \otimes \boldsymbol{X}) \mathcal{M}^{-1} \mathcal{D} (\boldsymbol{1}_T \otimes \boldsymbol{X}^\top \boldsymbol{e}_i),$$

where the expressions of D_{ij}^{lt} and Δ_{ij}^{lt} are given by

(C.5)
$$D_{ij}^{lt} = -(\boldsymbol{e}_t^\top \otimes \boldsymbol{e}_l^\top) [\boldsymbol{I}_{nT} - n^{-1} (\boldsymbol{I}_T \otimes \boldsymbol{X}) \mathcal{M}^{-1} \mathcal{D} (\boldsymbol{I}_T \otimes \boldsymbol{X}^\top)] ((\boldsymbol{H}^\top \boldsymbol{e}_j) \otimes \boldsymbol{e}_i)$$

(C.6)
$$\Delta_{ij}^{lt} = -n^{-1} (\boldsymbol{e}_t^\top \otimes \boldsymbol{e}_l^\top) (\boldsymbol{I}_T \otimes \boldsymbol{X}) \mathcal{M}^{-1} \mathcal{D} (\boldsymbol{F}^\top \otimes \boldsymbol{I}_p) (\boldsymbol{e}_i \otimes \boldsymbol{e}_j).$$

Here \mathcal{D} is defined in (2.7) and $\mathcal{M} = \mathbf{I}_{pT} + \mathcal{D}(\mathbf{I}_T \otimes \frac{\mathbf{X}^\top \mathbf{X}}{n}) - \mathcal{J}$ is defined in Lemma C.1. It immediately follows that

(C.7)
$$\sum_{i=1}^{n} D_{ij}^{it} = -\boldsymbol{e}_{t}^{\top} (\boldsymbol{n}\boldsymbol{I}_{T} - \widehat{\mathbf{A}}) \boldsymbol{H}^{\top} \boldsymbol{e}_{j} \quad and \quad \sum_{i=1}^{n} \sum_{t=1}^{T} D_{ij}^{it} \boldsymbol{e}_{t}^{\top} = -\boldsymbol{e}_{j}^{\top} \boldsymbol{H} (\boldsymbol{n}\boldsymbol{I}_{T} - \widehat{\mathbf{A}}^{\top}),$$

(C.8)
$$\operatorname{Tr}\left(\frac{\partial \mathbf{X}\hat{\mathbf{b}}^{t}}{\partial \boldsymbol{\varepsilon}}\right) = \sum_{l=1}^{n} \frac{\partial \mathbf{e}_{l}^{\top}\mathbf{X}\hat{\mathbf{b}}^{t}}{\partial \epsilon_{l}} = \mathbf{e}_{t}^{\top}\widehat{\mathbf{A}}\mathbf{1}_{T} \quad and \quad \operatorname{Tr}\left(\frac{\partial \mathbf{F}\mathbf{e}_{t}}{\partial \boldsymbol{\varepsilon}}\right) = \mathbf{e}_{t}^{\top}(n\mathbf{I}_{T} - \widehat{\mathbf{A}})\mathbf{1}_{T}.$$

Proof of Lemma C.1. By composition of locally Lipschitz functions, the map $(\mathbf{X}, \boldsymbol{\varepsilon}) \mapsto \hat{\mathbf{b}}^t$ is locally Lipschitz and thus differentiable almost everywhere. Let $(\dot{\mathbf{X}}, \dot{\boldsymbol{\varepsilon}})$ be a perturbation direction. We now compute the directional derivative of $\hat{\mathbf{b}}^t$ with respect to this direction by taking, for any function $F(\boldsymbol{\varepsilon}, \mathbf{X})$ the limit $u^{-1}(F(\boldsymbol{\varepsilon} + u\dot{\boldsymbol{\varepsilon}}, \mathbf{X} + u\dot{\mathbf{X}}) - F(\boldsymbol{\varepsilon}, \mathbf{X}))$ as $u \to 0$ and call the limit \dot{F} . For $\hat{\mathbf{b}}^t$, we denote the corresponding directional derivative by $\dot{\mathbf{b}}^t$, and for v^t by \dot{v}^t . By definition of $\hat{\mathbf{b}}^t$ in (2.8), we have almost surely by the chain rule (if necessary with modification from (Ambrosio and Dal Maso, 1990, Corollary 3.2) as explained after (2.11)),

(C.9)
$$\dot{\boldsymbol{b}}^t = \sum_{s=1}^{t-1} \boldsymbol{J}_{t,s} \dot{\boldsymbol{b}}^s + \boldsymbol{D}_{t,s} \dot{\boldsymbol{v}}^s.$$

Since $v^t = n^{-1} X^\top F e_t = n^{-1} X^\top (\varepsilon - X H e_t)$ and $\dot{H} e_t = \dot{b}^t$, we have by the product rule

(C.10)
$$\dot{\boldsymbol{v}}^{t} = -\frac{1}{n}\boldsymbol{X}^{\top}\boldsymbol{X}\dot{\boldsymbol{b}}^{t} + \underbrace{\frac{1}{n}\left[\dot{\boldsymbol{X}}^{\top}\boldsymbol{F}\boldsymbol{e}_{t} + \boldsymbol{X}^{\top}(\dot{\boldsymbol{\varepsilon}} - \dot{\boldsymbol{X}}\boldsymbol{H}\boldsymbol{e}_{t})\right]}_{\boldsymbol{a}^{t}}$$

where $a^t \in \mathbb{R}^p$. Substituting the expressions for \dot{v}^s into (C.9), we have

(C.11)
$$\dot{\boldsymbol{b}}^{t} = \sum_{s=1}^{t-1} (\boldsymbol{J}_{t,s} - \boldsymbol{D}_{t,s} \frac{\boldsymbol{X}^{\top} \boldsymbol{X}}{n}) \dot{\boldsymbol{b}}^{s} + \boldsymbol{D}_{t,s} \boldsymbol{a}^{s}$$

For the initial condition, we have $\dot{\boldsymbol{b}}^1 = \boldsymbol{0}$ since $\hat{\boldsymbol{b}}^1$ is a constant independent of \boldsymbol{X} . Similarly $\boldsymbol{D}_{2,0} = \boldsymbol{J}_{2,0} = \boldsymbol{0}$ since $\hat{\boldsymbol{b}}^0$ and \boldsymbol{v}^0 are set as constant vector $\boldsymbol{0}$. Therefore we can write (C.11) as a linear system of size pT:

$$\begin{bmatrix} I_p \\ D_{2,1} \frac{X^T X}{n} - J_{2,1} & I_p \\ D_{3,1} \frac{X^T X}{n} - J_{3,1} & D_{3,2} \frac{X^T X}{n} - J_{3,2} & I_p \\ \vdots & \ddots & \ddots & \ddots \\ D_{T,1} \frac{X^T X}{n} - J_{T,1} & \cdots & D_{T,T-2} \frac{X^T X}{n} - J_{T,T-2} & D_{T,T-1} \frac{X^T X}{n} - J_{T,T-1} & I_p \end{bmatrix} \underbrace{\begin{bmatrix} \dot{b}^1 \\ \dot{b}^2 \\ \dot{b}^3 \\ \vdots \\ \dot{b}^T \end{bmatrix}}_{\text{vec}(\dot{B})}$$

$$= \underbrace{\begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ D_{2,1} & 0 & 0 & 0 & 0 \\ D_{3,1} & D_{3,2} & 0 & 0 & 0 \\ \vdots & \ddots & \ddots & \ddots & \\ D_{T,1} & \cdots & D_{T,T-2} & D_{T,T-1} & 0 \end{bmatrix}}_{\mathcal{D}} \begin{bmatrix} a^1 \\ a^2 \\ a^3 \\ \vdots \\ a^T \end{bmatrix}}.$$

In the above equation, the matrix \mathcal{M} is the same as the one defined in Lemma C.1, i.e., $\mathcal{M} = \mathbf{I}_{pT} + \mathcal{D}(\mathbf{I}_T \otimes \frac{\mathbf{X}^{\top} \mathbf{X}}{n}) - \mathcal{J}$ for \mathcal{D}, \mathcal{J} in (2.10). Solving the linear system (C.11) for $\dot{\mathbf{b}}^t$, we obtain

$$\begin{split} \dot{\boldsymbol{b}}^t &= \operatorname{vec}(\dot{\boldsymbol{B}}\boldsymbol{e}_t) = (\boldsymbol{e}_t^\top \otimes \boldsymbol{I}_p) \operatorname{vec}(\dot{\boldsymbol{B}}) & \text{by (B.5)} \\ &= (\boldsymbol{e}_t^\top \otimes \boldsymbol{I}_p) \mathcal{M}^{-1} \mathcal{D} \boldsymbol{a} & \text{by (C.11).} \end{split}$$

By definition of $\boldsymbol{a} \in \mathbb{R}^{pT}$ and \boldsymbol{a}^t in (C.10), this completes the proof of (C.2) by taking $(\dot{\boldsymbol{\varepsilon}}, \dot{\boldsymbol{X}}) = (\boldsymbol{0}_n, \boldsymbol{e}_i \boldsymbol{e}_j^{\top})$ and of (C.3) by taking $(\dot{\boldsymbol{\varepsilon}}, \dot{\boldsymbol{X}}) = (\boldsymbol{e}_l, \boldsymbol{0}_{n \times p})$.

Appendix D: Change of variables

For the linear model $y = Xb^* + \varepsilon$, its design matrix X may not be isotropic. However, we can always consider the following change of variables:

(D.1)
$$X \rightsquigarrow X\Sigma^{-1/2} := G, \quad b^* \rightsquigarrow \Sigma^{1/2}b^* := \theta^*.$$

This way, the original linear model can be rewritten as

(D.2)
$$\boldsymbol{y} = \boldsymbol{G}\boldsymbol{\theta}^* + \boldsymbol{\varepsilon},$$

where \boldsymbol{G} is the design matrix with i.i.d. entries from N(0, 1), and $\boldsymbol{\theta}^*$ is the new unknown coefficient vector. For the linear model (D.2) with isotropic design matrix \boldsymbol{G} , we use $\hat{\boldsymbol{\theta}}^1, ..., \hat{\boldsymbol{\theta}}^T$ to denote the first T iterates of an iterative algorithm detailed in next paragraph, where $\hat{\boldsymbol{\theta}}^t$ are constructed such that $\hat{\boldsymbol{\theta}}^t = \boldsymbol{\Sigma}^{1/2} \hat{\boldsymbol{b}}^t$. Similar to the definition of $\boldsymbol{F}, \boldsymbol{H}$ in (C.1), for the linear model (D.2), we define

$$oldsymbol{F}^* = [oldsymbol{y} - oldsymbol{G}\widehat{oldsymbol{ heta}}^1, ..., oldsymbol{y} - oldsymbol{G}\widehat{oldsymbol{ heta}}^T], \quad oldsymbol{H}^* = [\widehat{oldsymbol{ heta}}^1 - oldsymbol{ heta}^*, ..., \widehat{oldsymbol{ heta}}^T - oldsymbol{ heta}^*].$$

Denoting with a superscript^{*} the quantities after the change of variable, we have $F^* = F$ and $H^* = \Sigma^{1/2} H$.

We now describe the iteration to generate the iterates $\hat{\theta}^1, ..., \hat{\theta}^T$ that guarantees $\hat{\theta}^t = \Sigma^{1/2} \hat{b}^t$. We start with $\hat{\theta}^1 = \Sigma^{1/2} \hat{b}^1$, and generate $\hat{\theta}^t$ for $t \ge 2$ by the recursion: $\hat{\theta}^t = \tilde{g}_t(\hat{\theta}^{t-1}, \tilde{v}^{t-1}, \hat{\theta}^{t-2}, \tilde{v}^{t-2})$, where $\tilde{v}^t = \frac{1}{n} \mathbf{G}^\top (\mathbf{y} - \mathbf{G} \hat{\theta}^t)$, and the iteration function \tilde{g}_t is defined as

(D.3)
$$\widetilde{g}_{t}(\widehat{\theta}^{t-1},\ldots,\widehat{\theta}^{1}, \quad \widetilde{v}^{t-1},\ldots,\widetilde{v}^{1}) = \Sigma^{1/2}g_{t}\left(\Sigma^{-1/2}\widehat{\theta}^{t-1},\ldots,\Sigma^{-1/2}\widehat{\theta}^{1}, \quad \Sigma^{1/2}\widetilde{v}^{t-1},\ldots,\Sigma^{1/2}\widetilde{v}^{1}\right)$$

Since g_t is ζ -Lipschitz continuous from Assumption 2.1, we have \tilde{g}_t is $\zeta\kappa$ -Lipschitz continuous using that $\|\Sigma\|_{\text{op}} \leq \|\Sigma\|_{\text{op}} \|\Sigma^{-1}\|_{\text{op}} \leq \kappa$ from Assumption 2.2. By construction, $\hat{\theta}^s = \Sigma^{1/2}\hat{b}^s$ for all $s \leq t-1$ implies $\hat{\theta}^t = \Sigma^{1/2}\hat{b}^t$, so by induction the relation holds for all $t \geq 1$. For the iteration function \tilde{g}_t in (D.3), similarly to (2.9), we define the derivative matrices with respect to each argument as

(D.4)
$$\boldsymbol{J}_{t,s}^* = \frac{\partial \widetilde{\boldsymbol{g}}_t}{\partial \boldsymbol{\theta}^s} \Big(\widehat{\boldsymbol{\theta}}^{t-1}, \dots, \widehat{\boldsymbol{\theta}}^1, \widetilde{\boldsymbol{v}}^{t-1}, \dots \widetilde{\boldsymbol{v}}^1 \Big), \qquad \boldsymbol{D}_{t,s}^* = \frac{\partial \widetilde{\boldsymbol{g}}_t}{\partial \widetilde{\boldsymbol{v}}^s} \Big(\widehat{\boldsymbol{\theta}}^{t-1}, \dots, \widehat{\boldsymbol{\theta}}^1, \widetilde{\boldsymbol{v}}^{t-1}, \dots \widetilde{\boldsymbol{v}}^1 \Big)$$

for each $s \leq t - 1$. Furthermore, we have by chain rule,

(D.5)
$$\boldsymbol{J}_{t,s}^{*} = \frac{\partial \widetilde{\boldsymbol{g}}_{t}}{\partial \widehat{\boldsymbol{\theta}}^{s}} = \boldsymbol{\Sigma}^{1/2} \frac{\partial \boldsymbol{g}_{t}}{\partial \widehat{\boldsymbol{b}}^{s}} \boldsymbol{\Sigma}^{-1/2} = \boldsymbol{\Sigma}^{1/2} \boldsymbol{J}_{t,s} \boldsymbol{\Sigma}^{-1/2},$$
$$\boldsymbol{D}_{t,t-1}^{*} = \frac{\partial \widetilde{\boldsymbol{g}}_{t}}{\partial \widetilde{\boldsymbol{v}}^{s}} = \boldsymbol{\Sigma}^{1/2} \frac{\partial \boldsymbol{g}_{t}}{\partial \boldsymbol{v}^{s}} \boldsymbol{\Sigma}^{1/2} = \boldsymbol{\Sigma}^{1/2} \boldsymbol{D}_{t,s} \boldsymbol{\Sigma}^{1/2}.$$

We may apply Lemma C.1 to \widetilde{g}_t , θ_t , G to obtain with $\mathcal{M}^* = I_{pT} + \mathcal{D}^*(I_T \otimes G^\top G/n) - \mathcal{J}^*$

$$\frac{\partial \widehat{\boldsymbol{\theta}}^t}{\partial g_{ik}} = n^{-1} (\boldsymbol{e}_t \otimes \boldsymbol{I}_p) (\mathcal{M}^*)^{-1} \mathcal{D}^* \sum_{j=1}^p \left[\left((\boldsymbol{F}^*)^\top \boldsymbol{e}_i \right) \otimes \boldsymbol{e}_k - \left((\boldsymbol{H}^*)^\top \boldsymbol{e}_k \right) \otimes (\boldsymbol{G}^\top \boldsymbol{e}_i) \right]$$

where $\mathcal{D}^* = \sum_{t=2}^T \sum_{s=1}^{t-1} (e_t e_s^{\top}) \otimes D_{t,s}^*$ and $\mathcal{J}^* = \sum_{t=2}^T \sum_{s=1}^{t-1} (e_t e_s^{\top}) \otimes J_{t,s}^*$ as in (2.10). Note that the relationships

(D.6)
$$\mathcal{M}^* = (\mathbf{I}_T \otimes \mathbf{\Sigma}^{1/2}) \mathcal{M}(\mathbf{I}_T \otimes \mathbf{\Sigma}^{-1/2}), \qquad \mathcal{D}^* = (\mathbf{I}_T \otimes \mathbf{\Sigma}^{1/2}) \mathcal{D}(\mathbf{I}_T \otimes \mathbf{\Sigma}^{1/2})$$

hold due to (D.5). Now we verify that $\widehat{\mathbf{A}}$ is unchanged by the change of variable, that is, $\widehat{\mathbf{A}} = \widehat{\mathbf{A}}^*$. By definition of $\widehat{\mathbf{A}}^*$ (as in (2.12)),

$$\widehat{\mathbf{A}}^* \stackrel{\text{def}}{=} \frac{1}{n} \sum_{i=1}^n (\mathbf{I}_T \otimes \mathbf{e}_i^\top \mathbf{G}) (\mathcal{M}^*)^{-1} \mathcal{D}^* (\mathbf{I}_T \otimes \mathbf{G}^\top \mathbf{e}_i) = \frac{1}{n} \sum_{i=1}^n (\mathbf{I}_T \otimes (\mathbf{e}_i^\top \mathbf{X})) \mathcal{M}^{-1} \mathcal{D} (\mathbf{I}_T \otimes (\mathbf{X}^\top \mathbf{e}_i))$$

Model	$oldsymbol{y} = oldsymbol{X} b^* + arepsilon$	$oldsymbol{y} = oldsymbol{G}oldsymbol{ heta}^* + oldsymbol{arepsilon}$	Relationship
Design matrix	X	G	$oldsymbol{X} = oldsymbol{G} oldsymbol{\Sigma}^{1/2}$
Covariance matrix	Σ	$oldsymbol{\Sigma}^* = oldsymbol{I}_p$	$\mathbf{\Sigma} = \mathbf{\Sigma} \mathbf{\Sigma}^*$
Coefficient vector	b *	θ^*	$oldsymbol{b}^* = oldsymbol{\Sigma}^{-1/2} oldsymbol{ heta}^*$
<i>t</i> -th iterate	$\widehat{m{b}}^t$	$\widehat{oldsymbol{ heta}}^t$	$\widehat{m{b}}^t = {m{\Sigma}}^{-1/2} \widehat{m{ heta}}^t$
Error matrix	$oldsymbol{H} = \sum_t (\widehat{oldsymbol{b}}^t - oldsymbol{b}^*) oldsymbol{e}_t^ op$	$oldsymbol{H}^* = \sum_t (\widehat{oldsymbol{ heta}}^t - oldsymbol{ heta}^*) oldsymbol{e}_t^ op$	$oldsymbol{H} = oldsymbol{\Sigma}^{-1/2} oldsymbol{H}^*$
Residual matrix	$F = \sum_{t} (\boldsymbol{y} - \boldsymbol{X} \widehat{\boldsymbol{b}}^{t}) \boldsymbol{e}_{t}^{\top}$	$oldsymbol{F}^* = \sum_t (oldsymbol{y} - oldsymbol{G} \widehat{oldsymbol{ heta}}^t) oldsymbol{e}_t^ op$	$F = F^*$
Memory matrix	Â	$\widehat{\mathbf{A}}^*$	$\widehat{\mathbf{A}} = \widehat{\mathbf{A}}^*$
TABLE 1			



using (D.6) for the second equality. The rightmost quantity is exactly $\hat{\mathbf{A}}$, so $\hat{\mathbf{A}} = \hat{\mathbf{A}}^*$ stays the same after the change of variable.

In summary, we present the relevant quantities for both the original model (1.1) and the new model (D.2) in Table 1. The benefit of this change of variable is that, the transformed model (D.2) has isotropic design matrix G, and the following quantities stay the same:

$$oldsymbol{F}=oldsymbol{F}^*,\quad \widehat{f A}=\widehat{f A}^*,\quad oldsymbol{\Sigma}^{1/2}oldsymbol{H}=oldsymbol{H}^*.$$

Therefore, Theorems 2.1 and 2.2 hold for general Σ if they hold for $\Sigma = I_p$. The only change is the Lipschitz constant of the function g_t changes to the Lipschitz constant of \tilde{g}_t , with an extra factor of κ by Assumption 2.2 as we argued below (D.3). Throughout the subsequent proofs of Theorems 2.1 and 2.2, we will assume $\Sigma = I_p$ without loss of generality. The proof for general Σ follows by changing the Lipschitz constant from ζ to $\kappa\zeta$.

Appendix E: Useful intermediate results

E.1. Deterministic operator norm bound

Lemma E.1. Under Assumption 2.1, for \mathcal{J}, \mathcal{D} in (2.10) we have

(E.1)
$$\max\{\|\mathcal{D}\|_{\mathrm{op}}, \|\mathcal{J}\|_{\mathrm{op}}\} \le T\zeta.$$

Proof of Lemma E.1. By Assumption 2.1 the function g_t is ζ -Lipschitz, thus the block row of size $p \times pT$ corresponding to g_t in \mathcal{D} and \mathcal{J} is bounded in operator norm by ζ . Since it has T such row-blocks of size $p \times pT$, we obtain the result by the triangle inequality.

Lemma E.2. With \mathcal{M} as in Lemma C.1 and $\mathbf{N} = n^{-1}(\mathbf{I}_T \otimes \mathbf{X})\mathcal{M}^{-1}\mathcal{D}(\mathbf{I}_T \otimes \mathbf{X}^{\top})$,

(E.2)
$$\|\mathcal{M}^{-1}\|_{\text{op}} \le C(\zeta, T)(1 + \|\boldsymbol{X}\|_{\text{op}}^2/n)^{T-1} \text{ and } \|\boldsymbol{N}\|_{\text{op}} \le C(\zeta, T)(1 + \|\boldsymbol{X}\|_{\text{op}}^2/n)^T$$

where $C(\zeta, T)$ is a constant depending on ζ and T only.

Proof of Lemma E.2. By definition, $\mathcal{M} = \mathbf{I}_{pT} - [\mathcal{J} - \mathcal{D}(\mathbf{I}_T \otimes \frac{\mathbf{X}^{\top} \mathbf{X}}{n})]$ and $(\mathbf{I}_{pT} - \mathcal{M})^T = \mathbf{0}_{pT \times pT}$ since $\mathbf{I}_{pT} - \mathcal{M}$ is lower triangular with zero diagonal blocks of size $p \times p$. Using the matrix identity $(\mathbf{I} - \mathbf{A})^{-1} = \sum_{k=0}^{\infty} \mathbf{A}^k = \sum_{k=1}^{T-1}$ for any matrix \mathbf{A} with $\mathbf{A}^T = 0$, we have $\mathcal{M}^{-1} = \sum_{k=0}^{T-1} [\mathcal{J} - \mathcal{D}(\mathbf{I}_T \otimes \frac{\mathbf{X}^{\top} \mathbf{X}}{n})]^k$. Furthermore for each $k = 0, ..., T_1$,

$$\begin{aligned} \|\mathcal{J} - \mathcal{D}(\boldsymbol{I}_T \otimes \frac{\boldsymbol{X}^{\top} \boldsymbol{X}}{n})\|_{\text{op}}^k &\leq (\|\mathcal{J}\|_{\text{op}} + \|\mathcal{D}\|_{\text{op}} \|\boldsymbol{X}\|_{\text{op}}^2/n)^k & \text{by (B.4)} \\ &\leq [(1 + \|\boldsymbol{X}\|_{\text{op}}^2/n)\zeta T]^k & \text{by (E.1)} \end{aligned}$$

This provides $\|\mathcal{M}\|_{\text{op}} \leq T(1+\zeta T)^{T-1}(1+\|\mathbf{X}\|_{\text{op}}^2/n)^{T-1}$. The bound on $\|\mathbf{N}\|_{\text{op}}$ follows from $\|\mathbf{N}\|_{\text{op}} \leq \|\mathcal{M}^{-1}\|_{\text{op}}\|\mathcal{D}\|_{\text{op}}\|\mathbf{X}\|_{\text{op}}^2/n$ and the previous bound.

Lemma E.3. Under Assumption 2.1, we have

(E.3)
$$\|\boldsymbol{I}_T - \widehat{\boldsymbol{A}}/n\|_{\text{op}} \le C(\zeta, T)(1 + \|\boldsymbol{X}\|_{\text{op}}^2/n)^T$$

(E.4)
$$\| (\boldsymbol{I}_T - \widehat{\boldsymbol{A}}/n)^{-1} \|_{\text{op}} \le C(\zeta, T) (1 + \| \boldsymbol{X} \|_{\text{op}}^2/n)^{T^2}.$$

Proof of Lemma E.3. Since $\widehat{\mathbf{A}} = \sum_{i=1}^{n} (\mathbf{I}_{T} \otimes \mathbf{e}_{i}^{\top}) \mathbf{N} (\mathbf{I}_{T} \otimes \mathbf{e}_{i})$ we have for any $\mathbf{u}, \mathbf{u} \in \mathbb{R}^{T}$ that $|\mathbf{u}^{\top} \widehat{\mathbf{A}} \mathbf{v}| = |\sum_{i=1}^{n} (\mathbf{u} \otimes \mathbf{e}_{i})^{\top} \mathbf{N} (\mathbf{v} \otimes \mathbf{e}_{i})| \leq ||\mathbf{N}||_{\text{op}} \sum_{i=1}^{n} ||\mathbf{u} \otimes \mathbf{e}_{i}|| ||\mathbf{v} \otimes \mathbf{e}_{i}|| \leq n ||\mathbf{N}||_{\text{op}}$ using (B.1) and (B.4). The bound on the operator norm of \mathbf{N} from Lemma E.2 gives (E.3).

Since $\widehat{\mathbf{A}}$ is a lower triangular matrix, we know $\widehat{\mathbf{A}}$ is a nilpotent matrix with $\widehat{\mathbf{A}}^k = 0$ if $k \ge T$. Consequently $(\mathbf{I}_T - \widehat{\mathbf{A}}/n)^{-1} = \sum_{k=0}^{\infty} (\widehat{\mathbf{A}}/n)^k = \sum_{k=0}^{T-1} (\widehat{\mathbf{A}}/n)^k$, hence

$$\|(\boldsymbol{I}_T - \frac{\widehat{\mathbf{A}}}{n})^{-1}\|_{\mathrm{op}} \le \sum_{k=0}^{T-1} \|\frac{\widehat{\mathbf{A}}}{n}\|_{\mathrm{op}}^k \le C(\zeta, T) \sum_{k=0}^{T-1} \left(1 + \frac{\|\boldsymbol{X}\|_{\mathrm{op}}^2}{n}\right)^{Tk} \le C(\zeta, T) (1 + \|\boldsymbol{X}\|_{\mathrm{op}}^2/n)^{T^2}.$$

This finishes the proof.

Lemma E.4. Under Assumption 2.1, let $\widehat{C} = \sum_{j=1}^{p} (I_T \otimes e_j^{\top}) \mathcal{M}^{-1} \mathcal{D}(I_T \otimes e_j)$, we have

(E.5)
$$\|\boldsymbol{I}_T + \widehat{\boldsymbol{C}}/n\|_{\text{op}} \le C(\zeta, T, \gamma)(1 + \|\boldsymbol{X}\|_{\text{op}}^2/n)^T,$$

(E.6)
$$\| (\boldsymbol{I}_T + \widehat{\boldsymbol{C}}/n)^{-1} \|_{\text{op}} \le C(\zeta, T, \gamma) (1 + \|\boldsymbol{X}\|_{\text{op}}^2/n)^{T^2}$$

Proof of Lemma E.4. By triangular inequality, we have

$$\begin{split} \|\widehat{\boldsymbol{C}}\|_{\text{op}}/n &\leq n^{-1} \sum_{j=1}^{p} \|(\boldsymbol{I}_{T} \otimes \boldsymbol{e}_{j}^{\top}) \mathcal{M}^{-1} \mathcal{D}(\boldsymbol{I}_{T} \otimes \boldsymbol{e}_{j})\|_{\text{op}} \\ &\leq p/n \|\mathcal{M}^{-1}\|_{\text{op}} \|\mathcal{D}\|_{\text{op}} \\ &\leq C(\zeta, T, \gamma)(1 + \|\boldsymbol{X}\|_{\text{op}}^{2}/n)^{T-1} \end{split}$$
 by Lemmas E.1 and E.2.

This directly implies (E.5) by the triangle inequality. Since \hat{C} is lower triangular by its definition, the same argument in the proof of Lemma E.3 gives (E.6).

Lemma E.5. Under Assumption 2.1, we have

(E.7)
$$\left\|\frac{\partial \boldsymbol{F}\boldsymbol{e}_t}{\partial \boldsymbol{\varepsilon}}\right\|_{\mathrm{op}} = \left\|\boldsymbol{I}_n - (\boldsymbol{e}_t \otimes \boldsymbol{I}_n)^\top \boldsymbol{N} (\boldsymbol{1}_T \otimes \boldsymbol{I}_n)\right\|_{\mathrm{op}} \le C(\zeta, T)(1 + \|\boldsymbol{X}\|_{\mathrm{op}}^2/n)^T,$$

(E.8)
$$\left\|\frac{\partial \boldsymbol{H}\boldsymbol{e}_t}{\partial \boldsymbol{\varepsilon}}\right\|_{\mathrm{op}} = \left\|\frac{1}{n}(\boldsymbol{e}_t \otimes \boldsymbol{I}_p)^\top \mathcal{M}^{-1} \mathcal{D}(\boldsymbol{1}_T \otimes \boldsymbol{X}^\top)\right\|_{\mathrm{op}} \le \frac{C(\zeta, T)}{\sqrt{n}} (1 + \|\boldsymbol{X}\|_{\mathrm{op}}^2/n)^T.$$

Proof of Lemma E.5. By Corollary C.2, we have

$$\frac{\partial \boldsymbol{F} \boldsymbol{e}_t}{\partial \boldsymbol{\varepsilon}} = \boldsymbol{I}_n - n^{-1} (\boldsymbol{e}_t^\top \otimes \boldsymbol{X}) \mathcal{M}^{-1} \mathcal{D} (\boldsymbol{1}_T \otimes \boldsymbol{X}^\top) = \boldsymbol{I}_n - (\boldsymbol{e}_t \otimes \boldsymbol{I}_n)^\top \boldsymbol{N} (\boldsymbol{1}_T \otimes \boldsymbol{I}_n)$$

so the bound for F follows from (E.2) and (B.4). The bound for H follows from (C.3) and the same argument with the operator norm bounds (E.1) and (E.2) for \mathcal{M} .

Lemma E.6. Assume Assumption 2.1 holds. Let $\frac{\partial \operatorname{vec}(F)}{\partial \operatorname{vec}(X)} \in \mathbb{R}^{nT \times np}$ be the Jacobian of the mapping $\mathbb{R}^{np} \to \mathbb{R}^n$: $\operatorname{vec}(X) \mapsto \operatorname{vec}(F)$. Then we have

(E.9)
$$\left\|\frac{\partial \operatorname{\mathbf{vec}}(\boldsymbol{F})}{\partial \operatorname{\mathbf{vec}}(\boldsymbol{X})}\right\|_{\mathrm{op}} \leq C(\zeta, T)(1 + \|\boldsymbol{X}\|_{\mathrm{op}}^2/n)^T(\|\boldsymbol{H}\|_{\mathrm{op}} + \|\boldsymbol{F}\|_{\mathrm{op}}/\sqrt{n}),$$

(E.10)
$$\left\|\frac{\partial \operatorname{vec}(\boldsymbol{F})}{\partial \operatorname{vec}(\boldsymbol{X})}\right\|_{\mathrm{F}} \leq C(\zeta, T)(1 + \|\boldsymbol{X}\|_{\mathrm{op}}^{2}/n)^{T}(\|\boldsymbol{H} \otimes \boldsymbol{I}_{n}\|_{\mathrm{F}} + \|\boldsymbol{F} \otimes \boldsymbol{I}_{p}\|_{\mathrm{F}}/\sqrt{n})$$

$$= C(\zeta, T)(1 + \|\boldsymbol{X}\|_{op}^{2}/n)^{T}(\|\boldsymbol{H}\|_{F}\sqrt{n} + \|\boldsymbol{F}\|_{F}\sqrt{p/n}).$$

Proof of Lemma E.6. With $\mathbf{F} = \sum_{lt} \mathbf{e}_l F_{lt} \mathbf{e}_t^{\top}$ we have $\mathbf{vec}(\mathbf{F}) = \sum_{lt} (\mathbf{e}_t \otimes \mathbf{e}_l) F_{lt}$ by (B.5) and so that

$$\frac{\partial \operatorname{\mathbf{vec}}(\boldsymbol{F})}{\partial \operatorname{\mathbf{vec}}(\boldsymbol{X})} = \sum_{l=1}^{n} \sum_{t=1}^{T} \sum_{i=1}^{n} \sum_{j=1}^{p} (\boldsymbol{e}_{t} \otimes \boldsymbol{e}_{l}) \frac{\partial F_{lt}}{\partial x_{ij}} (\boldsymbol{e}_{j}^{\top} \otimes \boldsymbol{e}_{i}^{\top}) = \sum_{lt,ij} (\boldsymbol{e}_{t} \otimes \boldsymbol{e}_{l}) (D_{ij}^{lt} + \Delta_{ij}^{lt}) (\boldsymbol{e}_{i}^{\top} \otimes \boldsymbol{e}_{j}^{\top})$$

where D_{ij}^{lt} and Δ_{ij}^{lt} are defined in (C.5) and (C.6). Since permuting the ordering of canonical basis vectors does not change the operator norm and the Frobenius norm, we find by (C.5) and the definition of N in Lemma E.2 that

(E.11)
$$\left\|\frac{\partial \operatorname{vec}(F)}{\partial \operatorname{vec}(X)}\right\|_{?} \leq \left\|N(H^{\top} \otimes I_{n})\right\|_{?} + \left\|n^{-1}(I_{T} \otimes X)\mathcal{M}^{-1}\mathcal{D}(F^{\top} \otimes I_{p})\right\|_{?}$$

where $\|\cdot\|_{?}$ is either the operator norm or the Frobenius norm. The property (B.4) of the Kronecker product and the operator norm bounds (E.2), (E.1) provide the two inequalities. For the last equality, we use $\|\boldsymbol{H} \otimes \boldsymbol{I}_n\|_{\mathrm{F}} = \|\boldsymbol{H}\|_{\mathrm{F}}\sqrt{n}$ and similarly for $\boldsymbol{F}^{\top} \otimes \boldsymbol{I}_p$ by (B.4).

Lemma E.7. Assume Assumption 2.1 holds. Let $\frac{\partial \operatorname{vec}(H)}{\partial \operatorname{vec}(X)} \in \mathbb{R}^{n \times np}$ be the Jacobian of the mapping $\mathbb{R}^{np} \to \mathbb{R}^n : \operatorname{vec}(X) \mapsto \operatorname{vec}(H)$. Then we have

(E.12)
$$\left\| \frac{\partial \operatorname{\mathbf{vec}}(\boldsymbol{H})}{\partial \operatorname{\mathbf{vec}}(\boldsymbol{X})} \right\|_{\mathrm{op}} \leq C(\zeta, T)(1 + \|\boldsymbol{X}\|_{\mathrm{op}}^2/n)^T \left(\|\boldsymbol{H}\|_{\mathrm{op}} + \|\boldsymbol{F}\|_{\mathrm{op}}/\sqrt{n} \right) \frac{1}{\sqrt{n}},$$

(E.13)
$$\left\| \frac{\partial \operatorname{\mathbf{vec}}(\boldsymbol{H})}{\partial \operatorname{\mathbf{vec}}(\boldsymbol{X})} \right\|_{\mathrm{F}} \leq C(\zeta, T)(1 + \|\boldsymbol{X}\|_{\mathrm{op}}^2/n)^T \left(\|\boldsymbol{F}^\top \otimes \boldsymbol{I}_p\|_{\mathrm{F}} + \sqrt{n} \|\boldsymbol{H} \otimes \boldsymbol{I}_n\|_{\mathrm{F}} \right) \frac{1}{n}$$

(3)
$$\| \overline{\partial \operatorname{vec}(\boldsymbol{X})} \|_{\mathrm{F}} \leq C(\zeta, T)(1 + \|\boldsymbol{X}\|_{\operatorname{op}}^{2}/n)^{T} \left(\|\boldsymbol{F}^{\top} \otimes \boldsymbol{I}_{p}\|_{\mathrm{F}} + \sqrt{n} \|\boldsymbol{H} \otimes \boldsymbol{I}_{n}\|_{\mathrm{F}} \right)$$
$$= C(\zeta, T)(1 + \|\boldsymbol{X}\|_{\operatorname{op}}^{2}/n)^{T} \left(\|\boldsymbol{F}n^{-1/2}\|_{\mathrm{F}}\sqrt{\gamma} + \|\boldsymbol{H}\|_{\mathrm{F}} \right).$$

Proof of Lemma E.7. By the same argument as in Lemma E.6, given (C.2),

$$\left\|\frac{\partial \operatorname{vec}(\boldsymbol{H})}{\partial \operatorname{vec}(\boldsymbol{X})}\right\|_{?} \leq \left\|n^{-1} \mathcal{M}^{-1} \mathcal{D}(\boldsymbol{F}^{\top} \otimes \boldsymbol{I}_{p})\right\|_{?} + \left\|n^{-1} \mathcal{M}^{-1} \mathcal{D}(\boldsymbol{I}_{T} \otimes \boldsymbol{X}^{\top})(\boldsymbol{H}^{\top} \otimes \boldsymbol{I}_{n})\right\|_{?}$$

where $\|\cdot\|_{?}$ is either the operator norm or the Frobenius norm. The property (B.4) of the Kronecker product and the operator norm bounds (E.2), (E.1) provide the two inequalities. For the last equality, we use $\|\mathbf{F}^{\top} \otimes \mathbf{I}_{p}\|_{\mathrm{F}} = \|\mathbf{F}\|_{\mathrm{F}}\sqrt{p}$ and similarly for $\mathbf{H}^{\top} \otimes \mathbf{I}_{n}$ by (B.4).

E.2. Moment bounds

Lemma E.8 (Moment bound of X). Under Assumptions 2.2 and 2.4, the following inequality holds for any positive, finite integer k:

$$\mathbb{E}[\|\boldsymbol{X}\boldsymbol{\Sigma}^{-1/2}/\sqrt{n}\|_{\mathrm{op}}^{k}] \le C(\gamma, k).$$

Proof of Lemma E.8. By (Davidson and Szarek, 2001, Theorem II.13), there exists a random variable $z \sim N(0,1)$ s.t. $\|\boldsymbol{X}\boldsymbol{\Sigma}^{-1/2}\|_{\text{op}} \leq \sqrt{n} + \sqrt{p} + z$ almost surely. Thus,

$$\mathbb{E}[\|\boldsymbol{X}\boldsymbol{\Sigma}^{-1/2}/\sqrt{n}\|_{\mathrm{op}}^{k}] \leq \mathbb{E}[(1+\sqrt{p/n}+z)^{k}] \leq C(\gamma,k).$$

The last inequality follows from $p/n \leq \gamma$ and the fact that $\mathbb{E}[z^k]$ is bounded for any finite k if $z \sim \mathsf{N}(0, 1)$. \Box

Lemma E.9 (Moment bound of ε). Under Assumption 2.3, for any positive finite integer k, there exists a constant C(k) depending only on k such that $\mathbb{E}[(\|\varepsilon\|^2/n)^k] \leq C(k)(\sigma^2)^k$.

This is a known bound on the finite moment of the χ_n^2 distribution. Alternatively, since ε/σ has a same distribution as any column of $X\Sigma^{-1/2}$, we have $\mathbb{E}[(\|\varepsilon\|^2/\sigma^2)^k] \leq \mathbb{E}[\|X\Sigma^{-1/2}\|_{op}^{2k}]$ so Lemma E.9 follows from Lemma E.8 with $\gamma = 1$.

Lemma E.10 (Moment bounds of H and F). If Assumptions 2.1 to 2.4 are fulfilled then

$$\mathbb{E}[\|\boldsymbol{\Sigma}^{1/2}\boldsymbol{H}\|_{\mathrm{F}}^{2}] \vee \mathbb{E}[\|\boldsymbol{\Sigma}^{1/2}\boldsymbol{H}\|_{\mathrm{F}}^{4}]^{1/2} \vee \mathbb{E}[\|\boldsymbol{\Sigma}^{1/2}\boldsymbol{H}\|_{\mathrm{F}}^{8}]^{1/4} \leq C(\zeta, T, \gamma, \kappa) \operatorname{var}(y_{1}), \\ \mathbb{E}[\|\boldsymbol{F}\|_{\mathrm{F}}^{2}/n] \vee \mathbb{E}[\|\boldsymbol{F}\|_{\mathrm{F}}^{4}/n^{2}]^{1/2} \vee \mathbb{E}[\|\boldsymbol{F}\|_{\mathrm{F}}^{8}/n^{4}]^{1/4} \leq C(\zeta, T, \gamma, \kappa) \operatorname{var}(y_{1}).$$

where y_1 is the first entry of the response vector and $var(y_1) = \|\Sigma^{1/2} b^*\|^2 + \sigma^2$. Consequently, by compactness, we can extract a subsequence of regression problems such that

(E.14)
$$\mathbb{E}[F^{\top}F/n] \to K, \text{ and } \mathbb{E}[H^{\top}\Sigma H + S] \to \bar{K},$$

where K and \overline{K} are two positive semi-definite deterministic matrices.

Proof of Lemma E.10. Without loss of generality, we assume $\Sigma = I_p$. Otherwise, if $\Sigma \neq I_p$, we apply the

change of variable (D.1), the desired result follows. Using the fact that $\|\boldsymbol{H}\|_{\mathrm{F}}^2 = \sum_{t=1}^T \|\boldsymbol{H}\boldsymbol{e}_t\|^2$ and $\|\boldsymbol{F}\|_{\mathrm{F}}^2 = \sum_{t=1}^T \|\boldsymbol{F}\boldsymbol{e}_t\|^2$, it suffices to bound the moments of $\|\boldsymbol{H}\boldsymbol{e}_t\|$ and $\|\boldsymbol{F}\boldsymbol{e}_t\|$ for each $t \in [T]$.

Let $a_s = \max\{\|[\hat{b}^s \mid \hat{b}^{s-1} \mid \dots \mid \hat{b}^1]\|_{\mathrm{F}}, n^{-1/2}\|[\boldsymbol{y} - \boldsymbol{X}\hat{b}^s \mid \boldsymbol{y} - \boldsymbol{X}\hat{b}^{s-1} \mid \boldsymbol{y} - \boldsymbol{X}\hat{b}^1]\|_{\mathrm{F}}\}$. By definition of \hat{b}^t in (2.8), using $g_t(\mathbf{0}) = \mathbf{0}$ and Assumption 2.1 we have

$$\begin{split} \|\widehat{\boldsymbol{b}}^{t} - \boldsymbol{0}\| &= \|\widehat{\boldsymbol{b}}^{t} - \boldsymbol{g}_{t}(\boldsymbol{0})\| \leq \zeta \| \left[\widehat{\boldsymbol{b}}^{t-1} \mid \widehat{\boldsymbol{b}}^{t-2} \mid \cdots \mid \widehat{\boldsymbol{b}}^{1} \mid \boldsymbol{v}^{t-1} \mid \cdots \mid \boldsymbol{v}^{1}\right] \|_{\mathrm{F}} \\ &\leq \zeta \| \left[\widehat{\boldsymbol{b}}^{t-1} \mid \widehat{\boldsymbol{b}}^{t-2} \mid \cdots \mid \widehat{\boldsymbol{b}}^{1}\right] \|_{\mathrm{F}} + \zeta \| \left[\boldsymbol{v}^{t-1} \mid \cdots \mid \boldsymbol{v}^{1}\right] \|_{\mathrm{F}} \\ &\leq \zeta (a_{t-1} + \| \boldsymbol{X} n^{-1/2} \|_{\mathrm{op}} a_{t-1}) \end{split}$$

and $\|\boldsymbol{y} - \boldsymbol{X} \hat{\boldsymbol{b}}^t\| \le \|\boldsymbol{y}\| + \|\boldsymbol{X} n^{-1/2}\|_{\text{op}} \|\hat{\boldsymbol{b}}^t\|$. Since $\boldsymbol{y} = \boldsymbol{y} - \boldsymbol{X} \hat{\boldsymbol{b}}^1$ since $\hat{\boldsymbol{b}}^1 = \boldsymbol{0}$, we also have $\|\boldsymbol{y}\|/\sqrt{n} = a_1 \le a_{t-1}$ and $\|\boldsymbol{y} - \boldsymbol{X} \widehat{\boldsymbol{b}}^t\| \leq \sqrt{n} a_{t-1} C(\zeta) (1 + \|\boldsymbol{X} n^{-1/2}\|_{op}^2)$. This proves

(E.15)
$$a_t \le C(\zeta)(1 + \|\boldsymbol{X}n^{-1/2}\|_{\text{op}}^2)a_{t-1}, \text{ and } a_T \le C(\zeta, T)(1 + \|\boldsymbol{X}n^{-1/2}\|_{\text{op}}^2)^T a_1$$

by induction, where $a_1 = \|\boldsymbol{y}\|/\sqrt{n}$. By the triangle inequality, $\|\boldsymbol{H}\|_{\rm F} \leq \sqrt{T} \|\boldsymbol{b}^*\| + a_T$, so we have established

$$\operatorname{var}(y_1)^{-1/2} \Big(\|\boldsymbol{H}\|_{\mathrm{F}} + \|\boldsymbol{F}\|_{\mathrm{F}} / \sqrt{n} \Big) \le C(\zeta, T) (1 + \|\boldsymbol{X}n^{-1/2}\|_{\operatorname{op}}^2)^T \Big(\frac{\|\boldsymbol{y}\|}{\sqrt{n} \operatorname{var}(y_1)^{1/2}} + 1 \Big).$$

The moments of order 2, 4 and 8 (and any other finite moment) of the right-hand side are bounded by $C(\zeta, T, \gamma)$ by Lemmas E.8 and E.9.

E.3. Frobenius norm bounds on Jacobians

Lemma E.11 (Frobenius norm bound of F w.r.t. X). Under Assumptions 2.1 and 2.4,

$$\frac{1}{n} \left\| \frac{\partial \operatorname{\mathbf{vec}}(\boldsymbol{F})}{\partial \operatorname{\mathbf{vec}}(\boldsymbol{X})} \right\|_{\mathrm{F}}^{2} = \frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{p} \left\| \frac{\partial \boldsymbol{F}}{\partial x_{ij}} \right\|_{\mathrm{F}}^{2} \le C(\zeta, T) \left(1 + \frac{1}{n} \| \boldsymbol{X} \|_{\mathrm{op}}^{2} \right)^{2T} \left(\| \boldsymbol{H} \|_{\mathrm{F}}^{2} + \gamma \| \boldsymbol{F} \|_{\mathrm{F}}^{2} / n \right),$$

Furthermore, if Assumptions 2.2 and 2.3 hold with $\Sigma = I_p$ then

$$\mathbb{E}\Big[\frac{1}{n}\sum_{i=1}^{n}\sum_{j=1}^{p}\left\|\frac{\partial \boldsymbol{F}}{\partial x_{ij}}\right\|_{\mathrm{F}}^{2}\Big] \leq \mathbb{E}\Big[\Big(\frac{1}{n}\sum_{i=1}^{n}\sum_{j=1}^{p}\left\|\frac{\partial \boldsymbol{F}}{\partial x_{ij}}\right\|_{\mathrm{F}}^{2}\Big)^{2}\Big]^{1/2} \leq C(\zeta, T, \gamma)\mathrm{var}(y_{1}).$$

Proof of Lemma E.11. The first line is proved in (E.10). For the second line, we use the Cauchy-Schwarz inequality with the moment bounds from Lemmas E.8 and E.10. Lemma E.12 (Frobenius norm bound of H w.r.t. X). Under Assumptions 2.1 and 2.4,

$$\sum_{i=1}^{n} \sum_{j=1}^{p} \left\| \frac{\partial \boldsymbol{H}}{\partial x_{ij}} \right\|_{\mathrm{F}}^{2} \leq \gamma C(\zeta, T) (1 + \|\boldsymbol{X}\|_{\mathrm{op}}^{2}/n)^{2T} (\|\boldsymbol{F}\|_{\mathrm{F}}^{2}/n + \|\boldsymbol{H}\|_{\mathrm{F}}^{2}).$$

In addition, if Assumptions 2.2 and 2.3 hold with $\Sigma = I_p$ then

$$\mathbb{E}\left[\sum_{i=1}^{n}\sum_{j=1}^{p}\left\|\frac{\partial \boldsymbol{H}}{\partial x_{ij}}\right\|_{\mathrm{F}}^{2}\right] \leq \mathbb{E}\left[\left(\sum_{i=1}^{n}\sum_{j=1}^{p}\left\|\frac{\partial \boldsymbol{H}}{\partial x_{ij}}\right\|_{\mathrm{F}}^{2}\right)^{2}\right]^{1/2} \leq C(\zeta, T, \gamma)\mathrm{var}(y_{1}).$$

Proof of Lemma E.12. The same argument as for (E.10) would provide the desired bound. We provide an alternative argument to showcase another means to control such quantities. By the expression of $\frac{\partial \hat{b}^t}{\partial x_{ij}}$ in (C.2), we have $\frac{\partial e_k^\top H e_t}{\partial x_{ij}} = \frac{\partial e_k^\top (\hat{b}^t - b^*)}{\partial x_{ij}} = \frac{\partial e_k^\top \hat{b}^t}{\partial x_{ij}}$ so that

$$\frac{\partial \boldsymbol{e}_{k}^{\top} \boldsymbol{H} \boldsymbol{e}_{t}}{\partial x_{ij}} = n^{-1} \boldsymbol{e}_{k}^{\top} (\boldsymbol{e}_{t}^{\top} \otimes \boldsymbol{I}_{p}) \mathcal{M}^{-1} \mathcal{D}[((\boldsymbol{F}^{\top} \boldsymbol{e}_{i}) \otimes \boldsymbol{e}_{j}) - ((\boldsymbol{H}^{\top} \boldsymbol{e}_{j}) \otimes (\boldsymbol{X}^{\top} \boldsymbol{e}_{i}))] \qquad \text{by (C.2)}$$
$$= n^{-1} (\boldsymbol{e}_{t}^{\top} \otimes \boldsymbol{e}_{k}^{\top}) \mathcal{M}^{-1} \mathcal{D}[(\boldsymbol{F}^{\top} \otimes \boldsymbol{I}_{p}) (\boldsymbol{e}_{i} \otimes \boldsymbol{e}_{j}) - (\boldsymbol{H}^{\top} \otimes \boldsymbol{X}^{\top}) (\boldsymbol{e}_{j} \otimes \boldsymbol{e}_{i})] \qquad \text{by (B.1)}.$$

Therefore, using $(a+b)^2 \leq 2a^2 + 2b^2$,

$$\begin{split} &\sum_{i=1}^{n} \sum_{j=1}^{p} \left\| \frac{\partial \boldsymbol{H}}{\partial x_{ij}} \right\|_{\mathrm{F}}^{2} = \sum_{ij,kt} \left(\frac{\partial \boldsymbol{e}_{k}^{\top} \boldsymbol{H} \boldsymbol{e}_{t}}{\partial x_{ij}} \right)^{2} \\ &\leq 2n^{-2} \| \mathcal{M}^{-1} \mathcal{D}(\boldsymbol{F}^{\top} \otimes \boldsymbol{I}_{p}) \|_{\mathrm{F}}^{2} + 2n^{-2} \| \mathcal{M}^{-1} \mathcal{D}(\boldsymbol{H}^{\top} \otimes \boldsymbol{X}^{\top}) \|_{\mathrm{F}}^{2} \\ &\leq 2n^{-2} \| \mathcal{M}^{-1} \mathcal{D} \|_{\mathrm{op}}^{2} \| \boldsymbol{F}^{\top} \otimes \boldsymbol{I}_{p} \|_{\mathrm{F}}^{2} + 2n^{-2} \| \mathcal{M}^{-1} \mathcal{D} \|_{\mathrm{op}}^{2} \| \boldsymbol{H}^{\top} \otimes \boldsymbol{X}^{\top} \|_{\mathrm{F}}^{2} \\ &= 2pn^{-2} \| \mathcal{M}^{-1} \mathcal{D} \|_{\mathrm{op}}^{2} \| \boldsymbol{F} \|_{\mathrm{F}}^{2} + 2n^{-2} \| \mathcal{M}^{-1} \mathcal{D} \|_{\mathrm{op}}^{2} \| \boldsymbol{H} \|_{\mathrm{F}}^{2} \| \boldsymbol{X} \|_{\mathrm{F}}^{2} \\ &\leq 2pn^{-2} \| \mathcal{M}^{-1} \mathcal{D} \|_{\mathrm{op}}^{2} (\| \boldsymbol{F} \|_{\mathrm{F}}^{2} + \| \boldsymbol{H} \|_{\mathrm{F}}^{2} \| \boldsymbol{X} \|_{\mathrm{op}}^{2}) \\ &\leq 2pn^{-2} \| \mathcal{M}^{-1} \|_{\mathrm{op}}^{2} \| \mathcal{D} \|_{\mathrm{op}}^{2} (\| \boldsymbol{F} \|_{\mathrm{F}}^{2} + \| \boldsymbol{H} \|_{\mathrm{F}}^{2} \| \boldsymbol{X} \|_{\mathrm{op}}^{2}) \\ &\leq 2pn^{-2} \| \mathcal{M}^{-1} \|_{\mathrm{op}}^{2} \| \mathcal{D} \|_{\mathrm{op}}^{2} (\| \boldsymbol{F} \|_{\mathrm{F}}^{2} + \| \boldsymbol{H} \|_{\mathrm{F}}^{2} \| \boldsymbol{X} \|_{\mathrm{op}}^{2}) \\ &\leq \gamma C(\zeta, T)(1 + \| \boldsymbol{X} \|_{\mathrm{op}}^{2}/n)^{2T} (\| \boldsymbol{F} \|_{\mathrm{F}}^{2}/n + \| \boldsymbol{H} \|_{\mathrm{F}}^{2}) \end{aligned}$$

For the upper bound on the moments, we use the Cauchy-Schwarz inequality with the moment bounds from Lemmas E.8 and E.10 as for the proof of Lemma E.11. \Box

Lemma E.13. Under Assumptions 2.1 to 2.4, we have

(E.16)
$$\mathbb{E}[\|\boldsymbol{F}^{\top}\boldsymbol{F}/n - \mathbb{E}[\boldsymbol{F}^{\top}\boldsymbol{F}/n]\|_{\mathrm{F}}^{2}] \leq C(\gamma, \zeta, T, \kappa) \mathrm{var}(y_{1})^{2}/n,$$

(E.17)
$$\mathbb{E}[\|\boldsymbol{H}^{\top}\boldsymbol{\Sigma}\boldsymbol{H} - \mathbb{E}[\boldsymbol{H}^{\top}\boldsymbol{\Sigma}\boldsymbol{H}]\|_{\mathrm{F}}^{2}] \leq C(\gamma,\zeta,T,\kappa)\mathrm{var}(y_{1})^{2}/n$$

Consequently, if $var(y_1)$ is bounded from above by a constant, by Markov's inequality,

(E.18)
$$\boldsymbol{F}^{\top}\boldsymbol{F}/n - \mathbb{E}(\boldsymbol{F}^{\top}\boldsymbol{F}/n) = O_P(n^{-1/2}) \text{ and } \boldsymbol{H}^{\top}\boldsymbol{\Sigma}\boldsymbol{H} - \mathbb{E}(\boldsymbol{H}^{\top}\boldsymbol{\Sigma}\boldsymbol{H}) = O_P(n^{-1/2}).$$

Proof of Lemma E.13. By the change of variable argument in Lemma E.10, it suffices to prove the results under $\Sigma = I_p$. We view F as a function of (X, ε) . By the Gaussian Poincaré inequality applied to $e_t^{\top} F^{\top} F e_s$ for each $t, s \in [T]$, we find

(E.19)
$$\operatorname{var}\left((\boldsymbol{F}\boldsymbol{e}_{t})^{\top}\boldsymbol{F}\boldsymbol{e}_{s}\right) \leq \mathbb{E}\sum_{i=1}^{n}\sigma^{2}\left(\frac{\partial(\boldsymbol{e}_{t}^{\top}\boldsymbol{F}^{\top}\boldsymbol{F}\boldsymbol{e}_{s})}{\partial\varepsilon_{i}}\right)^{2} + \mathbb{E}\sum_{i=1}^{n}\sum_{j=1}^{p}\left(\frac{\partial(\boldsymbol{e}_{t}^{\top}\boldsymbol{F}^{\top}\boldsymbol{F}\boldsymbol{e}_{s})}{\partial x_{ij}}\right)^{2}$$

Let ∂ denote either $\partial/\partial x_{ij}$ or $\partial/\partial \epsilon_i$. Using the product rule $\partial(\boldsymbol{e}_t^\top \boldsymbol{F}^\top \boldsymbol{F} \boldsymbol{e}_s)) = \boldsymbol{e}_t^\top (\partial \boldsymbol{F})^\top \boldsymbol{F} \boldsymbol{e}_s + \boldsymbol{e}_t^\top \boldsymbol{F}^\top (\partial \boldsymbol{F}) \boldsymbol{e}_s$ as well as $(a+b)^2 \leq 2a^2 + 2b^2$ and summing over all $s \in [T]$ and all $t \in [T]$,

(E.20)
$$\sum_{s=1}^{T} \sum_{t=1}^{T} \operatorname{var} \left((\boldsymbol{F} \boldsymbol{e}_{t})^{\top} \boldsymbol{F} \boldsymbol{e}_{s} \right) \leq 4\mathbb{E} \sum_{s=1}^{T} \sum_{t=1}^{T} \sum_{i=1}^{T} \left(\sigma^{2} \left(\boldsymbol{e}_{s}^{\top} \boldsymbol{F}^{\top} \frac{\partial \boldsymbol{F} \boldsymbol{e}_{t}}{\partial \epsilon_{i}} \right)^{2} + \sum_{j=1}^{p} \left(\boldsymbol{e}_{s}^{\top} \boldsymbol{F}^{\top} \frac{\partial \boldsymbol{F} \boldsymbol{e}_{t}}{\partial x_{ij}} \right)^{2} \right) \\ = 4\mathbb{E} \left[\sum_{i=1}^{n} \left(\sigma^{2} \| \boldsymbol{F}^{\top} \frac{\partial \boldsymbol{F}}{\partial \epsilon_{i}} \|_{\mathrm{F}}^{2} + \sum_{j=1}^{p} \| \boldsymbol{F}^{\top} \frac{\partial \boldsymbol{F}}{\partial x_{ij}} \|_{\mathrm{F}}^{2} \right) \right]$$

where we used $\sum_{s=1}^{T} \mathbf{e}_s \mathbf{e}_s^{\top} = \mathbf{I}_T$ and similarly for the sum over $t \in [T]$. We rewrite the above using the vectorization operator: $\|\mathbf{F}^{\top} \frac{\partial}{\partial x_{ij}} \mathbf{F}\|_{\mathrm{F}}^2 = \|(\mathbf{I}_T \otimes \mathbf{F}^{\top}) \operatorname{vec}(\frac{\partial}{\partial x_{ij}} \mathbf{F})\|^2$, which is also the squared norm of the (i, j)-th column of $(\mathbf{I}_T \otimes \mathbf{F}^{\top}) \frac{\partial \operatorname{vec} \mathbf{F}}{\partial \operatorname{vec} \mathbf{X}}$, so that

(E.21)
$$\sum_{i=1}^{n} \sum_{j=1}^{p} \| \boldsymbol{F}^{\top} \frac{\partial \boldsymbol{F}}{\partial x_{ij}} \|_{\mathrm{F}}^{2} = \left\| (\boldsymbol{I}_{T} \otimes \boldsymbol{F}^{\top}) \frac{\partial \operatorname{vec}(\boldsymbol{F})}{\partial \operatorname{vec}(\boldsymbol{X})} \right\|_{\mathrm{F}}^{2} \le T \| \boldsymbol{F} \|_{\mathrm{F}}^{2} \left\| \frac{\partial \operatorname{vec}(\boldsymbol{F})}{\partial \operatorname{vec}(\boldsymbol{X})} \right\|_{\mathrm{op}}^{2}$$

using $\|MM'\|_{\rm F} \leq \|M\|_{\rm F} \|M'\|_{\rm op}$ for the inequality. By the same argument,

(E.22)
$$\sum_{i=1}^{n} \| \boldsymbol{F}^{\top} \frac{\partial \boldsymbol{F}}{\partial \epsilon_{i}} \|_{\mathrm{F}}^{2} = \left\| (\boldsymbol{I}_{T} \otimes \boldsymbol{F}^{\top}) \frac{\partial \operatorname{\mathbf{vec}}(\boldsymbol{F})}{\partial \varepsilon} \right\|_{\mathrm{F}}^{2} \leq T \| \boldsymbol{F} \|_{\mathrm{F}}^{2} \left\| \frac{\partial \operatorname{\mathbf{vec}}(\boldsymbol{F})}{\partial \varepsilon} \right\|_{\mathrm{op}}^{2}.$$

By (E.9) and Equation (E.7), both previous displays are bounded from above by

$$C(\zeta, T, \gamma) \|\boldsymbol{F}\|_{\mathrm{F}}^{2} \max\{\sigma^{2}, \|\boldsymbol{H}\|_{\mathrm{F}}^{2} + \|\boldsymbol{F}\|_{\mathrm{F}}^{2}/n\}(1 + \|\boldsymbol{X}\|_{\mathrm{op}}^{2}/n)^{T}.$$

Using the Cauchy-Schwarz inequality to leverage the moment bounds (E.8) and (E.10), we find that (E.20) is bounded from above by $C(\zeta, T, \gamma)n$ and the proof of (E.16) is complete.

By exactly the same argument, (E.19), (E.20), (E.22) and (E.21) hold with F replaced by H. We use the upper bounds (E.12) and (E.8) to control the operator norm of $\frac{\partial \operatorname{vec}(F)}{\partial \operatorname{vec}(X)}$ and $\frac{\partial \operatorname{vec}(F)}{\partial \varepsilon}$, and the moment bounds (E.8) and (E.10) to obtain (E.17).

Appendix F: Proof of Theorem 2.2

Throughout this proof, we assume $\Sigma = I_p$, and the proof for general Σ follows the same line of argument by changing ζ to $\kappa \zeta$, thanks to the change of variables in Appendix D.

Before stating the proof, we recall a few definitions from (C.1):

$$\boldsymbol{H} = [\widehat{\boldsymbol{b}}^1 - \boldsymbol{b}^*, \dots, \widehat{\boldsymbol{b}}^T - \boldsymbol{b}^*] \in \mathbb{R}^{p \times T}, \quad \boldsymbol{F} = [\boldsymbol{y} - \boldsymbol{X}\widehat{\boldsymbol{b}}^1, \dots, \boldsymbol{y} - \boldsymbol{X}\widehat{\boldsymbol{b}}^T] \in \mathbb{R}^{n \times T}.$$

We first derive the upper bound of $\operatorname{var}(r_{tt'})$. By definition of $r_{tt'}$ and H, we know $r_{tt'}$ is the (t, t') entry of $H^{\top}H$. Thus,

$$\begin{aligned} &\operatorname{var}(r_{tt'}) \\ = & \mathbb{E}[(r_{tt'} - \mathbb{E}[r_{tt'}])^2] \\ = & \mathbb{E}[([\boldsymbol{H}^\top \boldsymbol{H}]_{t,t'} - \mathbb{E}[[\boldsymbol{H}^\top \boldsymbol{H}]_{t,t'}])^2] \\ \leq & \mathbb{E}[\|\boldsymbol{H}^\top \boldsymbol{H} - \mathbb{E}[\boldsymbol{H}^\top \boldsymbol{H}]\|_{\mathrm{F}}^2] \\ \leq & n^{-1}C(\gamma, \zeta, T, \kappa) \operatorname{var}(y_1)^2 \end{aligned}$$
 by Lemma E.13

It thus remains to show $\mathbb{E}[|r_{tt'} - \hat{r}_{tt'}|] \leq n^{-1/2}C(\gamma, \zeta, T, \kappa)\operatorname{var}(y_1)$. Define $\mathbf{S} = \sigma^2 \mathbf{1}_T \mathbf{1}_T^\top \in \mathbb{R}^{T \times T}$, then we have

$$\mathbb{E}[|r_{tt'} - \hat{r}_{tt'}|] = \mathbb{E}\Big[[\boldsymbol{H}^{\top}\boldsymbol{H} + \boldsymbol{S}]_{t,t'} - [(\boldsymbol{I}_T - \widehat{\mathbf{A}})^{-1}\boldsymbol{F}^{\top}\boldsymbol{F}/n(\boldsymbol{I}_T - \widehat{\mathbf{A}}^{\top})^{-1}]_{t,t'}\Big]$$
$$\leq \mathbb{E}\Big[\|\boldsymbol{H}^{\top}\boldsymbol{H} + \boldsymbol{S} - (\boldsymbol{I}_T - \widehat{\mathbf{A}})^{-1}\boldsymbol{F}^{\top}\boldsymbol{F}/n(\boldsymbol{I}_T - \widehat{\mathbf{A}}^{\top})^{-1}\|_{\mathrm{F}}\Big].$$

So it suffices to show

(F.1)
$$\mathbb{E}[\|\boldsymbol{H}^{\top}\boldsymbol{H} + \boldsymbol{S} - (\boldsymbol{I}_T - \widehat{\mathbf{A}})^{-1}\boldsymbol{F}^{\top}\boldsymbol{F}/n(\boldsymbol{I}_T - \widehat{\mathbf{A}}^{\top})^{-1}\|_{\mathrm{F}}] \leq n^{-1/2}C(\zeta, T, \gamma)\mathrm{var}(y_1).$$

To this end, we define

(F.2)
$$\widehat{\boldsymbol{C}} = \sum_{j=1}^{p} (\boldsymbol{I}_T \otimes \boldsymbol{e}_j^{\top}) \mathcal{M}^{-1} \mathcal{D} (\boldsymbol{I}_T \otimes \boldsymbol{e}_j) \in \mathbb{R}^{T \times T},$$

where $\mathcal{M} = \mathbf{I}_{pT} + \mathcal{D}(\mathbf{I}_T \otimes \frac{\mathbf{X}^\top \mathbf{X}}{n}) - \mathcal{J}$ as in Lemma C.1. We also define the matrices $\mathbf{Q}_1, \mathbf{Q}_2 \in \mathbb{R}^{T \times T}$ that are bounded in Propositions F.1 and F.2 below:

$$Q_1 = n^{-1/2} \left[\boldsymbol{F}^\top \boldsymbol{F} (\boldsymbol{I}_T + \widehat{\boldsymbol{C}}/n)^\top - (n\boldsymbol{I}_T - \widehat{\mathbf{A}})(\boldsymbol{H}^\top \boldsymbol{H} + \boldsymbol{S}) \right],$$

$$Q_2 = n^{-1/2} \left[n(\boldsymbol{H}^\top \boldsymbol{H} + \boldsymbol{S}) - (\boldsymbol{I}_T + \widehat{\boldsymbol{C}}/n) \boldsymbol{F}^\top \boldsymbol{F} (\boldsymbol{I}_T + \widehat{\boldsymbol{C}}/n)^\top \right].$$

Proposition F.1 (Proof is given in Appendix F.1). Let Assumptions 2.1 to 2.4 be fulfilled and $\Sigma = I_p$, then we have $\mathbb{E}[\|Q_1\|_F^2] \leq C(\zeta, T, \gamma) \operatorname{var}(y_1)^2$. As a consequence, by Jensen's inequality, $\mathbb{E}[\|Q_1\|_F^2] \leq C(\zeta, T, \gamma) \operatorname{var}(y_1)^2$.

Proposition F.2 (Proof is given in Appendix F.2). Let Assumptions 2.1 to 2.4 be fulfilled and $\Sigma = I_p$, then $\mathbb{E}[\|Q_2\|_F] \leq C(\zeta, T, \gamma) \operatorname{var}(y_1)$.

Now we are ready to prove Equation (F.1) using the above two propositions. For brevity, let $\boldsymbol{V} = [-\boldsymbol{H}^{\top}, \sigma \mathbf{1}_T]^{\top} \in \mathbb{R}^{(p+1)\times T}$ and the lower triangular matrices $\boldsymbol{L} = \boldsymbol{I}_T - \widehat{\mathbf{A}}/n$ and $\boldsymbol{T} = \boldsymbol{I}_T + \widehat{\boldsymbol{C}}/n$. With this notation,

(F.3)
$$\boldsymbol{Q}_1 = \sqrt{n} [(\boldsymbol{F}^\top \boldsymbol{F}/n) \boldsymbol{T}^\top - \boldsymbol{L} \boldsymbol{V}^\top \boldsymbol{V}],$$

(F.4)
$$\boldsymbol{Q}_2 = \sqrt{n} [\boldsymbol{V}^\top \boldsymbol{V} - \boldsymbol{T} (\boldsymbol{F}^\top \boldsymbol{F}/n) \boldsymbol{T}^\top].$$

By expanding the expressions of Q_1 and Q_2 in (F.3)-(F.4), we have by simple algebra

(F.5)
$$n^{-1/2} \left[\boldsymbol{Q}_{1}^{\top} (\boldsymbol{L}^{\top})^{-1} + (\boldsymbol{L}^{-1} \boldsymbol{Q}_{1} + \boldsymbol{Q}_{2}) (\boldsymbol{T}^{\top})^{-1} (\boldsymbol{L}^{\top})^{-1} \right] \\= \begin{cases} \boldsymbol{T} (\boldsymbol{F}^{\top} \boldsymbol{F} / n) (\boldsymbol{L}^{\top})^{-1} - \boldsymbol{V}^{\top} \boldsymbol{V} \\ + \boldsymbol{L}^{-1} (\boldsymbol{F}^{\top} \boldsymbol{F} / n) (\boldsymbol{L}^{\top})^{-1} - \boldsymbol{V}^{\top} \boldsymbol{V} (\boldsymbol{T}^{\top})^{-1} (\boldsymbol{L}^{\top})^{-1} \\ + \boldsymbol{V}^{\top} \boldsymbol{V} (\boldsymbol{T}^{\top})^{-1} (\boldsymbol{L}^{\top})^{-1} - \boldsymbol{T} (\boldsymbol{F}^{\top} \boldsymbol{F} / n) (\boldsymbol{L}^{\top})^{-1} \\ = \boldsymbol{L}^{-1} (\boldsymbol{F}^{\top} \boldsymbol{F} / n) (\boldsymbol{L}^{\top})^{-1} - \boldsymbol{V}^{\top} \boldsymbol{V} \\ = (\boldsymbol{I}_{T} - \frac{1}{n} \widehat{\mathbf{A}})^{-1} (\boldsymbol{F}^{\top} \boldsymbol{F} / n) (\boldsymbol{I}_{T} - \frac{1}{n} \widehat{\mathbf{A}}^{\top})^{-1} - (\boldsymbol{H}^{\top} \boldsymbol{H} + \boldsymbol{S}) \end{cases}$$

as all terms except two cancel out. Consequently by the triangle inequality,

$$\sqrt{n} \| \boldsymbol{L}^{-1} (\boldsymbol{F}^{\top} \boldsymbol{F} / n) (\boldsymbol{L}^{\top})^{-1} - \boldsymbol{V}^{\top} \boldsymbol{V} \|_{\mathrm{F}} \le \max\{1, \| \boldsymbol{L}^{-1} \|_{\mathrm{op}}^{3}, \| \boldsymbol{T} \|_{\mathrm{op}}^{3}\} (2 \| \boldsymbol{Q}_{1} \|_{\mathrm{F}} + \| \boldsymbol{Q}_{2} \|_{\mathrm{F}}).$$

Let $\Omega = \{ \mathbf{X} \in \mathbb{R}^{n \times p} : \|\mathbf{X}\|_{\text{op}}/\sqrt{n} \leq 2 + \sqrt{\gamma} \}$. Under Assumption 2.2 and here $\mathbf{\Sigma} = \mathbf{I}_p$, (Davidson and Szarek, 2001, Theorem II.13) implies that $\mathbb{P}(\Omega) \geq 1 - e^{-n}$. Then in the event Ω , we have by Lemmas E.3 and E.4,

(F.6)
$$\max\{\|\boldsymbol{L}\|_{\rm op}, \|\boldsymbol{L}^{-1}\|_{\rm op}, \|\boldsymbol{T}\|_{\rm op}, \|\boldsymbol{T}^{-1}\|_{\rm op}\} \le C(\zeta, T, \gamma),$$

so that by the previous display and Propositions F.1 and F.2,

(F.7)
$$\mathbb{E}[\mathbb{I}(\Omega)\sqrt{n}\|\boldsymbol{L}^{-1}(\boldsymbol{F}^{\top}\boldsymbol{F}/n)(\boldsymbol{L}^{\top})^{-1} - \boldsymbol{V}^{\top}\boldsymbol{V}\|_{\mathrm{F}}] \leq C(T,\zeta,\gamma)\mathbb{E}[\|\boldsymbol{Q}_{1}\|_{\mathrm{F}} + \|\boldsymbol{Q}_{2}\|_{\mathrm{F}}] \leq C(T,\zeta,\gamma)\mathrm{var}(y_{1}).$$

On the other hand, the same expectation with Ω^c is exponentially small due to

$$\mathbb{E}[\mathbb{I}(\Omega^{c})\|(\mathbf{F}.5)\|_{\mathbf{F}}] \leq \mathbb{P}(\Omega^{c})^{1/2} \mathbb{E}[\{(1+\|\boldsymbol{L}\|_{\mathrm{op}}^{2})(\|\boldsymbol{F}\|_{\mathbf{F}}^{2}/n+\|\boldsymbol{V}\|_{\mathbf{F}}^{2})\}^{2}]^{1/2}$$
(C. Schwarz)

$$\leq \mathbb{P}(\Omega^{c})^{1/2} \mathbb{E}[(1+\|\boldsymbol{L}\|_{\mathrm{op}}^{2})^{4}]^{1/4} \mathbb{E}[(\|\boldsymbol{F}\|_{\mathbf{F}}^{2}/n+\|\boldsymbol{V}\|_{\mathbf{F}}^{2})^{4}]^{1/4}$$
(C. Schwarz)

(F.8) $\leq e^{-n/2}C(\zeta, T, \gamma)\operatorname{var}(y_1)$

thanks to Lemmas E.3, E.4 and E.8 and $\mathbb{P}(\Omega) \leq e^{-n}$ for the last line. This completes the proof of Theorem 2.2 for $\Sigma = I_p$.

For $\Sigma \neq I_p$, we apply the change of variables argument presented in Appendix D to achieve the desired result. In this context, the constant C is dependent on ζ, T, γ, κ . This concludes the proof of Theorem 2.2. In passing, let us mention that we also have by definitions of Q_1 and Q_2 that

(F.9)
$$[\boldsymbol{L}^{-1}\boldsymbol{Q}_1(\boldsymbol{T}^{\top})^{-1} + \boldsymbol{Q}_2(\boldsymbol{T}^{\top})^{-1}](\boldsymbol{L}^{-1} - \boldsymbol{T})^{\top} = \sqrt{n}(\boldsymbol{L}^{-1} - \boldsymbol{T})(\boldsymbol{F}^{\top}\boldsymbol{F}/n)(\boldsymbol{L}^{-1} - \boldsymbol{T})^{\top}$$

holds. By the same argument as in (F.7)-(F.8), that the right-hand side of the previous display is bounded as

(F.10)
$$\sqrt{n}\mathbb{E}[\|(\boldsymbol{L}^{-1}-\boldsymbol{T})\boldsymbol{F}^{\top}\boldsymbol{n}^{-1/2}\|_{\mathrm{F}}^{2}] \leq C(T,\zeta,\gamma)\mathrm{var}(y_{1})$$

F.1. Proofs of Proposition F.1

We frist write

$$oldsymbol{F}^{ op}oldsymbol{F} = oldsymbol{F}^{ op}igg[X,rac{oldsymbol{arepsilon}}{\sigma}igg]igg[-oldsymbol{H}^{ op},\sigmaoldsymbol{1}_Tigg]^{ op}$$

Applying (Tan et al., 2022, Lemma E.10) to $\boldsymbol{U} = \boldsymbol{F} \in \mathbb{R}^{n \times T}, \ \boldsymbol{Z} = [\boldsymbol{X}, \boldsymbol{\varepsilon}/\sigma] \in \mathbb{R}^{n \times (p+1)}, \text{ and } \boldsymbol{V} = [-\boldsymbol{H}^{\top}, \sigma \mathbf{1}_T]^{\top} \in \mathbb{R}^{(p+1) \times T}$ gives

(F.11)
$$\mathbb{E}\left[\left\|\boldsymbol{U}^{\top}\boldsymbol{Z}\boldsymbol{V}-\sum_{j=1}^{p+1}\sum_{i=1}^{n}\frac{\partial}{\partial z_{ij}}\left(\boldsymbol{U}^{\top}\boldsymbol{e}_{i}\boldsymbol{e}_{j}^{\top}\boldsymbol{V}\right)\right\|_{\mathrm{F}}^{2}\right]$$

(F.12)
$$\leq \mathbb{E}[\|\boldsymbol{U}\|_{\mathrm{F}}^{2}\|\boldsymbol{V}\|_{\mathrm{F}}^{2}] + \mathbb{E}\sum_{i=1}^{n}\sum_{j=1}^{p+1}\left[2\|\boldsymbol{V}\|_{\mathrm{F}}^{2}\left\|\frac{\partial\boldsymbol{U}}{\partial z_{ij}}\right\|_{\mathrm{F}}^{2} + 2\|\boldsymbol{U}\|_{\mathrm{F}}^{2}\left\|\frac{\partial\boldsymbol{V}}{\partial z_{ij}}\right\|_{\mathrm{F}}^{2}\right].$$

To prove Proposition F.1, we need the following two lemmas.

Lemma F.3 (Proof is given on Page 47). Let the assumptions of Proposition F.1 be fulfilled. For U = F, $Z = [X, \varepsilon/\sigma]$, and $V = [-H^{\top}, \sigma \mathbf{1}_T]^{\top}$, we have

$$\boldsymbol{U}^{\top} \boldsymbol{Z} \boldsymbol{V} - \sum_{j=1}^{p+1} \sum_{i=1}^{n} \frac{\partial}{\partial z_{ij}} \left(\boldsymbol{U}^{\top} \boldsymbol{e}_{i} \boldsymbol{e}_{j}^{\top} \boldsymbol{V} \right) = \sqrt{n} \boldsymbol{Q}_{1} + \operatorname{Rem}_{1}$$

where Rem_1 is a $T \times T$ matrix satisfying $\mathbb{E}[\|\operatorname{Rem}_1\|_{\mathrm{F}}^2] \leq nC(\zeta, T, \gamma)\operatorname{var}(y_1)^2$.

Lemma F.4 (Proof is given on Page 48). Let the assumptions of Proposition F.1 be fulfilled, then

$$(\mathbf{F.12}) \le nC(\zeta, T, \gamma)\operatorname{var}(y_1)^2.$$

Now we prove Proposition F.1 using the above two lemmas. According to Lemma F.3, we have $\sqrt{n}Q_1 = U^{\top}ZV - \sum_{j=1}^{p+1}\sum_{i=1}^{n}\frac{\partial}{\partial z_{ii}}(U^{\top}e_ie_j^{\top}V) - \text{Rem}_1$. By triangular inequality, we obtain

$$n\mathbb{E}[\|\boldsymbol{Q}_{1}\|_{\mathrm{F}}^{2}]$$

$$\leq 2\mathbb{E}\Big[\|\boldsymbol{U}^{\top}\boldsymbol{Z}\boldsymbol{V} - \sum_{j=1}^{p+1}\sum_{i=1}^{n}\frac{\partial}{\partial z_{ij}}(\boldsymbol{U}^{\top}\boldsymbol{e}_{i}\boldsymbol{e}_{j}^{\top}\boldsymbol{V})\|_{\mathrm{F}}^{2}\Big] + 2\mathbb{E}[\|\mathrm{Rem}_{1}\|_{\mathrm{F}}^{2}]$$

$$\leq 2\Big((\mathrm{F}.12) + \mathbb{E}[\|\mathrm{Rem}_{1}\|_{\mathrm{F}}^{2}]\Big)$$

$$\leq nC(\zeta, T, \gamma)\mathrm{var}(y_{1})^{2} \qquad \text{by Lemmas F.3 and F.4.}$$

This completes the proof of Proposition F.1.

F.2. Proofs of Proposition F.2

We first state a useful lemma, which is an extension of Lemma E.12 in Tan et al. (2022) to allow $\|\boldsymbol{U}\|_{\rm F} \ge 1$ and $\|\boldsymbol{V}\|_{\rm F} \ge 1$.

Lemma F.5 (Proof is given on Page 49). Let $U, V : \mathbb{R}^{n \times p} \to \mathbb{R}^{n \times T}$ be two locally Lipschitz functions of Z with *i.i.d.* N(0,1) entries. Provided the following expectations are finite, we have

$$\begin{split} & \mathbb{E}\Big[\Big\|p\boldsymbol{U}^{\top}\boldsymbol{V} - \sum_{j=1}^{p}\Big(\sum_{i=1}^{n}\partial_{ij}\boldsymbol{U}^{\top}\boldsymbol{e}_{i} - \boldsymbol{U}^{\top}\boldsymbol{Z}\boldsymbol{e}_{j}\Big)\Big(\sum_{i=1}^{n}\partial_{ij}\boldsymbol{e}_{i}^{\top}\boldsymbol{V} - \boldsymbol{e}_{j}^{\top}\boldsymbol{Z}^{\top}\boldsymbol{V}\Big)\Big\|_{\mathrm{F}}\Big] \\ & \leq \ (1 + 2\sqrt{p})\Big(\mathbb{E}[\|\boldsymbol{U}\|_{\mathrm{F}}^{4}]^{1/2} + \mathbb{E}[\|\boldsymbol{V}\|_{\mathrm{F}}^{4}]^{1/2} + \mathbb{E}[\|\boldsymbol{U}\|_{\partial}^{4}]^{1/2} + \mathbb{E}[\|\boldsymbol{V}\|_{\partial}^{4}]^{1/2} \Big), \end{split}$$

where $\partial_{ij} U = \partial U / \partial z_{ij}$ and $\|U\|_{\partial} = (\sum_{i=1}^n \sum_{j=1}^p \|\partial_{ij} U\|_{\mathrm{F}}^2)^{1/2}$.

To apply Lemma F.5, we consider the following mapping:

$$\mathbb{R}^{(p+1)\times n} \to \mathbb{R}^{(p+1)\times T} : \boldsymbol{Z}^\top \mapsto \boldsymbol{V}$$

where $\boldsymbol{Z} = [\boldsymbol{X}, \frac{\boldsymbol{\varepsilon}}{\sigma}]$ and $\boldsymbol{V} = [-\boldsymbol{H}^{\top}, \sigma \boldsymbol{1}_T]^{\top}$. Applying Lemma F.5 to $\boldsymbol{U} = \boldsymbol{V} = [-\boldsymbol{H}^{\top}, \sigma \boldsymbol{1}_T]^{\top}$ and the Gaussian matrix \boldsymbol{Z}^{\top} , we have

(F.13)
$$\mathbb{E}\left[\left\|n\boldsymbol{V}^{\top}\boldsymbol{V}-\sum_{i=1}^{n}\left(\sum_{j=1}^{p+1}\frac{\partial\boldsymbol{V}^{\top}}{\partial z_{ij}}\boldsymbol{e}_{j}-\boldsymbol{V}^{\top}\boldsymbol{Z}^{\top}\boldsymbol{e}_{i}\right)\left(\sum_{j=1}^{p+1}\frac{\partial\boldsymbol{e}_{j}^{\top}\boldsymbol{V}}{\partial z_{ij}}-\boldsymbol{e}_{i}^{\top}\boldsymbol{Z}\boldsymbol{V}\right)\right\|_{\mathrm{F}}\right] \\ \leq 2(1+2\sqrt{n})\left(\mathbb{E}[\|\boldsymbol{V}\|_{\mathrm{F}}^{4}]^{1/2}+\mathbb{E}[\|\boldsymbol{V}\|_{\partial}^{4}]^{1/2}\right),$$

where $\|\boldsymbol{V}\|_{\partial} := (\sum_{i=1}^{n} \sum_{j=1}^{p+1} \|\frac{\partial \boldsymbol{V}}{\partial z_{ij}}\|_{\mathrm{F}}^{2})^{1/2}$. The desired bound of $\mathbb{E}[\|\boldsymbol{Q}_{2}\|_{\mathrm{F}}]$ then follows from the subsequent two lemmas.

Lemma F.6 (Proof is given on Page 53). Let the assumptions of Proposition F.2 be fulfilled. For $\mathbf{Z} = [\mathbf{X}, \frac{\varepsilon}{\sigma}]$ and $\mathbf{V} = [-\mathbf{H}^{\top}, \sigma \mathbf{1}_T]^{\top}$, we have

(F.14)
$$n \boldsymbol{V}^{\top} \boldsymbol{V} - \sum_{i=1}^{n} \left(\sum_{j=1}^{p+1} \frac{\partial \boldsymbol{V}^{\top}}{\partial z_{ij}} \boldsymbol{e}_{j} - \boldsymbol{V}^{\top} \boldsymbol{Z}^{\top} \boldsymbol{e}_{i} \right) \left(\sum_{j=1}^{p+1} \frac{\partial \boldsymbol{e}_{j}^{\top} \boldsymbol{V}}{\partial z_{ij}} - \boldsymbol{e}_{i}^{\top} \boldsymbol{Z} \boldsymbol{V} \right) = \sqrt{n} \boldsymbol{Q}_{2} - \operatorname{Rem}_{2},$$

where Rem_2 is a $T \times T$ matrix satisfying $\mathbb{E}[\|\operatorname{Rem}_2\|_{\mathrm{F}}] \leq \sqrt{n}C(\zeta, T, \gamma)\operatorname{var}(y_1)$.

Lemma F.7 (Proof is given on Page 53). Under the same conditions of Proposition F.2, for $\mathbf{V} = [-\mathbf{H}^{\top}, \sigma \mathbf{1}_T]^{\top}$, we have

$$2(1+2\sqrt{n}) \left(\mathbb{E}[\|\boldsymbol{V}\|_{\mathrm{F}}^{4}]^{1/2} + \mathbb{E}[\|\boldsymbol{V}\|_{\partial}^{4}]^{1/2} \right) \leq \sqrt{n} C(\zeta, T, \gamma) \operatorname{var}(y_{1}).$$

Now we are ready to prove Proposition F.2. By the triangle inequality, we have

$$\begin{split} & \mathbb{E}[\|\sqrt{n}\boldsymbol{Q}_{2}\|_{\mathrm{F}}] \\ \leq & \mathbb{E}[\|\mathrm{Rem}_{2}\|_{\mathrm{F}}] + 2(1+2\sqrt{n}) \big(\mathbb{E}[\|\boldsymbol{V}\|_{\mathrm{F}}^{4}]^{1/2} + \mathbb{E}[\|\boldsymbol{V}\|_{\partial}^{4}]^{1/2} \big) \qquad \text{by (F.13) and (F.14)} \\ \leq & \sqrt{n}C(\zeta,T,\gamma) \mathrm{var}(y_{1}) \qquad \text{by Lemmas F.6 and F.7.} \end{split}$$

This finishes the proof of Proposition F.2.

F.3. Proofs of supporting lemmas

Proof of Lemma F.3. First, by definitions of U, Z, V in Lemma F.3, we have

$$\boldsymbol{U}^{\top}\boldsymbol{Z}\boldsymbol{V}=\boldsymbol{F}^{\top}\boldsymbol{F}.$$

Next, by product rule and spliting the summation over j into two parts: $j \in [p]$ and j = p + 1, we have

(F.15)

$$\sum_{j=1}^{p+1} \sum_{i=1}^{n} \frac{\partial}{\partial z_{ij}} \left(\boldsymbol{U}^{\top} \boldsymbol{e}_{i} \boldsymbol{e}_{j}^{\top} \boldsymbol{V} \right)$$

$$= \sum_{j=1}^{p+1} \sum_{i=1}^{n} \left(\frac{\partial \boldsymbol{U}^{\top}}{\partial z_{ij}} \boldsymbol{e}_{i} \boldsymbol{e}_{j}^{\top} \boldsymbol{V} + \boldsymbol{U}^{\top} \boldsymbol{e}_{i} \boldsymbol{e}_{j}^{\top} \frac{\partial \boldsymbol{V}}{\partial z_{ij}} \right)$$

$$= \sum_{j=1}^{p} \sum_{i=1}^{n} \left(\frac{\partial \boldsymbol{F}^{\top}}{\partial x_{ij}} \boldsymbol{e}_{i} \boldsymbol{e}_{j}^{\top} (-\boldsymbol{H}) \right) + \sum_{i=1}^{n} \frac{\partial \boldsymbol{F}^{\top}}{\partial \epsilon_{i} / \sigma} \boldsymbol{e}_{i} \sigma \mathbf{1}_{T}^{\top} - \sum_{i=1}^{n} \sum_{j=1}^{p} \boldsymbol{F}^{\top} \boldsymbol{e}_{i} \boldsymbol{e}_{j}^{\top} \frac{\partial \boldsymbol{H}}{\partial x_{ij}}$$

$$= -\sum_{j=1}^{p} \sum_{i=1}^{n} \left(\frac{\partial \boldsymbol{F}^{\top}}{\partial x_{ij}} \boldsymbol{e}_{i} \boldsymbol{e}_{j}^{\top} \boldsymbol{H} \right) + \sigma^{2} \sum_{i=1}^{n} \frac{\partial \boldsymbol{F}^{\top}}{\partial \epsilon_{i}} \boldsymbol{e}_{i} \mathbf{1}_{T}^{\top} - \sum_{i=1}^{n} \sum_{j=1}^{p} \boldsymbol{F}^{\top} \boldsymbol{e}_{i} \boldsymbol{e}_{j}^{\top} \frac{\partial \boldsymbol{H}}{\partial x_{ij}}.$$

For the first term in (F.15), we have its transpose is

$$-\boldsymbol{H}^{\top}\sum_{j=1}^{p}\sum_{i=1}^{n}\boldsymbol{e}_{j}\boldsymbol{e}_{i}^{\top}\frac{\partial \boldsymbol{F}}{\partial x_{ij}}=\boldsymbol{H}^{\top}\boldsymbol{H}(n\boldsymbol{I}_{T}-\widehat{\mathbf{A}})^{\top}-\operatorname{Rem}_{1,1}$$

by (F.16). For the second term in (F.15), we have its transpose is

$$\sigma^{2} \mathbf{1}_{T} \sum_{i=1}^{n} \mathbf{e}_{i}^{\top} \frac{\partial \mathbf{F}}{\partial \epsilon_{i}}$$

$$= \sigma^{2} \mathbf{1}_{T} \sum_{i=1}^{n} \sum_{t=1}^{T} \mathbf{e}_{i}^{\top} \frac{\partial \mathbf{F} \mathbf{e}_{t}}{\partial \epsilon_{i}} \mathbf{e}_{t}^{\top}$$

$$= \sigma^{2} \mathbf{1}_{T} \sum_{t=1}^{T} \operatorname{Tr} \left(\frac{\partial \mathbf{F} \mathbf{e}_{t}}{\partial \epsilon} \right) \mathbf{e}_{t}^{\top}$$

$$= \sigma^{2} \mathbf{1}_{T} \sum_{t=1}^{T} \mathbf{e}_{t}^{\top} (n \mathbf{I}_{T} - \widehat{\mathbf{A}}) \mathbf{1}_{T} \mathbf{e}_{t}^{\top}$$
by (C.8)
$$= \sigma^{2} \mathbf{1}_{T} \mathbf{1}_{T}^{\top} (n \mathbf{I}_{T} - \widehat{\mathbf{A}})^{\top}$$

$$= \mathbf{S} (n \mathbf{I}_{T} - \widehat{\mathbf{A}})^{\top}.$$

For the third term in (F.15), we have by (F.17),

$$\sum_{i=1}^{n} \sum_{j=1}^{p} \boldsymbol{F}^{\top} \boldsymbol{e}_{i} \boldsymbol{e}_{j}^{\top} \frac{\partial \boldsymbol{H}}{\partial x_{ij}} = \boldsymbol{F}^{\top} \boldsymbol{F} \widehat{\boldsymbol{C}}^{\top} / n + \operatorname{Rem}_{1,2}.$$

Combining the three terms in (F.15), we have

$$(\mathbf{F}.15) = (n\mathbf{I}_T - \widehat{\mathbf{A}})(\mathbf{H}^\top \mathbf{H} + \mathbf{S}) - \mathbf{F}^\top \mathbf{F} \widehat{\mathbf{C}}^\top / n - \operatorname{Rem}_{1,1}^\top - \operatorname{Rem}_{1,2}^\top.$$

It follows that

$$\boldsymbol{U}^{\top} \boldsymbol{Z} \boldsymbol{V} - \sum_{j=1}^{p+1} \sum_{i=1}^{n} \frac{\partial}{\partial z_{ij}} \left(\boldsymbol{U}^{\top} \boldsymbol{e}_{i} \boldsymbol{e}_{j}^{\top} \boldsymbol{V} \right)$$

= $\boldsymbol{F}^{\top} \boldsymbol{F} (\boldsymbol{I}_{T} + \hat{\boldsymbol{C}}/n)^{\top} - (n \boldsymbol{I}_{T} - \hat{\boldsymbol{A}}) (\boldsymbol{H}^{\top} \boldsymbol{H} + \boldsymbol{S}) + (\operatorname{Rem}_{1,1}^{\top} + \operatorname{Rem}_{1,2})$
= $\sqrt{n} \boldsymbol{Q}_{1} + \operatorname{Rem}_{1},$

where $\operatorname{Rem}_1 = (\operatorname{Rem}_{1,1}^\top + \operatorname{Rem}_{1,2})$, and $\operatorname{Rem}_{1,1}$ and $\operatorname{Rem}_{1,2}$ are defined in Lemma F.8. It remains to bound $\mathbb{E}[\|\operatorname{Rem}_1\|_F^2]$. By the triangle inequality,

$$\mathbb{E}[\|\operatorname{Rem}_{1}\|_{\mathrm{F}}^{2}] \leq 2\mathbb{E}[\|\operatorname{Rem}_{1,1}\|_{\mathrm{F}}^{2}] + 2\mathbb{E}[\|\operatorname{Rem}_{1,2}\|_{\mathrm{F}}^{2}]$$
$$\leq nC(\zeta, T, \gamma)\operatorname{var}(y_{1})^{2}$$

This concludes the proof of Lemma F.3.

Proof of Lemma F.4. Let us recall (F.12) here for convenience:

$$(F.12) = \mathbb{E}\Big[\|\boldsymbol{U}\|_{F}^{2}\|\boldsymbol{V}\|_{F}^{2}\Big] + 2\mathbb{E}\Big[\|\boldsymbol{V}\|_{F}^{2}\sum_{i=1}^{n}\sum_{j=1}^{p+1}\left\|\frac{\partial\boldsymbol{U}}{\partial z_{ij}}\right\|_{F}^{2}\Big] + 2\mathbb{E}\Big[\|\boldsymbol{U}\|_{F}^{2}\sum_{i=1}^{n}\sum_{j=1}^{p+1}\left\|\frac{\partial\boldsymbol{V}}{\partial z_{ij}}\right\|_{F}^{2}\Big].$$

For the first term in (F.12), since $\|\boldsymbol{V}\|_{\rm F}^2 = \|\boldsymbol{H}\|_{\rm F}^2 + T\sigma^2$, we have

$$\begin{split} \mathbb{E}[\|\boldsymbol{U}\|_{\rm F}^2 \|\boldsymbol{V}\|_{\rm F}^2] = & \mathbb{E}[\|\boldsymbol{F}\|_{\rm F}^2 (\|\boldsymbol{H}\|_{\rm F}^2 + T\sigma^2)] \\ \leq & \mathbb{E}[\|\boldsymbol{F}\|_{\rm F}^4]^{1/2} \mathbb{E}[\|\boldsymbol{H}\|_{\rm F}^4 + T^2\sigma^4]^{1/2} \\ \leq & nC(\zeta, T, \gamma) \operatorname{var}(y_1)^2 \end{split}$$

For the second term in (F.12), we have

$$\begin{split} & \mathbb{E}\Big[\|\boldsymbol{V}\|_{\mathrm{F}}^{2}\sum_{i=1}^{n}\sum_{j=1}^{p+1} \left\|\frac{\partial \boldsymbol{U}}{\partial z_{ij}}\right\|_{\mathrm{F}}^{2}\Big] \\ =& \mathbb{E}\Big[(\|\boldsymbol{H}\|_{\mathrm{F}}^{2}+T\sigma^{2})\Big(\sum_{i=1}^{n}\sum_{j=1}^{p}\left\|\frac{\partial \boldsymbol{F}}{\partial x_{ij}}\right\|_{\mathrm{F}}^{2}+\sigma^{2}\sum_{i=1}^{n}\left\|\frac{\partial \boldsymbol{F}}{\partial \epsilon_{i}}\right\|_{\mathrm{F}}^{2}\Big)\Big] \\ =& \mathbb{E}\Big[(\|\boldsymbol{H}\|_{\mathrm{F}}^{2}+T\sigma^{2})\Big(\left\|\frac{\partial\operatorname{vec}(\boldsymbol{F})}{\partial\operatorname{vec}(\boldsymbol{X})}\right\|_{\mathrm{F}}^{2}+\sigma^{2}\left\|\frac{\partial\operatorname{vec}(\boldsymbol{F})}{\partial\varepsilon}\right\|_{\mathrm{F}}^{2}\Big)\Big] \\ \leq& \mathbb{E}\Big[(\|\boldsymbol{H}\|_{\mathrm{F}}^{2}+T\sigma^{2})\Big(\left\|\frac{\partial\operatorname{vec}(\boldsymbol{F})}{\partial\operatorname{vec}(\boldsymbol{X})}\right\|_{\mathrm{F}}^{2}+\sigma^{2}\left\|\frac{\partial\operatorname{vec}(\boldsymbol{F})}{\partial\varepsilon}\right\|_{\mathrm{F}}^{2}\Big)\Big] \\ \leq& C(\zeta,T)\mathbb{E}[(\|\boldsymbol{H}\|_{\mathrm{F}}^{2}+T\sigma^{2})(1+\|\boldsymbol{X}\|_{\mathrm{op}}^{2}/n)^{2T}(\|\boldsymbol{H}\|_{\mathrm{F}}^{2}+\gamma\|\boldsymbol{F}\|_{\mathrm{F}}^{2}/n)] \\ & +n\sigma^{2}C(\zeta,T)\mathbb{E}[(\|\boldsymbol{H}\|_{\mathrm{F}}^{2}+T\sigma^{2})(1+\|\boldsymbol{X}\|_{\mathrm{op}}^{2}/n)^{2T}] \\ \leq& nC(\zeta,T,\gamma)\operatorname{var}(y_{1})^{2} \end{split}$$

For the third term in (F.12), since $\boldsymbol{V} = \begin{bmatrix} -\boldsymbol{H} \\ \sigma \boldsymbol{1}_T^\top \end{bmatrix}$, we have

by Lemma E.11

by (F.20).

by C. Schwarz by Lemma E.10.

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by (E.7) by Lemmas E.8 and E.10.

13) 8) nmas E.8 and E.10.

= 0

Combining the above three bounds gives the desired bound for (F.12). This concludes the proof. Lemma F.8 (Proof is given on Page 53). Under the same conditions of Proposition F.1, we have

(F.16)
$$\boldsymbol{H}^{\top} \sum_{i=1}^{n} \sum_{j=1}^{p} \boldsymbol{e}_{j} \boldsymbol{e}_{i}^{\top} \frac{\partial \boldsymbol{F}}{\partial x_{ij}} = -\boldsymbol{H}^{\top} \boldsymbol{H} (n\boldsymbol{I}_{T} - \widehat{\boldsymbol{A}}^{\top}) + \operatorname{Rem}_{1,1},$$

(F.17)
$$\sum_{i=1}^{n} \sum_{j=1}^{p} \boldsymbol{F}^{\top} \boldsymbol{e}_{i} \boldsymbol{e}_{j}^{\top} \frac{\partial \boldsymbol{H}}{\partial x_{ij}} = \boldsymbol{F}^{\top} \boldsymbol{F} \widehat{\boldsymbol{C}}^{\top} / n + \operatorname{Rem}_{1,2},$$

where

(F.21)

(F.18)
$$\operatorname{Rem}_{1,1} = \boldsymbol{H}^{\top} \sum_{i=1}^{n} \sum_{j=1}^{p} \boldsymbol{e}_{j} \sum_{t} \Delta_{ij}^{it} \boldsymbol{e}_{t}^{\top},$$

(F.19)
$$\operatorname{Rem}_{1,2} = -n^{-1} \sum_{i=1}^{n} \sum_{j=1}^{p} \sum_{t=1}^{T} \boldsymbol{F}^{\top} \boldsymbol{e}_{i} \boldsymbol{e}_{j}^{\top} (\boldsymbol{e}_{t}^{\top} \otimes \boldsymbol{I}_{p}) \mathcal{M}^{-1} \mathcal{D} ((\boldsymbol{H}^{\top} \boldsymbol{e}_{j}) \otimes (\boldsymbol{X}^{\top} \boldsymbol{e}_{i})) \boldsymbol{e}_{t}^{\top}.$$

In addition, we have

(F.20)
$$\mathbb{E}[\|\operatorname{Rem}_{1,1}\|_{\mathrm{F}}^2] \leq nC(\zeta, T, \gamma)\operatorname{var}(y_1)^2, \\ \mathbb{E}[\|\operatorname{Rem}_{1,2}\|_{\mathrm{F}}^2] \leq nC(\zeta, T, \gamma)\operatorname{var}(y_1)^2.$$

Proof of Lemma F.5. For each $j \in [p]$, let $\mathbb{E}_j[\cdot]$ denote the conditional expectation $\mathbb{E}[\cdot|\{\mathbf{Z}\mathbf{e}_k, k \neq j\}]$. The left-hand side of the desired inequality can be rewritten as

$$\mathbb{E}\Big[\big\|p\boldsymbol{U}^{\top}\boldsymbol{V}-\sum_{j=1}^{p}(\mathbb{E}_{j}[\boldsymbol{U}]^{\top}\boldsymbol{Z}-\boldsymbol{L}^{\top})\boldsymbol{e}_{j}\boldsymbol{e}_{j}^{\top}(\boldsymbol{Z}^{\top}\mathbb{E}_{j}[\boldsymbol{V}]-\hat{\boldsymbol{L}})\big\|_{\mathrm{F}}\Big]$$

with $\boldsymbol{L} \in \mathbb{R}^{p \times T}$ defined by $\boldsymbol{L}^{\top} \boldsymbol{e}_j = \mathbb{E}_j [\boldsymbol{U}]^{\top} \boldsymbol{Z} \boldsymbol{e}_j - \boldsymbol{U}^{\top} \boldsymbol{Z} \boldsymbol{e}_j + \sum_{i=1}^n \partial_{ij} \boldsymbol{U}^{\top} \boldsymbol{e}_i$ and $\hat{\boldsymbol{L}}$ defined similarly with \boldsymbol{U} replaced by \boldsymbol{V} . We develop the terms in the sum over j as follows:

$$p \boldsymbol{U}^{\top} \boldsymbol{V} - \sum_{j} (\mathbb{E}_{j} [\boldsymbol{U}]^{\top} \boldsymbol{Z} - \boldsymbol{L}^{\top}) \boldsymbol{e}_{j} \boldsymbol{e}_{j}^{\top} (\boldsymbol{Z}^{\top} \mathbb{E}_{j} [\boldsymbol{V}] - \hat{\boldsymbol{L}})$$
$$= \sum_{j} \left(\boldsymbol{U}^{\top} \boldsymbol{V} - \mathbb{E}_{j} [\boldsymbol{U}]^{\top} \mathbb{E}_{j} [\boldsymbol{V}] \right)$$

(F.22)
$$+ \sum_{j} \Big(\mathbb{E}_{j}[\boldsymbol{U}]^{\top} \mathbb{E}_{j}[\boldsymbol{V}] - \mathbb{E}_{j}[\boldsymbol{U}]^{\top} \boldsymbol{Z} \boldsymbol{e}_{j} \boldsymbol{e}_{j}^{\top} \boldsymbol{Z}^{\top} \mathbb{E}_{j}[\boldsymbol{V}] \Big)$$

(F.23)
$$- \boldsymbol{L}^{\top} \hat{\boldsymbol{L}}$$

(F.24)
$$+ \sum_{j} \left(\mathbb{E}_{j} [\boldsymbol{U}]^{\top} \boldsymbol{Z} \boldsymbol{e}_{j} \boldsymbol{e}_{j}^{\top} \hat{\boldsymbol{L}} \right) + \left(\boldsymbol{L}^{\top} \boldsymbol{e}_{j} \boldsymbol{e}_{j}^{\top} \boldsymbol{Z}^{\top} \mathbb{E}_{j} [\boldsymbol{V}] \right).$$

The following proof is dedicated to bounding the expectation of Frobenius norm of each term in (F.21)-(F.24). We now bound (F.23), (F.24), (F.21), and (F.22) in order.

For (F.23). We have by the Cauchy-Schwarz inequality $\mathbb{E}[\|\boldsymbol{L}^{\top}\hat{\boldsymbol{L}}\|_{\mathrm{F}}] \leq \mathbb{E}[\|\boldsymbol{L}\|_{\mathrm{F}}^{2}]^{\frac{1}{2}}\mathbb{E}[\|\hat{\boldsymbol{L}}\|_{\mathrm{F}}^{2}]^{\frac{1}{2}}$. For a fixed $j \in [p]$ and $t \in [T]$,

$$\begin{split} \mathbb{E}[(\boldsymbol{e}_{j}^{\top}\boldsymbol{L}\boldsymbol{e}_{t})^{2}] &\leq \sum_{i=1}^{n} \mathbb{E}[(\boldsymbol{e}_{i}^{\top}(\mathbb{E}_{j}[\boldsymbol{U}]-\boldsymbol{U})\boldsymbol{e}_{t})^{2}] + \mathbb{E}\sum_{i=1}^{n}\sum_{l=1}^{n} \left(\frac{\boldsymbol{e}_{i}^{\top}\partial\boldsymbol{U}\boldsymbol{e}_{t}}{\partial z_{lj}}\right)^{2} \\ &\leq 2\mathbb{E}\sum_{i=1}^{n}\sum_{l=1}^{n} \left(\frac{\boldsymbol{e}_{i}^{\top}\partial\boldsymbol{U}\boldsymbol{e}_{t}}{\partial z_{lj}}\right)^{2}, \end{split}$$

where the two inequalities are due to the second-order stein inequality in Bellec and Zhang (2021), and Gaussian-Poincaré inequality in (Boucheron et al., 2013, Theorem 3.20), respectively. Summing over $j \in [p]$ and $t \in [T]$ we obtain $\mathbb{E}[\|\boldsymbol{L}\|_{\mathrm{F}}^2] \leq 2\mathbb{E}\sum_{lj} \|\partial_{lj}\boldsymbol{U}\|_{\mathrm{F}}^2 = 2\mathbb{E}[\|\boldsymbol{U}\|_{\partial}^2]$. Combined with the same bound for $\hat{\boldsymbol{L}}$, we obtain

$$\mathbb{E}[\|(\mathbf{F}.23)\|_{\mathbf{F}}] \le 2\mathbb{E}[\|\boldsymbol{U}\|_{\partial}^{2}]^{1/2}\mathbb{E}[\|\boldsymbol{V}\|_{\partial}^{2}]^{1/2}$$

For (F.24). We focus on the first term in (F.24); the similar bound applies to the second term by exchanging the role of U and V. For the first term, we have

$$\begin{split} \mathbb{E}\Big[\|\sum_{j} \mathbb{E}_{j}[\boldsymbol{U}]^{\top} \boldsymbol{Z} \boldsymbol{e}_{j} \boldsymbol{e}_{j}^{\top} \hat{\boldsymbol{L}}\|_{\mathrm{F}}\Big] &\leq \sum_{j} \mathbb{E}\Big[\|\mathbb{E}_{j}[\boldsymbol{U}]^{\top} \boldsymbol{Z} \boldsymbol{e}_{j}\|_{2} \|\boldsymbol{e}_{j}^{\top} \hat{\boldsymbol{L}}\|_{2}\Big] \\ &\leq \mathbb{E}[\sum_{j} \|\mathbb{E}_{j}[\boldsymbol{U}]^{\top} \boldsymbol{Z} \boldsymbol{e}_{j}\|_{2}^{2}]^{\frac{1}{2}} \mathbb{E}[\sum_{j} \|\boldsymbol{e}_{j}^{\top} \hat{\boldsymbol{L}}\|_{2}^{2}]^{\frac{1}{2}} \\ &\leq (p\mathbb{E}[\|\boldsymbol{U}\|_{\mathrm{F}}^{2}])^{\frac{1}{2}} \mathbb{E}[\|\hat{\boldsymbol{L}}\|_{\mathrm{F}}^{2}]^{\frac{1}{2}} \\ &\leq (p\mathbb{E}[\|\boldsymbol{U}\|_{\mathrm{F}}^{2}])^{\frac{1}{2}} \sqrt{2} \mathbb{E}[\|\boldsymbol{V}\|_{\partial}^{2}]^{1/2}, \end{split}$$

where we used that $\|\boldsymbol{a}\boldsymbol{b}^{\top}\|_{\mathrm{F}} = \|\boldsymbol{a}\|_{2}\|\boldsymbol{b}\|_{2}$ for two vectors $\boldsymbol{a}, \boldsymbol{b}$, the Cauchy-Schwarz inequality, $\mathbb{E}[\|\boldsymbol{A}\boldsymbol{z}_{j}\|_{2}^{2}|\boldsymbol{A}] = \|\boldsymbol{A}\|_{\mathrm{F}}^{2}$ if matrix \boldsymbol{A} is independent of $\boldsymbol{z}_{j} \sim \mathsf{N}(0, \boldsymbol{I}_{n})$ (set $\boldsymbol{z}_{j} = \boldsymbol{Z}\boldsymbol{e}_{j}$), and Jensen's inequality. By symmetry of the two terms in (F.24), we have

$$\mathbb{E}\|(\mathbf{F}.24)\|_{\mathbf{F}} \le \sqrt{2p} \mathbb{E}[\|\boldsymbol{U}\|_{\mathbf{F}}^2]^{\frac{1}{2}} \mathbb{E}[\|\boldsymbol{V}\|_{\partial}^2]^{1/2} + \sqrt{2p} \mathbb{E}[\|\boldsymbol{V}\|_{\mathbf{F}}^2]^{\frac{1}{2}} \mathbb{E}[\|\boldsymbol{U}\|_{\partial}^2]^{1/2}.$$

For (F.21). We decompose (F.21) as $\sum_{j} U^{\top} (V - \mathbb{E}_{j}[V]) + \sum_{j} (U - \mathbb{E}_{j}[U])^{\top} \mathbb{E}_{j}[V]$. We focus on the left term; similar bound will apply to the second term by exchanging the roles of V and U. For the first term, we have by the submultiplicativity of the Frobenius norm and the Cauchy-Schwarz inequality

$$egin{aligned} \mathbb{E}[\|oldsymbol{U}^{ op}\sum_j(oldsymbol{V}-\mathbb{E}_j[oldsymbol{V}])\|_{ ext{F}}] &\leq \mathbb{E}[p\|oldsymbol{U}\|_{ ext{F}}^2]^{rac{1}{2}}\mathbb{E}[\sum_j\|oldsymbol{V}-\mathbb{E}_j[oldsymbol{V}]\|_{ ext{F}}^2]^{rac{1}{2}} & \leq \mathbb{E}[p\|oldsymbol{U}\|_{ ext{F}}^2]^{rac{1}{2}}\mathbb{E}[\sum_j\|oldsymbol{V}-\mathbb{E}_j[oldsymbol{V}]\|_{ ext{F}}^2]^{rac{1}{2}} \end{aligned}$$

By the Gaussian Poincaré inequality applied p times, $\mathbb{E}[\sum_{j} \|\boldsymbol{V} - \mathbb{E}_{j}[\boldsymbol{V}]\|_{\mathrm{F}}^{2}] \leq \mathbb{E}[\|\boldsymbol{V}\|_{\partial}^{2}]$, so that the previous display is bounded from above by $\sqrt{p}\mathbb{E}[\|\boldsymbol{U}\|_{\mathrm{F}}^{2}]^{\frac{1}{2}}\mathbb{E}[\|\boldsymbol{V}\|_{\partial}^{2}]^{\frac{1}{2}}$. Using the same argument, we have

$$\mathbb{E}[\|\sum_{j} (\boldsymbol{U} - \mathbb{E}_{j}[\boldsymbol{U}])^{\top} \mathbb{E}_{j}[\boldsymbol{V}]\|_{\mathrm{F}}] \leq \sqrt{p} \mathbb{E}[\|\boldsymbol{V}\|_{\mathrm{F}}^{2}]^{\frac{1}{2}} \mathbb{E}[\|\boldsymbol{U}\|_{\partial}^{2}]^{\frac{1}{2}}.$$

Hence,

$$\mathbb{E}[\|(\mathbf{F}.21)\|_{\mathbf{F}}] \le \sqrt{p} \mathbb{E}[\|\boldsymbol{U}\|_{\mathbf{F}}^{2}]^{1/2} \mathbb{E}[\|\boldsymbol{V}\|_{\partial}^{2}]^{\frac{1}{2}} + \sqrt{p} \mathbb{E}[\|\boldsymbol{V}\|_{\mathbf{F}}^{2}]^{1/2} \mathbb{E}[\|\boldsymbol{U}\|_{\partial}^{2}]^{\frac{1}{2}}$$

For (F.22). We first use $\mathbb{E}[\|(F.22)\|_F] \leq \mathbb{E}[\|(F.22)\|_F^2]^{\frac{1}{2}}$ by Jensen's inequality and now proceed to bound $\mathbb{E}\|(F.22)\|_F^2$. We have

$$\|(\mathbf{F}.22)\|_{\mathbf{F}}^2 = \|\sum_j \mathbb{E}_j[\boldsymbol{U}]^\top \mathbb{E}_j[\boldsymbol{V}] - \mathbb{E}_j[\boldsymbol{U}]^\top \boldsymbol{Z} \boldsymbol{e}_j \boldsymbol{e}_j^\top \boldsymbol{Z}^\top \mathbb{E}_j[\boldsymbol{V}]\|_{\mathbf{F}}^2 = \sum_{j,k} \operatorname{Tr}[\boldsymbol{M}_j^\top \boldsymbol{M}_k],$$

where $M_j = \mathbb{E}_j[U]^\top \mathbb{E}_j[V] - \mathbb{E}_j[U]^\top Z e_j e_j^\top Z^\top \mathbb{E}_j[V]$. For the summation $\sum_{j,k}$, we split it into two cases $\sum_{j=k}$ and $\sum_{j\neq k}$. We first bound $\mathbb{E}[\sum_j ||M_j||_F^2]$. Since the variance of $a^\top b - a^\top g g^\top b$ for standard normal $g \sim \mathsf{N}(0, I_p)$ is $2||(ab^\top + ba^\top)/2||_F^2 \leq 2||a||_2^2||b||_2^2$, applying this variance bound on each pair of coordinates $(t, t') \in [T] \times [T]$ gives $\sum_j ||M_j||_F^2 \leq \sum_j 2||\mathbb{E}_j[U]||_F^2||\mathbb{E}_j[V]||_F^2$. Hence, using the Cauchy-Schwarz inequality and Jensen's inequality, we have

$$\mathbb{E}[\sum_{j} \|\boldsymbol{M}_{j}\|_{\mathrm{F}}^{2}] \leq 2 \sum_{j} \mathbb{E}[\|\mathbb{E}_{j}[\boldsymbol{U}]\|_{\mathrm{F}}^{2} \|\mathbb{E}_{j}[\boldsymbol{V}]\|_{\mathrm{F}}^{2}] \leq 2p \mathbb{E}[\|\boldsymbol{U}\|_{\mathrm{F}}^{4}]^{1/2} \mathbb{E}[\|\boldsymbol{V}\|_{\mathrm{F}}^{4}]^{1/2}$$

We now bound $\sum_{j \neq k} \operatorname{Tr}[\boldsymbol{M}_j^\top \boldsymbol{M}_k]$. Setting $\boldsymbol{z}_j = \boldsymbol{Z} \boldsymbol{e}_j \sim \mathsf{N}(0, \boldsymbol{I}_n)$ for every $j \in [p]$, we will use many times the identity

(F.25)
$$\mathbb{E}[(\boldsymbol{z}_j^{\top} f(\boldsymbol{Z}) - \sum_i \partial_{ij} f(\boldsymbol{Z})^{\top} \boldsymbol{e}_i) g(\boldsymbol{Z}) = \mathbb{E}[\sum_i f(\boldsymbol{Z})^{\top} \boldsymbol{e}_i \partial_{ij} g(\boldsymbol{Z})]$$

which follows from Stein's formula for $f : \mathbb{R}^{n \times p} \to \mathbb{R}^n$ and $g : \mathbb{R}^{n \times p} \to \mathbb{R}$. With $f^{tt'}(\mathbf{Z}) = (\mathbf{z}_j^\top \mathbb{E}_j[\mathbf{U}]\mathbf{e}_{t'})\mathbb{E}_j[\mathbf{V}]\mathbf{e}_t$ and $g^{tt'}(\mathbf{Z}) = \mathbf{e}_{t'}^\top \mathbf{M}_k \mathbf{e}_t$, we find

$$\mathbb{E} \operatorname{Tr}[\boldsymbol{M}_{j}^{\top}\boldsymbol{M}_{k}] = \mathbb{E} \operatorname{Tr}[\boldsymbol{M}_{j}^{\top}\sum_{t'} \boldsymbol{e}_{t'} \boldsymbol{e}_{t'}^{\top}\boldsymbol{M}_{k}] = \mathbb{E}[\sum_{tt'} \boldsymbol{e}_{t}^{\top}\boldsymbol{M}_{j}^{\top} \boldsymbol{e}_{t'} \boldsymbol{e}_{t'}^{\top}\boldsymbol{M}_{k} \boldsymbol{e}_{t}]$$
$$= \mathbb{E} \sum_{tt'} \left(\boldsymbol{z}_{j}^{\top} f^{tt'}(\boldsymbol{Z}) - \sum_{i} \boldsymbol{e}_{i}^{\top} \partial_{ij} f^{tt'}(\boldsymbol{Z})\right) g^{tt'}(\boldsymbol{Z})$$
$$= \mathbb{E} \sum_{tt'} \sum_{i} \boldsymbol{e}_{i}^{\top} f^{tt'}(\boldsymbol{Z}) \partial_{ij} g^{tt'}(\boldsymbol{Z}).$$

where $g_{tt'}(\boldsymbol{Z}) = (\boldsymbol{e}_t^\top \mathbb{E}_k \boldsymbol{V}^\top \mathbb{E}_k \boldsymbol{V} \boldsymbol{e}_t' - \boldsymbol{e}_t^\top \mathbb{E}_k \boldsymbol{U}^\top \boldsymbol{z}_k \boldsymbol{z}_k^\top \mathbb{E}_k \boldsymbol{V} \boldsymbol{e}_t')$ and

$$\partial_{ij}g_{tt'} = \partial_{ij}\boldsymbol{e}_{t'}^{\top}\boldsymbol{M}_{k}\boldsymbol{e}_{t} = \boldsymbol{e}_{t'}^{\top}\partial_{ij}[\mathbb{E}_{k}\boldsymbol{U}^{\top}\mathbb{E}_{k}\boldsymbol{V}]\boldsymbol{e}_{t} - \boldsymbol{z}_{k}^{\top}\partial_{ij}[\mathbb{E}_{k}\boldsymbol{U}\boldsymbol{e}_{t'}\boldsymbol{e}_{t}^{\top}\mathbb{E}_{k}\boldsymbol{U}^{\top}]\boldsymbol{z}_{k}.$$

Now define $\tilde{f}^{tt'}(\boldsymbol{Z}) = \partial_{ij}[\mathbb{E}_k \boldsymbol{U} \boldsymbol{e}_{t'} \boldsymbol{e}_t^\top \mathbb{E}_k \boldsymbol{U}^\top] \boldsymbol{z}_k$ and $\tilde{g}^{tt'}(\boldsymbol{Z}) = \sum_i \boldsymbol{e}_i^\top f^{tt'}(\boldsymbol{Z})$. By definition of $\tilde{f}^{tt'}(\boldsymbol{Z})$, the previous display is equal to $\boldsymbol{z}_k^\top \tilde{f}^{tt'}(\boldsymbol{Z}) - \sum_l \partial_{lk} \boldsymbol{e}_l^\top \tilde{f}^{tt'}(\boldsymbol{Z})$. We apply (F.25) again with respect to \boldsymbol{z}_k , so that

$$\begin{split} \mathbb{E} \operatorname{Tr}[\boldsymbol{M}_{j}^{\top}\boldsymbol{M}_{k}] &= \sum_{il,tt'} \boldsymbol{e}_{i}^{\top} \partial_{lk} [f^{tt'}(\boldsymbol{Z})] \boldsymbol{e}_{l}^{\top} \tilde{f}^{tt'}(\boldsymbol{Z}) \\ &= \sum_{il,tt'} \Big(\boldsymbol{e}_{i}^{\top} \partial_{lk} \Big[\mathbb{E}_{j}[\boldsymbol{V}] \boldsymbol{e}_{t} \boldsymbol{e}_{t'}^{\top} \mathbb{E}_{j}[\boldsymbol{U}]^{\top} \Big] \boldsymbol{z}_{j} \Big) \Big(\boldsymbol{e}_{l}^{\top} \partial_{ij} \Big[\mathbb{E}_{k}[\boldsymbol{U}] \boldsymbol{e}_{t'} \boldsymbol{e}_{t}^{\top} \mathbb{E}_{k}[\boldsymbol{V}]^{\top} \Big] \boldsymbol{z}_{k} \Big). \end{split}$$

To remove the indices t, t', we rewrite the above using $\sum_t e_t e_t^{\top} = I_T$ and $\sum_{t'} e_{t'} e_{t'}^{\top} = I_T$ so that it equals

$$\mathbb{E}\sum_{il} \operatorname{Tr} \Big\{ \partial_{lk} \Big[\mathbb{E}_{j}[\boldsymbol{U}]^{\top} \boldsymbol{z}_{j} \boldsymbol{e}_{i}^{\top} \mathbb{E}_{j}[\boldsymbol{V}] \Big] \partial_{ij} \Big[\mathbb{E}_{k}[\boldsymbol{V}]^{\top} \boldsymbol{z}_{k} \boldsymbol{e}_{l}^{\top} \mathbb{E}_{k}[\boldsymbol{U}] \Big] \Big\}$$

Summing over j, k, using $\operatorname{Tr}[\mathbf{A}^{\top}\mathbf{B}] \leq \|\mathbf{A}\|_{\mathrm{F}} \|\mathbf{B}\|_{\mathrm{F}}$ and the Cauchy-Schwarz inequality, the above is bounded from above by

(F.26)
$$\left\{\mathbb{E}\sum_{jk,il} \left\|\partial_{lk} \left[\mathbb{E}_{j}[\boldsymbol{U}]^{\top} \boldsymbol{z}_{j} \boldsymbol{e}_{i}^{\top} \mathbb{E}_{j}[\boldsymbol{V}]\right]\right\|_{\mathrm{F}}^{2}\right\}^{\frac{1}{2}} \left\{\mathbb{E}\sum_{jk,il} \left\|\partial_{ij} \left[\mathbb{E}_{k}[\boldsymbol{V}]^{\top} \boldsymbol{z}_{k} \boldsymbol{e}_{l}^{\top} \mathbb{E}_{k}[\boldsymbol{U}]\right]\right\|_{\mathrm{F}}^{2}\right\}^{\frac{1}{2}}$$

At this point the two factors are symmetric, with (V, U) in the left factor replaced with (U, V) on the right factor. We focus on the left factor; similar bound will apply to the right one by exchanging the roles of V and U. If z_j is independent of matrices $A^{(q)}$, then $\mathbb{E}_j[\|\sum_{q=1}^n (e_q^\top z_j)A^{(q)}\|_F^2] = \sum_{q=1}^n \|A^{(q)}\|_F^2$. So that with $A^{(q)} = \partial_{lk}[\mathbb{E}_j[U]^\top e_q e_i^\top \mathbb{E}_j[U]]$, the first factor in the above display is equal to

$$\left\{ \mathbb{E} \sum_{jk,ilq} \left\| \partial_{lk} \left(\mathbb{E}_{j}[\boldsymbol{U}]^{\top} \boldsymbol{e}_{q} \boldsymbol{e}_{i}^{\top} \mathbb{E}_{j}[\boldsymbol{V}] \right) \right\|_{\mathrm{F}}^{2} \right\}^{\frac{1}{2}}$$

$$\stackrel{(\mathrm{i})}{=} \left\{ \mathbb{E} \sum_{jk,ilq} \left\| \partial_{lk} \left(\mathbb{E}_{j}[\boldsymbol{U}]^{\top} \right) \boldsymbol{e}_{q} \boldsymbol{e}_{i}^{\top} \mathbb{E}_{j}[\boldsymbol{V}] + \mathbb{E}_{j}[\boldsymbol{U}]^{\top} \boldsymbol{e}_{q} \boldsymbol{e}_{i}^{\top} \partial_{lk} \left(\mathbb{E}_{j}[\boldsymbol{V}] \right) \right\|_{\mathrm{F}}^{2} \right\}^{\frac{1}{2}}$$

$$\stackrel{(\mathrm{ii})}{\leq} \left\{ \mathbb{E} \sum_{jk,ilq} \left\| \partial_{lk} \left(\mathbb{E}_{j}[\boldsymbol{U}]^{\top} \right) \boldsymbol{e}_{q} \boldsymbol{e}_{i}^{\top} \mathbb{E}_{j}[\boldsymbol{V}] \right\|_{\mathrm{F}}^{2} \right\}^{\frac{1}{2}} + \left\{ \mathbb{E} \sum_{jk,ilq} \left\| \mathbb{E}_{j}[\boldsymbol{U}]^{\top} \boldsymbol{e}_{q} \boldsymbol{e}_{i}^{\top} \partial_{lk} \left(\mathbb{E}_{j}[\boldsymbol{V}] \right) \right\|_{\mathrm{F}}^{2} \right\}^{\frac{1}{2}}$$

$$\stackrel{(\mathrm{iii})}{=} \left\{ \mathbb{E} \sum_{jk,ilq} \left\| \mathbb{E}_{j}[\partial_{lk}\boldsymbol{U}]^{\top} \boldsymbol{e}_{q} \right\|_{2}^{2} \left\| \boldsymbol{e}_{i}^{\top} \mathbb{E}_{j}[\boldsymbol{V}] \right\|_{2}^{2} \right\}^{\frac{1}{2}} + \left\{ \mathbb{E} \sum_{jk,ilq} \left\| \mathbb{E}_{j}[\boldsymbol{U}]^{\top} \boldsymbol{e}_{q} \right\|_{2}^{2} \left\| \boldsymbol{e}_{i}^{\top} \mathbb{E}_{j}[\partial_{lk}\boldsymbol{V}] \right\|_{2}^{2} \right\}^{\frac{1}{2}}$$

$$\stackrel{(\mathrm{iv})}{=} \left\{ \mathbb{E} \sum_{jk,l} \left\| \mathbb{E}_{j}[\partial_{lk}\boldsymbol{U}]^{\top} \right\|_{\mathrm{F}}^{2} \left\| \mathbb{E}_{j}[\boldsymbol{V}] \right\|_{\mathrm{F}}^{2} \right\}^{\frac{1}{2}} + \left\{ \mathbb{E} \sum_{jk,l} \left\| \mathbb{E}_{j}[\boldsymbol{U}]^{\top} \right\|_{\mathrm{F}}^{2} \left\| \mathbb{E}_{j}[\partial_{lk}\boldsymbol{V}] \right\|_{\mathrm{F}}^{2} \right\}^{\frac{1}{2}} ,$$

where (i) is the chain rule, (ii) the triangle inequality, (iii) holds provided that the order of the derivation ∂_{lk} and the expectation sign \mathbb{E}_j can be switched (thanks to dominant convergence theorem) and using $\|\boldsymbol{a}\boldsymbol{b}^{\top}\|_{\mathrm{F}}^2 = \|\boldsymbol{a}\|_2^2 \|\boldsymbol{b}\|_2^2$ for vectors $\boldsymbol{a}, \boldsymbol{b}$, and (iv) holds using $\sum_i \|\boldsymbol{A}\boldsymbol{e}_i\|_2^2 = \|\boldsymbol{A}\|_{\mathrm{F}}^2 = \sum_q \|\boldsymbol{A}\boldsymbol{e}_q\|_2^2$ for a matrix \boldsymbol{A} with n columns. Finally, by Jensen's inequality, the above display is bounded by

$$\left\{\mathbb{E}\sum_{k,l}\left\|\partial_{lk}\boldsymbol{U}\right\|_{\mathrm{F}}^{2}\sum_{j}\left\|\mathbb{E}_{j}[\boldsymbol{V}]\right\|_{\mathrm{F}}^{2}\right\}^{\frac{1}{2}}+\left\{\mathbb{E}\sum_{k,l}\left\|\partial_{lk}\boldsymbol{V}\right\|_{\mathrm{F}}^{2}\sum_{j}\left\|\mathbb{E}_{j}[\boldsymbol{U}]\right\|_{\mathrm{F}}^{2}\right\}^{\frac{1}{2}}.$$

By the Cauchy-Schwarz inequality, the first term in the above display is bounded by

$$\begin{split} &\left\{\sum_{j} \sqrt{\mathbb{E}\left[\left(\sum_{k,l} \|\partial_{lk}\boldsymbol{U}\|_{\mathrm{F}}^{2}\right)^{2}\right]} \sqrt{\mathbb{E}\|\mathbb{E}_{j}[\boldsymbol{V}]\|_{\mathrm{F}}^{4}}\right\}^{1/2} \\ &\leq \left\{p \sqrt{\mathbb{E}\left[\left(\sum_{k,l} \|\partial_{lk}\boldsymbol{U}\|_{\mathrm{F}}^{2}\right)^{2}\right]} \sqrt{\mathbb{E}\|\boldsymbol{V}\|_{\mathrm{F}}^{4}}\right\}^{1/2} \\ &= \sqrt{p}\mathbb{E}[\|\boldsymbol{U}\|_{\partial}^{4}]^{1/4}\mathbb{E}[\|\boldsymbol{V}\|_{\mathrm{F}}^{4}]^{1/4}, \end{split}$$

where we used $\|\mathbb{E}_{j}[V]\|_{\mathrm{F}}^{4} \leq \mathbb{E}_{j}[\|V\|_{\mathrm{F}}^{4}]$ by Jensen's inequality. Hence,

$$\begin{aligned} (\mathbf{F}.26) &\leq \left(\sqrt{p}\mathbb{E}[\|\boldsymbol{U}\|_{\partial}^{4}]^{1/4}\mathbb{E}[\|\boldsymbol{V}\|_{\mathbf{F}}^{4}]^{1/4} + \mathbb{E}[\|\boldsymbol{V}\|_{\partial}^{4}]^{1/4}\mathbb{E}[\|\boldsymbol{U}\|_{\mathbf{F}}^{4}]^{1/4}\right)^{2} \\ &\leq 2p\mathbb{E}[\|\boldsymbol{U}\|_{\partial}^{4}]^{1/2}\mathbb{E}[\|\boldsymbol{V}\|_{\mathbf{F}}^{4}]^{1/2} + 2p\mathbb{E}[\|\boldsymbol{V}\|_{\partial}^{4}]^{1/2}\mathbb{E}[\|\boldsymbol{U}\|_{\mathbf{F}}^{4}]^{1/2}, \end{aligned}$$

where we uses $(a + b)^2 \le 2a^2 + 2b^2$.

Combining the above bounds of $\sum_{j=k} \operatorname{Tr}[\boldsymbol{M}_j^{\top} \boldsymbol{M}_k]$ and $\sum_{j\neq k} \operatorname{Tr}[\boldsymbol{M}_j^{\top} \boldsymbol{M}_k]$, we have

$$\begin{split} & \mathbb{E}[\|(\mathbf{F}.22)\|_{\mathbf{F}}] \\ \leq & \mathbb{E}[\|(\mathbf{F}.22)\|_{\mathbf{F}}^{2}]^{\frac{1}{2}} \\ \leq & (2p\mathbb{E}[\|\boldsymbol{U}\|_{\mathbf{F}}^{4}]^{1/2}\mathbb{E}[\|\boldsymbol{V}\|_{\mathbf{F}}^{4}]^{1/2} + 2p\mathbb{E}[\|\boldsymbol{U}\|_{\partial}^{4}]^{1/2}\mathbb{E}[\|\boldsymbol{V}\|_{\mathbf{F}}^{4}]^{1/2} + 2p\mathbb{E}[\|\boldsymbol{U}\|_{\mathbf{F}}^{4}]^{1/2}\mathbb{E}[\|\boldsymbol{U}\|_{\mathbf{F}}^{4}]^{1/2} \\ \leq & \sqrt{2p} \Big(\mathbb{E}[\|\boldsymbol{U}\|_{\mathbf{F}}^{4}]^{1/4}\mathbb{E}[\|\boldsymbol{V}\|_{\mathbf{F}}^{4}]^{1/4} + \mathbb{E}[\|\boldsymbol{U}\|_{\partial}^{4}]^{1/4}\mathbb{E}[\|\boldsymbol{V}\|_{\mathbf{F}}^{4}]^{1/4} + \mathbb{E}[\|\boldsymbol{V}\|_{\partial}^{4}]^{1/4}\mathbb{E}[\|\boldsymbol{V}\|_{\mathbf{F}}^{4}]^{1/4} \\ \end{split}$$

where the last inequality uses $(a + b + c)^{1/2} \le a^{1/2} + b^{1/2} + c^{1/2}$ for non-negative a, b, and c.

Now, combining the bounds on the terms (F.21)-(F.22)-(F.23)-(F.24) with the triangle inequality, the expectation in the lemma statement can be bounded from above by

$$\begin{split} & \mathbb{E}\Big[\Big\|p\boldsymbol{U}^{\top}\boldsymbol{V} - \sum_{j=1}^{p} \Big(\sum_{i=1}^{n} \partial_{ij}\boldsymbol{U}^{\top}\boldsymbol{e}_{i} - \boldsymbol{U}^{\top}\boldsymbol{Z}\boldsymbol{e}_{j}\Big)\Big(\sum_{i=1}^{n} \partial_{ij}\boldsymbol{e}_{i}^{\top}\boldsymbol{V} - \boldsymbol{e}_{j}^{\top}\boldsymbol{Z}^{\top}\boldsymbol{V}\Big)\Big\|_{\mathrm{F}}\Big] \\ & \leq 2\mathbb{E}[\|\boldsymbol{U}\|_{\partial}^{2}]^{1/2}\mathbb{E}[\|\boldsymbol{V}\|_{\partial}^{2}]^{1/2} \\ & + (1 + \sqrt{2})\sqrt{p}\Big(\mathbb{E}[\|\boldsymbol{U}\|_{\mathrm{F}}^{2}]^{\frac{1}{2}}\mathbb{E}[\|\boldsymbol{V}\|_{\partial}^{2}]^{1/2} + \mathbb{E}[\|\boldsymbol{V}\|_{\mathrm{F}}^{2}]^{\frac{1}{2}}\mathbb{E}[\|\boldsymbol{U}\|_{\partial}^{2}]^{1/2}\Big) \\ & + \sqrt{2p}\Big(\mathbb{E}[\|\boldsymbol{U}\|_{\mathrm{F}}^{4}]^{1/4}\mathbb{E}[\|\boldsymbol{V}\|_{\partial}^{4}]^{1/4} + \mathbb{E}[\|\boldsymbol{U}\|_{\partial}^{4}]^{1/4}\mathbb{E}[\|\boldsymbol{V}\|_{\mathrm{F}}^{4}]^{1/4} + \mathbb{E}[\|\boldsymbol{V}\|_{\partial}^{4}]^{1/4}\mathbb{E}[\|\boldsymbol{U}\|_{\mathrm{F}}^{4}]^{1/4}\Big) \\ & \leq \mathbb{E}[\|\boldsymbol{U}\|_{\partial}^{2}] + \mathbb{E}[\|\boldsymbol{V}\|_{\partial}^{2}] \\ & + (1 + \sqrt{2})\sqrt{p}/2\Big(\mathbb{E}[\|\boldsymbol{U}\|_{\mathrm{F}}^{2}] + \mathbb{E}[\|\boldsymbol{V}\|_{\partial}^{2}] + \mathbb{E}[\|\boldsymbol{V}\|_{\mathrm{F}}^{2}] + \mathbb{E}[\|\boldsymbol{U}\|_{\partial}^{2}]\Big) \\ & + \sqrt{2p}/2\Big(\mathbb{E}[\|\boldsymbol{U}\|_{\mathrm{F}}^{4}]^{1/2} + \mathbb{E}[\|\boldsymbol{V}\|_{\mathrm{F}}^{4}]^{1/2} + \mathbb{E}[\|\boldsymbol{V}\|_{\partial}^{4}]^{1/2} + \mathbb{E}[\|\boldsymbol{V}\|_{\mathrm{F}}^{4}]^{1/2} + \mathbb{E}[\|\boldsymbol{V}\|_{\partial}^{4}]^{1/2} + \mathbb{E}[\|\boldsymbol{V}\|_{\partial}^{4}]^{1/2} \Big), \end{split}$$

where the second inequality uses $ab \leq (a^2 + b^2)/2$ and the last inequality uses

$$\mathbb{E}[\|\boldsymbol{U}\|_{\mathrm{F}}^2]^{1/2} \leq \mathbb{E}[\|\boldsymbol{U}\|_{\mathrm{F}}^4]^{1/4} \text{ and } \mathbb{E}[\|\boldsymbol{U}\|_{\partial}^2]^{1/2} \leq \mathbb{E}[\|\boldsymbol{U}\|_{\partial}^4]^{1/4}$$

from Jensen's inequality. This completes the proof of Lemma F.5.

Proof of Lemma F.6. For notation simplicity, we define

$$oldsymbol{
ho}_i = \sum_{j=1}^{p+1} rac{\partial oldsymbol{V}^ op}{\partial z_{ij}} oldsymbol{e}_j - oldsymbol{V}^ op oldsymbol{Z}^ op oldsymbol{e}_i.$$

Then the left-hand side of (F.14) can be written as $n \mathbf{V}^{\top} \mathbf{V} - \sum_{i=1}^{n} \boldsymbol{\rho}_{i} \boldsymbol{\rho}_{i}^{\top}$. Since $\mathbf{V} = [-\mathbf{H}^{\top}, \sigma \mathbf{1}_{T}]^{\top}$, we have $\mathbf{V}^{\top} \mathbf{V} = \mathbf{H}^{\top} \mathbf{H} + \mathbf{S}$. We need the following lemma for this proof.

Lemma F.9 (Proof is given on Page 56). We have

(F.27)
$$\boldsymbol{\rho}_{i}^{\top} = \sum_{j=1}^{p+1} \frac{\partial \boldsymbol{e}_{j}^{\top} \boldsymbol{V}}{\partial z_{ij}} - \boldsymbol{e}_{i}^{\top} \boldsymbol{Z} \boldsymbol{V} = -\boldsymbol{e}_{i}^{\top} \boldsymbol{F} (\boldsymbol{I}_{T} + \widehat{\boldsymbol{C}}/n)^{\top} + \boldsymbol{e}_{i}^{\top} \boldsymbol{\Xi},$$

where $\boldsymbol{\Xi} = n^{-1} \sum_{j=1}^{p} \boldsymbol{X} \big((\boldsymbol{e}_{j}^{\top} \boldsymbol{H}) \otimes \boldsymbol{I}_{p} \big) (\mathcal{M}^{-1} \mathcal{D})^{\top} (\boldsymbol{I}_{T} \otimes \boldsymbol{e}_{j})$ and it satisfies

$$\|\boldsymbol{\Xi}\|_{\mathrm{op}} \leq C(\zeta, T, \gamma) \|\boldsymbol{H}\|_{\mathrm{F}} (1 + \|\boldsymbol{X}\|_{\mathrm{op}}^2/n)^T$$

By Lemma F.9,

$$n\boldsymbol{V}^{\top}\boldsymbol{V} - \sum_{i=1}^{n} \boldsymbol{\rho}_{i}\boldsymbol{\rho}_{i}^{\top}$$

= $n(\boldsymbol{H}^{\top}\boldsymbol{H} + \boldsymbol{S}) - ((\boldsymbol{I}_{T} + \hat{\boldsymbol{C}}/n)\boldsymbol{F}^{\top} + \boldsymbol{\Xi}^{\top})(\boldsymbol{F}(\boldsymbol{I}_{T} + \hat{\boldsymbol{C}}/n)^{\top} + \boldsymbol{\Xi})$
= $n(\boldsymbol{H}^{\top}\boldsymbol{H} + \boldsymbol{S}) - (\boldsymbol{I}_{T} + \hat{\boldsymbol{C}}/n)\boldsymbol{F}^{\top}\boldsymbol{F}(\boldsymbol{I}_{T} + \hat{\boldsymbol{C}}/n)^{\top}$
 $-\underbrace{\boldsymbol{\Xi}^{\top}\boldsymbol{F}(\boldsymbol{I}_{T} + \hat{\boldsymbol{C}}/n)^{\top} - (\boldsymbol{I}_{T} + \hat{\boldsymbol{C}}/n)\boldsymbol{F}^{\top}\boldsymbol{\Xi} - \boldsymbol{\Xi}^{\top}\boldsymbol{\Xi}}_{\text{Rem}_{2}}$
= $\sqrt{n}\boldsymbol{Q}_{2} - \text{Rem}_{2}.$

The desired bound for $\mathbb{E}[\|\text{Rem}_2\|_{\text{F}}]$ then follows from the Cauchy-Schwarz inequality, Lemmas E.4, E.8 and E.10 and the operator norm bound of Ξ from Lemma F.9. This completes the proof of Lemma F.6. \Box

Proof of Lemma F.7. We need to bound $\mathbb{E}[\|\boldsymbol{V}\|_{\mathrm{F}}^4]^{1/2}$ and $\mathbb{E}[\|\boldsymbol{V}\|_{\partial}^4]^{1/2}$. For the first term, since $\|\boldsymbol{V}\|_{\mathrm{F}}^2 = \|\boldsymbol{H}\|_{\mathrm{F}}^2 + T\sigma^2$, we have by Lemma E.10,

$$\mathbb{E}[\|\boldsymbol{V}\|_{\mathrm{F}}^{4}]^{1/2} = \mathbb{E}[(\|\boldsymbol{H}\|_{\mathrm{F}}^{2} + T\sigma^{2})^{2}]^{1/2} \le 2\mathbb{E}[\|\boldsymbol{H}\|_{\mathrm{F}}^{4}]^{1/2} + 2T\sigma^{2} \le C(\zeta, T, \gamma)\operatorname{var}(y_{1}).$$

For the second term, we have

$$\|\boldsymbol{V}\|_{\partial}^{2} = \sum_{i=1}^{n} \sum_{j=1}^{p+1} \|\frac{\partial \boldsymbol{V}}{\partial z_{ij}}\|_{\mathrm{F}}^{2} = \sum_{i=1}^{n} \sum_{j=1}^{p} \|\frac{\partial \boldsymbol{H}}{\partial x_{ij}}\|_{\mathrm{F}}^{2} = \|\frac{\partial \operatorname{\mathbf{vec}}(\boldsymbol{H})}{\partial \operatorname{\mathbf{vec}}(\boldsymbol{X})}\|_{\mathrm{F}}.$$

Applying (E.13), and the moment bound of F, H, X in Lemmas E.8 and E.10, we have

$$\mathbb{E}[\|\boldsymbol{V}\|_{\partial}^4]^{1/2} \le C(\zeta, T, \gamma) \operatorname{var}(y_1).$$

Combining the above two bounds, we have the desired inequality. This completes the proof of Lemma F.7. \Box Proof of Lemma F.8. By Corollary C.2, we have $\frac{\partial F_{lt}}{\partial x_{ij}} = D_{ij}^{lt} + \Delta_{ij}^{lt}$, where

$$D_{ij}^{lt} = -(\boldsymbol{e}_t^{\top} \otimes \boldsymbol{e}_l^{\top})(\boldsymbol{I}_{nT} - \boldsymbol{N})((\boldsymbol{H}^{\top}\boldsymbol{e}_j) \otimes \boldsymbol{e}_i),$$

$$\Delta_{ij}^{lt} = -n^{-1}(\boldsymbol{e}_t^{\top} \otimes \boldsymbol{e}_l^{\top})(\boldsymbol{I}_T \otimes \boldsymbol{X})\mathcal{M}^{-1}\mathcal{D}\big(\boldsymbol{F}^{\top} \otimes \boldsymbol{I}_p\big)(\boldsymbol{e}_i \otimes \boldsymbol{e}_j).$$

We first prove (F.16). Since $e_i^{\top} \frac{\partial F}{\partial x_{ij}} = \sum_t \frac{\partial F_{it}}{\partial x_{ij}} e_t^{\top} = \sum_t (D_{ij}^{it} + \Delta_{ij}^{it}) e_t^{\top}$, we have

$$\boldsymbol{H}^{\top} \sum_{i=1}^{n} \sum_{j=1}^{p} \boldsymbol{e}_{j} \boldsymbol{e}_{i}^{\top} \frac{\partial \boldsymbol{F}}{\partial x_{ij}}$$

$$= \boldsymbol{H}^{\top} \sum_{ij} \boldsymbol{e}_{j} \sum_{t=1}^{T} (D_{ij}^{it} + \Delta_{ij}^{it}) \boldsymbol{e}_{t}^{\top}$$

$$= \boldsymbol{H}^{\top} \sum_{ij} \boldsymbol{e}_{j} \sum_{t} D_{ij}^{it} \boldsymbol{e}_{t}^{\top} + \underbrace{\boldsymbol{H}^{\top} \sum_{ij} \boldsymbol{e}_{j} \sum_{t} \Delta_{ij}^{it} \boldsymbol{e}_{t}^{\top}}_{\text{Rem}_{1,1}}.$$

The first term in the last line can be simplified as below,

$$\boldsymbol{H}^{\top} \sum_{j=1}^{p} \sum_{i=1}^{n} \boldsymbol{e}_{j} \sum_{t=1}^{T} D_{ij}^{it} \boldsymbol{e}_{t}^{\top}$$

$$= -\boldsymbol{H}^{\top} \sum_{j=1}^{p} \sum_{i=1}^{n} \boldsymbol{e}_{j} \sum_{t=1}^{T} (\boldsymbol{e}_{j}^{\top} \boldsymbol{H} \otimes \boldsymbol{e}_{i}^{\top}) (\boldsymbol{I}_{nT} - \boldsymbol{N}^{\top}) (\boldsymbol{e}_{t} \otimes \boldsymbol{e}_{i}) \boldsymbol{e}_{t}^{\top}$$
 by (C.5)
$$= -\boldsymbol{H}^{\top} \boldsymbol{H} \Big[\sum_{i=1}^{n} (\boldsymbol{I}_{T} \otimes \boldsymbol{e}_{i}^{\top}) (\boldsymbol{I}_{nT} - \boldsymbol{N}^{\top}) (\boldsymbol{I}_{T} \otimes \boldsymbol{e}_{i}) \Big]$$

$$= -\boldsymbol{H}^{\top} \boldsymbol{H} (n \boldsymbol{I}_{T} - \hat{\boldsymbol{A}}^{\top})$$
 by (2.12).

Next, we prove (F.17).

$$\sum_{i=1}^{n} \sum_{j=1}^{p} \mathbf{F}^{\mathsf{T}} \mathbf{e}_{i} \mathbf{e}_{j}^{\mathsf{T}} \frac{\partial \mathbf{H}}{\partial x_{ij}}$$

$$= \sum_{i=1}^{n} \sum_{j=1}^{p} \sum_{t=1}^{T} \mathbf{F}^{\mathsf{T}} \mathbf{e}_{i} \mathbf{e}_{j}^{\mathsf{T}} \frac{\partial \hat{\mathbf{b}}^{t}}{\partial x_{ij}} \mathbf{e}_{t}^{\mathsf{T}}$$

$$= n^{-1} \sum_{i=1}^{n} \sum_{j=1}^{p} \sum_{t=1}^{T} \mathbf{F}^{\mathsf{T}} \mathbf{e}_{i} \mathbf{e}_{j}^{\mathsf{T}} (\mathbf{e}_{t}^{\mathsf{T}} \otimes \mathbf{I}_{p}) \mathcal{M}^{-1} \mathcal{D} \Big((\mathbf{F}^{\mathsf{T}} \mathbf{e}_{i}) \otimes \mathbf{e}_{j} \Big) \mathbf{e}_{t}^{\mathsf{T}} + \operatorname{Rem}_{1,2} \qquad \text{by (C.2)}$$

$$= n^{-1} \sum_{i=1}^{n} \sum_{j=1}^{p} \sum_{t=1}^{T} \mathbf{F}^{\mathsf{T}} \mathbf{e}_{i} \Big[(\mathbf{e}_{t}^{\mathsf{T}} \otimes \mathbf{e}_{j}^{\mathsf{T}}) \mathcal{M}^{-1} \mathcal{D} \Big((\mathbf{F}^{\mathsf{T}} \mathbf{e}_{i}) \otimes \mathbf{e}_{j} \Big) \Big]^{\mathsf{T}} \mathbf{e}_{t}^{\mathsf{T}} + \operatorname{Rem}_{1,2}$$

$$= n^{-1} \sum_{i=1}^{n} \sum_{j=1}^{p} \sum_{t=1}^{T} \mathbf{F}^{\mathsf{T}} \mathbf{e}_{i} \Big((\mathbf{e}_{t}^{\mathsf{T}} \mathbf{F}) \otimes \mathbf{e}_{j}^{\mathsf{T}} \Big) (\mathcal{M}^{-1} \mathcal{D})^{\mathsf{T}} (\mathbf{e}_{t} \otimes \mathbf{e}_{j}) \mathbf{e}_{t}^{\mathsf{T}} + \operatorname{Rem}_{1,2} \qquad \text{by (B.1)}$$

$$=n^{-1}\boldsymbol{F}^{\top}\boldsymbol{F}\sum_{j=1}^{r}(\boldsymbol{I}_{T}\otimes\boldsymbol{e}_{j}^{\top})(\mathcal{M}^{-1}\mathcal{D})^{\top}(\boldsymbol{I}_{T}\otimes\boldsymbol{e}_{j}) + \operatorname{Rem}_{1,2} \qquad \text{by (B.1)}$$

$$= \mathbf{F}^{\top} \mathbf{F} \widehat{\mathbf{C}}^{\top} / n + \operatorname{Rem}_{1,2}$$
 by (F.2).

It remains to bound $\mathbb{E}[\|\operatorname{Rem}_{1,1}\|_{\mathrm{F}}^2]$ and $\mathbb{E}[\|\operatorname{Rem}_{1,2}\|_{\mathrm{F}}^2]$. By expression of $\operatorname{Rem}_{1,1}$ in (F.18), we have

 $\operatorname{Rem}_{1,1}$

$$= \boldsymbol{H}^{\top} \sum_{i=1}^{n} \sum_{j=1}^{p} \boldsymbol{e}_{j} \sum_{t=1}^{T} \Delta_{ij}^{it} \boldsymbol{e}_{t}^{\top},$$

$$= -n^{-1} \boldsymbol{H}^{\top} \sum_{i=1}^{n} \sum_{j=1}^{p} \sum_{t=1}^{T} \boldsymbol{e}_{j} (\boldsymbol{e}_{t}^{\top} \otimes \boldsymbol{e}_{i}^{\top}) (\boldsymbol{I}_{T} \otimes \boldsymbol{X}) \mathcal{M}^{-1} \mathcal{D} (\boldsymbol{F}^{\top} \otimes \boldsymbol{I}_{p}) (\boldsymbol{e}_{i} \otimes \boldsymbol{e}_{j}) \boldsymbol{e}_{t}^{\top} \qquad \text{by (C.6)}$$

$$= -n^{-1} \boldsymbol{H}^{\top} \sum_{i=1}^{n} \sum_{j=1}^{p} \sum_{t=1}^{T} \boldsymbol{e}_{j} [(\boldsymbol{e}_{t}^{\top} \otimes \boldsymbol{e}_{i}^{\top}) (\boldsymbol{I}_{T} \otimes \boldsymbol{X}) \mathcal{M}^{-1} \mathcal{D} (\boldsymbol{F}^{\top} \otimes \boldsymbol{I}_{p}) (\boldsymbol{e}_{i} \otimes \boldsymbol{e}_{j})]^{\top} \boldsymbol{e}_{t}^{\top}$$

$$= -n^{-1} \boldsymbol{H}^{\top} \sum_{i=1}^{n} \sum_{j=1}^{p} \sum_{t=1}^{T} \boldsymbol{e}_{j} (\boldsymbol{e}_{i}^{\top} \otimes \boldsymbol{e}_{i}^{\top}) (\boldsymbol{F} \otimes \boldsymbol{I}_{p}) (\mathcal{M}^{-1} \mathcal{D})^{\top} (\boldsymbol{I}_{T} \otimes \boldsymbol{X}^{\top}) (\boldsymbol{e}_{t} \otimes \boldsymbol{e}_{i}) \boldsymbol{e}_{t}^{\top}$$

$$= -n^{-1} \boldsymbol{H}^{\top} \sum_{i=1}^{n} (\boldsymbol{e}_{i}^{\top} \otimes \boldsymbol{I}_{p}) (\boldsymbol{F} \otimes \boldsymbol{I}_{p}) (\mathcal{M}^{-1} \mathcal{D})^{\top} (\boldsymbol{I}_{T} \otimes \boldsymbol{X}^{\top}) (\boldsymbol{I}_{T} \otimes \boldsymbol{e}_{i}) \qquad \text{by (B.1)}$$

$$= -n^{-1} \boldsymbol{H}^{\top} \sum_{i=1}^{n} ((\boldsymbol{e}_{i}^{\top} \boldsymbol{F}) \otimes \boldsymbol{I}_{p}) (\mathcal{M}^{-1} \mathcal{D})^{\top} (\boldsymbol{I}_{T} \otimes (\boldsymbol{X}^{\top} \boldsymbol{e}_{i})) \qquad \text{by (B.1)}.$$

Using the fact that $\|\boldsymbol{M}\|_{\mathrm{F}} \leq \sqrt{T} \|\boldsymbol{M}\|_{\mathrm{op}}$ for $\boldsymbol{M} \in \mathbb{R}^{T \times T}$ and the triangular inequality, we have

 $\left\|\operatorname{Rem}_{1,1}\right\|_{F}$

$$\leq \sqrt{T}n^{-1} \|\boldsymbol{H}\|_{\mathrm{op}} \|\mathcal{M}^{-1}\mathcal{D}\|_{\mathrm{op}} \sum_{i=1}^{n} \|(\boldsymbol{e}_{i}^{\top}\boldsymbol{F}) \otimes \boldsymbol{I}_{p}\|_{\mathrm{op}} \|\boldsymbol{I}_{T} \otimes (\boldsymbol{X}^{\top}\boldsymbol{e}_{i})\|_{\mathrm{op}}$$

$$\leq \sqrt{T}n^{-1} \|\boldsymbol{H}\|_{\mathrm{op}} \|\mathcal{M}^{-1}\mathcal{D}\|_{\mathrm{op}} \Big[\sum_{i=1}^{n} \|(\boldsymbol{e}_{i}^{\top}\boldsymbol{F}) \otimes \boldsymbol{I}_{p}\|_{\mathrm{op}}^{2}\Big]^{1/2} \Big[\sum_{i=1}^{n} \|\boldsymbol{I}_{T} \otimes (\boldsymbol{X}^{\top}\boldsymbol{e}_{i})\|_{\mathrm{op}}^{2}\Big]^{1/2}$$

$$\leq \sqrt{T}n^{-1} \|\boldsymbol{H}\|_{\mathrm{F}} \|\boldsymbol{F}\|_{\mathrm{F}} \|\boldsymbol{X}\|_{\mathrm{F}} \|\mathcal{M}^{-1}\|_{\mathrm{op}} \|\mathcal{D}\|_{\mathrm{op}}$$

$$\leq \sqrt{T}n^{-1/2} \|\boldsymbol{H}\|_{\mathrm{F}} \|\boldsymbol{F}\|_{\mathrm{F}} \|\boldsymbol{X}\|_{\mathrm{op}} \|\mathcal{M}^{-1}\|_{\mathrm{op}} \|\mathcal{D}\|_{\mathrm{op}}$$

$$\leq C(\zeta, T, \gamma) \|\boldsymbol{F}\|_{\mathrm{F}} \|\boldsymbol{H}\|_{\mathrm{F}} (1 + \|\boldsymbol{X}\|_{\mathrm{op}}^{2}/n)^{T}$$
by Lemmas E.1 and E.2.

It follows by the Cauchy-Schwarz inequality and Lemmas E.8 and E.10 that

$$\mathbb{E}[\|\operatorname{Rem}_{1,1}\|_{\mathrm{F}}^2] \le nC(\zeta, T, \gamma)\operatorname{var}(y_1)^2.$$

We next bound $\mathbb{E}[\|\operatorname{Rem}_{1,2}\|_{\mathrm{F}}^2]$. By the expression of $\operatorname{Rem}_{1,2}$ in (F.19), we have

$$-\operatorname{Rem}_{1,2} = n^{-1} \sum_{i=1}^{n} \sum_{j=1}^{p} \sum_{t=1}^{T} \boldsymbol{F}^{\top} \boldsymbol{e}_{i} \boldsymbol{e}_{j}^{\top} (\boldsymbol{e}_{t}^{\top} \otimes \boldsymbol{I}_{p}) \mathcal{M}^{-1} \mathcal{D} ((\boldsymbol{H}^{\top} \boldsymbol{e}_{j}) \otimes (\boldsymbol{X}^{\top} \boldsymbol{e}_{i})) \boldsymbol{e}_{t}^{\top}$$
$$= n^{-1} \sum_{i=1}^{n} \sum_{j=1}^{p} \sum_{t=1}^{T} \boldsymbol{F}^{\top} \boldsymbol{e}_{i} \Big[(\boldsymbol{e}_{t}^{\top} \otimes \boldsymbol{e}_{j}^{\top}) \mathcal{M}^{-1} \mathcal{D} ((\boldsymbol{H}^{\top} \boldsymbol{e}_{j}) \otimes (\boldsymbol{X}^{\top} \boldsymbol{e}_{i})) \Big]^{\top} \boldsymbol{e}_{t}^{\top}$$
$$= n^{-1} \sum_{i=1}^{n} \sum_{j=1}^{p} \sum_{t=1}^{T} \boldsymbol{F}^{\top} \boldsymbol{e}_{i} ((\boldsymbol{e}_{j}^{\top} \boldsymbol{H}) \otimes (\boldsymbol{e}_{i}^{\top} \boldsymbol{X})) (\mathcal{M}^{-1} \mathcal{D})^{\top} (\boldsymbol{e}_{t} \otimes \boldsymbol{e}_{j}) \boldsymbol{e}_{t}^{\top}$$
$$= n^{-1} \sum_{j=1}^{p} \Big((\boldsymbol{e}_{j}^{\top} \boldsymbol{H}) \otimes (\boldsymbol{F}^{\top} \boldsymbol{X}) \Big) (\mathcal{M}^{-1} \mathcal{D})^{\top} (\boldsymbol{I}_{T} \otimes \boldsymbol{e}_{j}).$$

Using the same argument that we used to bound $\mathbb{E}[\|\operatorname{Rem}_{1,1}\|_{\mathrm{F}}^2]$, we have

$$\mathbb{E}[\|\operatorname{Rem}_{1,2}\|_{\mathrm{F}}^2] \le nC(\zeta, T, \gamma)\operatorname{var}(y_1)^2.$$

This completes the proof of Lemma F.8.

Proof of Lemma F.9. By the definition of V, we have

$$\sum_{j=1}^{p+1} \frac{\partial \mathbf{e}_{j}^{\top} \mathbf{V}}{\partial z_{ij}}$$

$$= -\sum_{j=1}^{p} \frac{\partial \mathbf{e}_{j}^{\top} \mathbf{H}}{\partial x_{ij}}$$

$$= -\sum_{j=1}^{p} \sum_{t=1}^{T} \frac{\partial \mathbf{e}_{j}^{\top} \hat{\mathbf{b}}^{t}}{\partial x_{ij}} \mathbf{e}_{t}^{\top}$$

$$= -n^{-1} \sum_{j=1}^{p} \sum_{t=1}^{T} (\mathbf{e}_{t}^{\top} \otimes \mathbf{e}_{j}^{\top}) \mathcal{M}^{-1} \mathcal{D} ((\mathbf{F}^{\top} \mathbf{e}_{i}) \otimes \mathbf{e}_{j}) \mathbf{e}_{t}^{\top} + \mathbf{\Delta}_{i} \qquad \text{by (C.2)}$$

$$= -n^{-1} \sum_{j=1}^{p} \sum_{t=1}^{T} [\mathbf{e}_{t} (\mathbf{e}_{t}^{\top} \otimes \mathbf{e}_{j}^{\top}) \mathcal{M}^{-1} \mathcal{D} ((\mathbf{F}^{\top} \mathbf{e}_{i}) \otimes \mathbf{e}_{j})]^{\top} + \mathbf{\Delta}_{i}$$

$$= -n^{-1} \sum_{j=1}^{p} [(\mathbf{I}_{T} \otimes \mathbf{e}_{j}^{\top}) \mathcal{M}^{-1} \mathcal{D} (\mathbf{I}_{T} \otimes \mathbf{e}_{j}) \mathbf{F}^{\top} \mathbf{e}_{i}]^{\top} + \mathbf{\Delta}_{i}$$

$$= -\mathbf{e}_{i}^{\top} \mathbf{F} \widehat{\mathbf{C}}^{\top} / n + \mathbf{\Delta}_{i},$$

where $\boldsymbol{\Delta}_{i} = n^{-1} \sum_{j=1}^{p} \sum_{t=1}^{T} \boldsymbol{e}_{j}^{\top} (\boldsymbol{e}_{t}^{\top} \otimes \boldsymbol{I}_{p}) \mathcal{M}^{-1} \mathcal{D} ((\boldsymbol{H}^{\top} \boldsymbol{e}_{j}) \otimes (\boldsymbol{X}^{\top} \boldsymbol{e}_{i})) \boldsymbol{e}_{t}^{\top}.$ We claim that

(F.28)
$$\boldsymbol{\Delta}_i = \boldsymbol{e}_i^\top \boldsymbol{\Xi}.$$

Therefore, using $\mathbf{Z}\mathbf{V} = \mathbf{F}$, we have

$$egin{aligned} oldsymbol{
ho}_i^{ op} &= \sum_{j=1}^{p+1} rac{\partial oldsymbol{e}_j^{ op} oldsymbol{V}}{\partial z_{ij}} - oldsymbol{e}_i^{ op} oldsymbol{Z} oldsymbol{V} \ &= -oldsymbol{e}_i^{ op} oldsymbol{F} \widehat{oldsymbol{C}}^{ op} / n + oldsymbol{\Delta}_i - oldsymbol{e}_i^{ op} oldsymbol{F} \ &= -oldsymbol{e}_i^{ op} oldsymbol{F} (oldsymbol{I}_T + oldsymbol{\widehat{C}} / n)^{ op} + oldsymbol{e}_i^{ op} oldsymbol{\Xi}. \end{aligned}$$

Now we prove the claim (F.28). By definition,

$$\begin{split} \boldsymbol{\Delta}_{i} &= n^{-1} \sum_{j=1}^{p} \sum_{t=1}^{T} \boldsymbol{e}_{j}^{\top} (\boldsymbol{e}_{t}^{\top} \otimes \boldsymbol{I}_{p}) \mathcal{M}^{-1} \mathcal{D} \big((\boldsymbol{H}^{\top} \boldsymbol{e}_{j}) \otimes (\boldsymbol{X}^{\top} \boldsymbol{e}_{i}) \big) \boldsymbol{e}_{t}^{\top} \\ &= n^{-1} \sum_{j=1}^{p} \sum_{t=1}^{T} (\boldsymbol{e}_{t}^{\top} \otimes \boldsymbol{e}_{j}^{\top}) \mathcal{M}^{-1} \mathcal{D} \big((\boldsymbol{H}^{\top} \boldsymbol{e}_{j}) \otimes (\boldsymbol{X}^{\top} \boldsymbol{e}_{i}) \big) \boldsymbol{e}_{t}^{\top} \\ &= n^{-1} \sum_{j=1}^{p} \sum_{t=1}^{T} \left[\boldsymbol{e}_{t} (\boldsymbol{e}_{t}^{\top} \otimes \boldsymbol{e}_{j}^{\top}) \mathcal{M}^{-1} \mathcal{D} \big((\boldsymbol{H}^{\top} \boldsymbol{e}_{j}) \otimes (\boldsymbol{X}^{\top} \boldsymbol{e}_{i}) \big) \right]^{\top} \\ &= n^{-1} \sum_{j=1}^{p} \left[(\boldsymbol{I}_{T} \otimes \boldsymbol{e}_{j}^{\top}) \mathcal{M}^{-1} \mathcal{D} \big((\boldsymbol{H}^{\top} \boldsymbol{e}_{j}) \otimes (\boldsymbol{X}^{\top} \boldsymbol{e}_{i}) \big) \right]^{\top} \\ &= n^{-1} \sum_{j=1}^{p} \left[(\boldsymbol{e}_{j}^{\top} \boldsymbol{H}) \otimes (\boldsymbol{e}_{i}^{\top} \boldsymbol{X}) \big) (\mathcal{M}^{-1} \mathcal{D})^{\top} (\boldsymbol{I}_{T} \otimes \boldsymbol{e}_{j}) \\ &= n^{-1} \sum_{j=1}^{p} \boldsymbol{e}_{i}^{\top} \boldsymbol{X} \big((\boldsymbol{e}_{j}^{\top} \boldsymbol{H}) \otimes \boldsymbol{I}_{p} \big) (\mathcal{M}^{-1} \mathcal{D})^{\top} (\boldsymbol{I}_{T} \otimes \boldsymbol{e}_{j}) \\ &= \boldsymbol{e}_{i}^{\top} \boldsymbol{\Xi}. \end{split}$$

It remains to bound $\|\Xi\|_{op}$. By definition of Ξ , we have

$$\begin{split} \|\mathbf{\Xi}\|_{\mathrm{op}} \\ &= n^{-1} \|\sum_{j=1}^{p} \mathbf{X} \left((\mathbf{e}_{j}^{\top} \mathbf{H}) \otimes \mathbf{I}_{p} \right) (\mathcal{M}^{-1} \mathcal{D})^{\top} (\mathbf{I}_{T} \otimes \mathbf{e}_{j}) \|_{\mathrm{op}} \\ &\leq n^{-1} \sum_{j=1}^{p} \|\mathbf{X} \left((\mathbf{e}_{j}^{\top} \mathbf{H}) \otimes \mathbf{I}_{p} \right) (\mathcal{M}^{-1} \mathcal{D})^{\top} (\mathbf{I}_{T} \otimes \mathbf{e}_{j}) \|_{\mathrm{op}} \\ &\leq n^{-1} \|\mathbf{X}\|_{\mathrm{op}} \|\mathcal{M}^{-1}\|_{\mathrm{op}} \|\mathcal{D}\|_{\mathrm{op}} \sum_{j=1}^{p} \|(\mathbf{e}_{j}^{\top} \mathbf{H}) \otimes \mathbf{I}_{p}\|_{\mathrm{op}} \|\mathbf{I}_{T} \otimes \mathbf{e}_{j}\|_{\mathrm{op}} \\ &\leq n^{-1} \|\mathbf{X}\|_{\mathrm{op}} \|\mathcal{M}^{-1}\|_{\mathrm{op}} \|\mathcal{D}\|_{\mathrm{op}} [\sum_{j=1}^{p} \|(\mathbf{e}_{j}^{\top} \mathbf{H}) \otimes \mathbf{I}_{p}\|_{\mathrm{op}}^{2}]^{1/2} [\sum_{j} \|\mathbf{I}_{T} \otimes \mathbf{e}_{j}\|_{\mathrm{op}}^{2}]^{1/2} \\ &\leq n^{-1} \|\mathbf{X}\|_{\mathrm{op}} \|\mathcal{M}^{-1}\|_{\mathrm{op}} \|\mathcal{D}\|_{\mathrm{op}} \|\mathbf{H}\|_{\mathrm{F}} \sqrt{Tp} \\ &\leq C(\zeta, T, \gamma) \|\mathbf{H}\|_{\mathrm{F}} (1 + \|\mathbf{X}\|_{\mathrm{op}}^{2}/n)^{T} \qquad \text{by Lemmas E.1 and E.2.} \end{split}$$

This completes the proof of Lemma F.9.

Appendix G: Proof of Theorem 2.1

Proof of Theorem 2.1. By definition, we know $\hat{r}_t = \hat{r}_{t,t}$ and $r_t = r_{t,t}$. Thus the result of this theorem follows directly from the result of Theorem 2.2.

Appendix H: Proof of Corollary 2.3

Proof of Corollary 2.3. By the definition of r_t in (2.14), it suffices to show that

$$\mathbb{P}\Big(r_{\hat{t}} - \min_{s \in [T]} r_s \ge \frac{\operatorname{var}(y_1)}{n^{1/2-c}}\Big) \le \frac{C(\zeta, \gamma, T, \kappa)}{n^c}.$$

To see this, we have

$$\begin{split} & \mathbb{P}\left(r_{\hat{t}} - \min_{s \in [T]} r_{s} \geq \frac{\operatorname{var}(y_{1})}{n^{1/2-c}}\right) \\ & \leq \frac{n^{1/2-c}}{\operatorname{var}(y_{1})} \mathbb{E}\left[r_{\hat{t}} - \min_{s \in [T]} r_{s}\right] & \text{Markov's inequality} \\ & \leq \frac{n^{1/2-c}}{\operatorname{var}(y_{1})} \left(\mathbb{E}[|r_{\hat{t}} - \hat{r}_{\hat{t}}|] + \mathbb{E}[|\hat{r}_{\hat{t}} - \min_{s \in [T]} r_{s}|]\right) & \text{triangle inequality} \\ & = \frac{n^{1/2-c}}{\operatorname{var}(y_{1})} \left(\mathbb{E}[|r_{\hat{t}} - \hat{r}_{\hat{t}}|] + \mathbb{E}[|\min_{s \in [T]} \hat{r}_{s} - \min_{s \in [T]} r_{s}|]\right) & \text{by definition of } \hat{t} \\ & \leq \frac{n^{1/2-c}}{\operatorname{var}(y_{1})} \left(\mathbb{E}[|r_{\hat{t}} - \hat{r}_{\hat{t}}|] + \mathbb{E}[\max_{s \in [T]} |\hat{r}_{s} - r_{s}|]\right) & \text{by |} \min_{s} a_{s} - \min_{s} b_{s}| \leq \max_{s} |a_{s} - b_{s}| \\ & \leq \frac{n^{1/2-c}}{\operatorname{var}(y_{1})} \left(\mathbb{E}[|r_{\hat{t}} - \hat{r}_{\hat{t}}|] + \max_{s \in [T]} \mathbb{E}[|\hat{r}_{s} - r_{s}|]\right) & \text{Jensen's inequality} \\ & \leq \frac{C(\zeta, \gamma, T, \kappa)}{n^{c}} & \text{by Theorem 2.1.} \end{split}$$

This concludes the proof.

Appendix I: Proof of Theorem 2.4

Note that for this proof, we will consider general Σ directly. We first present two lemmas that will be useful. **Lemma I.1.** Under the same condition of Theorem 2.4. For $\operatorname{Rem}_j = \sum_{i=1}^n \sum_{t=1}^T \Delta_{ij}^{it} e_t^\top \frac{1}{\|\Sigma^{-1/2} e_j\|}$, we have

$$\mathbb{E}\left[\sum_{j=1}^{p} \|\operatorname{Rem}_{j}\|^{2}\right] \leq nC(\zeta, T, \kappa, \gamma)\operatorname{var}(y_{1}).$$

Proof of Lemma I.1. By definition, Rem_{i} is a row vector in \mathbb{R}^{T} , and its *t*-th entry is

$$\operatorname{Rem}_{jt} = \sum_{i=1}^{n} \Delta_{ij}^{it} \frac{1}{\|\boldsymbol{\Sigma}^{-1/2} \boldsymbol{e}_{j}\|}$$
$$= -n^{-1} \sum_{i=1}^{n} (\boldsymbol{e}_{t}^{\top} \otimes (\boldsymbol{e}_{i}^{\top} \boldsymbol{X})) \mathcal{M}^{-1} \mathcal{D}((\boldsymbol{F}^{\top} \boldsymbol{e}_{i}) \otimes \boldsymbol{e}_{j}) \frac{1}{\|\boldsymbol{\Sigma}^{-1/2} \boldsymbol{e}_{j}\|} \qquad \text{by (C.6)}$$
$$= -n^{-1} \sum_{i=1}^{n} \boldsymbol{e}_{i}^{\top} (\boldsymbol{e}_{t}^{\top} \otimes \boldsymbol{X}) \mathcal{M}^{-1} \mathcal{D}(\boldsymbol{F}^{\top} \otimes \boldsymbol{e}_{j}) \boldsymbol{e}_{i} \frac{1}{\|\boldsymbol{\Sigma}^{-1/2} \boldsymbol{e}_{j}\|} \qquad \text{by (B.1)}$$

$$= -n^{-1} \frac{1}{\|\boldsymbol{\Sigma}^{-1/2} \boldsymbol{e}_j\|} \operatorname{Tr} \big((\boldsymbol{e}_t^\top \otimes \boldsymbol{X}) \mathcal{M}^{-1} \mathcal{D} (\boldsymbol{F}^\top \otimes \boldsymbol{e}_j) \big).$$

For the trace in the last line above, we have for each $j \in [p], t \in [T]$, the following holds,

Since $(\mathbf{F}^{\top} \otimes \mathbf{e}_j) = (\mathbf{I}_T \otimes \mathbf{e}_j) \mathbf{F}^{\top}$, whose rank is at most T, we have

$$\begin{aligned} &\operatorname{Tr}\left((\boldsymbol{e}_{t}^{\top}\otimes\boldsymbol{X})\mathcal{M}^{-1}\mathcal{D}(\boldsymbol{F}^{\top}\otimes\boldsymbol{e}_{j})\right) \\ &\leq T\|(\boldsymbol{e}_{t}^{\top}\otimes\boldsymbol{X})\mathcal{M}^{-1}\mathcal{D}(\boldsymbol{F}^{\top}\otimes\boldsymbol{e}_{j})\|_{\operatorname{op}} \\ &\leq T\|(\boldsymbol{e}_{t}^{\top}\otimes\boldsymbol{X})\|_{\operatorname{op}}\|\mathcal{M}^{-1}\|_{\operatorname{op}}\|\mathcal{D}\|_{\operatorname{op}}\|(\boldsymbol{F}^{\top}\otimes\boldsymbol{e}_{j})\|_{\operatorname{op}} \qquad \text{submultiplicativity of } \|\cdot\|_{\operatorname{op}} \\ &= \sqrt{T}\|\boldsymbol{X}\|_{\operatorname{op}}\|\mathcal{M}^{-1}\|_{\operatorname{op}}\|\mathcal{D}\|_{\operatorname{op}}\|\boldsymbol{F}\|_{\operatorname{op}} \qquad \text{by (B.4)} \\ &\leq C(\zeta,T)\|\boldsymbol{X}\|_{\operatorname{op}}(1+\|\boldsymbol{X}\|_{\operatorname{op}}^{2}/n)^{T-1}\|\boldsymbol{F}\|_{\operatorname{F}} \qquad \text{by (E.1) and (E.2)} \\ &\leq C(\zeta,T)\sqrt{n}(1+\|\boldsymbol{X}\|_{\operatorname{op}}^{2}/n)^{T}\|\boldsymbol{F}\|_{\operatorname{F}}. \qquad \text{by } \|\boldsymbol{X}\|_{\operatorname{op}}/\sqrt{n} \leq (1+\|\boldsymbol{X}\|_{\operatorname{op}}^{2}/n)/2 \end{aligned}$$

Thus, using $\max_{j \in [p]} \frac{1}{\|\boldsymbol{\Sigma}^{-1/2} \boldsymbol{e}_j\|^2} \leq \|\boldsymbol{\Sigma}\|_{\text{op}}$ and above inequality for the trace, we have

$$\begin{split} &\sum_{j=1}^{p} \|\operatorname{Rem}_{j}\|^{2} \\ &= \sum_{j=1}^{p} \sum_{t=1}^{T} (\operatorname{Rem}_{jt})^{2} \\ &\leq n^{-2} \|\boldsymbol{\Sigma}\|_{\operatorname{op}} \sum_{j=1}^{p} \sum_{t=1}^{T} \operatorname{Tr} \left((\boldsymbol{e}_{t}^{\top} \otimes \boldsymbol{X}) \mathcal{M}^{-1} \mathcal{D}(\boldsymbol{F}^{\top} \otimes \boldsymbol{e}_{j}) \right)^{2} \\ &\leq n^{-1} p \|\boldsymbol{\Sigma}\|_{\operatorname{op}} C(\zeta, T) (1 + \|\boldsymbol{X}\|_{\operatorname{op}}^{2}/n)^{2T} \|\boldsymbol{F}\|_{\operatorname{F}}^{2} \\ &\leq \gamma \kappa C(\zeta, T) (1 + \|\boldsymbol{X}\|_{\operatorname{op}}^{2}/n)^{2T} \|\boldsymbol{F}\|_{\operatorname{F}}^{2}. \end{split} \quad \text{by } p/n \leq \gamma \text{ and } \|\boldsymbol{\Sigma}\|_{\operatorname{op}} \leq \kappa \text{ from Assumption 2.2} \end{split}$$

Therefore, Taking expectation using the Cauchy-Schwarz inequality and Lemmas E.8 and E.10, we have

$$\mathbb{E}\left[\sum_{j=1}^{p} \|\operatorname{Rem}_{j}\|^{2}\right] \leq nC(\zeta, T, \kappa, \gamma)\operatorname{var}(y_{1}).$$

This completes the proof of Lemma I.1.

Lemma I.2. Under Assumptions 2.1 to 2.4, we have

$$n^{-1}\mathbb{E}\Big[\sum_{t=1}^{T}\sum_{i=1}^{n}\sum_{j=1}^{p}(\boldsymbol{e}_{j}^{\top}\boldsymbol{\Sigma}^{-1}\boldsymbol{e}_{j})^{-1}\left\|\frac{\partial\boldsymbol{F}\boldsymbol{e}_{t}}{\partial\boldsymbol{x}_{ij}}\right\|_{\mathrm{F}}^{2}\Big] \leq C(\zeta,T,\kappa,\gamma)\mathrm{var}(y_{1}).$$

Proof of Lemma I.2. By Lemma E.6 the mapping $\mathbb{R}^{n \times p} \to \mathbb{R}^n : \mathbf{X} \mapsto \mathbf{F}\mathbf{e}_t$ is Lipschitz. Since the Frobenius norm of the Jacobian of an L_* -Lipschitz function valued in \mathbb{R}^n is at most $L_*\sqrt{n}$, we have the Frobenius norm of the Jacobian of the mapping $\mathbb{R}^{n \times p} \to \mathbb{R}^n : \mathbf{X} \mapsto \mathbf{F}\mathbf{e}_t$ is bounded by

$$\sqrt{n}C(\zeta,T)(1+\|\boldsymbol{X}\|_{\mathrm{op}}^2/n)^T(\|\boldsymbol{H}\|_{\mathrm{F}}+\|\boldsymbol{F}\|_{\mathrm{F}}/\sqrt{n}).$$

Therefore, using $\max_{j \in [p]} (\boldsymbol{e}_j^\top \boldsymbol{\Sigma}^{-1} \boldsymbol{e}_j)^{-1} \leq (\lambda_{\min}(\boldsymbol{\Sigma}^{-1}))^{-1} = \|\boldsymbol{\Sigma}\|_{\text{op}}$, we have

$$\begin{split} n^{-1} \sum_{t=1}^{T} \sum_{i=1}^{n} \sum_{j=1}^{p} (\boldsymbol{e}_{j}^{\top} \boldsymbol{\Sigma}^{-1} \boldsymbol{e}_{j})^{-1} \left\| \frac{\partial \boldsymbol{F} \boldsymbol{e}_{t}}{\partial \boldsymbol{x}_{ij}} \right\|_{\mathrm{F}}^{2} \\ &\leq n^{-1} \| \boldsymbol{\Sigma} \|_{\mathrm{op}} \sum_{t=1}^{T} \sum_{i=1}^{n} \sum_{j=1}^{p} \left\| \frac{\partial \boldsymbol{F} \boldsymbol{e}_{t}}{\partial \boldsymbol{x}_{ij}} \right\|_{\mathrm{F}}^{2} \\ &\leq n^{-1} \| \boldsymbol{\Sigma} \|_{\mathrm{op}} \sum_{t=1}^{T} \left\| \frac{\partial \boldsymbol{F} \boldsymbol{e}_{t}}{\partial \operatorname{vec}(\boldsymbol{X})} \right\|_{\mathrm{F}}^{2} \\ &\leq \| \boldsymbol{\Sigma} \|_{\mathrm{op}} C(\boldsymbol{\zeta}, T) (1 + \| \boldsymbol{X} \|_{\mathrm{op}}^{2} / n)^{2T} (\| \boldsymbol{H} \|_{\mathrm{F}} + \| \boldsymbol{F} \|_{\mathrm{F}} / \sqrt{n})^{2}. \end{split}$$

Taking expectations, using the Cauchy-Schwarz inequality and Lemmas E.8 and E.10, we have

$$n^{-1}\mathbb{E}\Big[\sum_{t=1}^{T}\sum_{i=1}^{n}\sum_{j=1}^{p}(\boldsymbol{e}_{j}^{\top}\boldsymbol{\Sigma}^{-1}\boldsymbol{e}_{j})^{-1}\left\|\frac{\partial\boldsymbol{F}\boldsymbol{e}_{t}}{\partial x_{ij}}\right\|_{\mathrm{F}}^{2}\Big]$$
$$\leq C(\zeta,T,\kappa,\gamma)\mathrm{var}(y_{1}).$$

Proof of Theorem 2.4. For any $j \in [p]$, $e_j \in \mathbb{R}^p$, let $z_j = X\Sigma^{-1}e_j/\|\Sigma^{-1/2}e_j\|$, then $z_j \sim \mathsf{N}(\mathbf{0}, I_n)$. Let $F(z_j) = Y - X\widehat{B} \in \mathbb{R}^{n \times T}$. Since

$$oldsymbol{X} = oldsymbol{X}(oldsymbol{I}_p - rac{oldsymbol{\Sigma}^{-1}oldsymbol{e}_joldsymbol{e}_j^{ op}}{\|oldsymbol{\Sigma}^{-1/2}oldsymbol{e}_j\|^2}) + oldsymbol{X}rac{oldsymbol{\Sigma}^{-1}oldsymbol{e}_joldsymbol{e}_j^{ op}}{\|oldsymbol{\Sigma}^{-1/2}oldsymbol{e}_j\|^2} := oldsymbol{X} oldsymbol{\Pi}_j + oldsymbol{z}_jrac{oldsymbol{e}_j^{ op}}{\|oldsymbol{\Sigma}^{-1/2}oldsymbol{e}_j\|^2},$$

where $\mathbf{\Pi}_j = \mathbf{I}_p - \frac{\mathbf{\Sigma}^{-1} \mathbf{e}_j \mathbf{e}_j^\top}{\|\mathbf{\Sigma}^{-1/2} \mathbf{e}_j\|^2}.$

We now show $\operatorname{vec}(X\Pi_j)$ is independent of z_j . Let $G = X\Sigma^{-1/2}$, we have

$$\mathbf{vec}(oldsymbol{X}oldsymbol{\Pi}_j) = \mathbf{vec}(oldsymbol{G}oldsymbol{\Sigma}^{1/2}oldsymbol{\Pi}_j) = (oldsymbol{\Sigma}^{1/2}oldsymbol{\Pi}_j\otimesoldsymbol{I}_n)\,\mathbf{vec}(oldsymbol{G})$$

and

(I.2)

$$oldsymbol{z}_j = oldsymbol{G} oldsymbol{\Sigma}^{-1/2} oldsymbol{e}_j ig\| = rac{1}{ig\| oldsymbol{\Sigma}^{-1/2} oldsymbol{e}_j ig\|} (oldsymbol{e}_j^ op oldsymbol{\Sigma}^{-1/2} \otimes oldsymbol{I}_n) \operatorname{vec}(oldsymbol{G}).$$

Since $\operatorname{vec}(G)$ is a standard Gaussian vector in \mathbb{R}^{np} , the above two vectors $\operatorname{vec}(X\Pi_j)$ and z_j are two Gaussian vectors. It suffices to show that $\operatorname{vec}(X\Pi_j)$ and z_j are uncorrelated, which can be shown by verifying that

$$(\boldsymbol{e}_j^{\top}\boldsymbol{\Sigma}^{-1/2}\otimes \boldsymbol{I}_n)(\boldsymbol{\Sigma}^{1/2}\boldsymbol{\Pi}_j\otimes \boldsymbol{I}_n)=(\boldsymbol{e}_j^{\top}\boldsymbol{\Pi}_j\otimes \boldsymbol{I}_n)=\boldsymbol{0}$$

thanks to $\Pi_i^{\top} e_j = \mathbf{0}$ from definition of Π_j .

Applying (Tan and Bellec, 2024, Lemma S5.3) to the mapping: $\mathbf{z}_j \mapsto \mathbf{F}(\mathbf{z}_j)/\sqrt{n}$, using $z_{ij} = \mathbf{e}_i^\top \mathbf{z}_j$, we have

(I.1)
$$\mathbb{E}\left[\left\|\frac{\boldsymbol{z}_{j}^{\top}\boldsymbol{F}(\boldsymbol{z}_{j})}{\sqrt{n}}-\frac{1}{\sqrt{n}}\sum_{i=1}^{n}\frac{\partial\boldsymbol{e}_{i}^{\top}\boldsymbol{F}(\boldsymbol{z}_{j})}{\partial z_{ij}}-\frac{\boldsymbol{z}_{j}^{\top}\boldsymbol{F}(\tilde{\boldsymbol{z}}_{j})}{\sqrt{n}}\right\|^{2}\right] \leq \frac{3}{n}\mathbb{E}\sum_{i=1}^{n}\left\|\frac{\partial\boldsymbol{F}(\boldsymbol{z}_{j})}{\partial z_{ij}}\right\|_{\mathrm{F}}^{2},$$

where $\tilde{z}_j \sim \mathsf{N}(\mathbf{0}, I_n)$ is independent of (X, y).

We want to compute the derivative of $F(z_j)$ with respect to z_{ij} . Since $X = X\Pi_j + z_j \frac{e_j^{\dagger}}{\|\Sigma^{-1/2} e_j\|}$. Conditional on $X\Pi_j$ (that is, with $X\Pi_j$ held fixed), we have $\frac{\partial F}{\partial z_{ij}} = \frac{\partial F}{\partial x_{ij}} \frac{1}{\|\Sigma^{-1/2} e_j\|}$. According to the expression of $\frac{\partial F_{lt}}{\partial x_{ij}}$ in Corollary C.2, we have

$$\sum_{i=1}^{n} \frac{\partial \boldsymbol{e}_{i}^{\top} \boldsymbol{F}}{\partial z_{ij}} = \sum_{i=1}^{n} \frac{\partial \boldsymbol{e}_{i}^{\top} \boldsymbol{F}}{\partial x_{ij}} \frac{1}{\|\boldsymbol{\Sigma}^{-1/2} \boldsymbol{e}_{j}\|}$$
$$= \sum_{i=1}^{n} \sum_{t=1}^{T} (D_{ij}^{it} + \Delta_{ij}^{it}) \boldsymbol{e}_{t}^{\top} \frac{1}{\|\boldsymbol{\Sigma}^{-1/2} \boldsymbol{e}_{j}\|}$$
$$= \frac{-\boldsymbol{e}_{j}^{\top} (\hat{\boldsymbol{B}} - \boldsymbol{B}^{*}) (n\boldsymbol{I}_{T} - \hat{\boldsymbol{A}})^{\top}}{\|\boldsymbol{\Sigma}^{-1/2} \boldsymbol{e}_{j}\|} + \operatorname{Rem}_{j} \qquad \text{by (C.7)},$$

where $\operatorname{Rem}_j = \sum_{i=1}^n \sum_{t=1}^T \Delta_{ij}^{it} \boldsymbol{e}_t^\top \frac{1}{\|\boldsymbol{\Sigma}^{-1/2} \boldsymbol{e}_j\|}$. Define $\boldsymbol{w}_j \in \mathbb{R}^T$ by

$$\boldsymbol{w}_{j}^{\top} \stackrel{\text{def}}{=} \frac{\boldsymbol{e}_{j}^{\top} \boldsymbol{\Sigma}^{-1} \boldsymbol{X}^{\top} (\boldsymbol{Y} - \boldsymbol{X} \hat{\boldsymbol{B}}) + \boldsymbol{e}_{j}^{\top} (\hat{\boldsymbol{B}} - \boldsymbol{B}^{*}) (n \boldsymbol{I}_{T} - \hat{\boldsymbol{A}})^{\top}}{\sqrt{n} \|\boldsymbol{\Sigma}^{-1/2} \boldsymbol{e}_{j}\|} - \frac{\boldsymbol{z}_{j}^{\top} \boldsymbol{F}(\tilde{\boldsymbol{z}}_{j})}{\sqrt{n}}$$

Combining (I.1) and (I.2), by the triangle inequality,

$$\sum_{j=1}^{p} \mathbb{E}\left[\left\|\boldsymbol{w}_{j}^{\top}\right\|^{2}\right] = \sum_{j=1}^{p} \mathbb{E}\left[\left\|\frac{\boldsymbol{z}_{j}^{\top}\boldsymbol{F}(\boldsymbol{z}_{j})}{\sqrt{n}} - \sum_{i}\frac{\partial\boldsymbol{e}_{i}^{\top}\boldsymbol{F}(\boldsymbol{z}_{j})}{\partial\boldsymbol{z}_{ij}}/\sqrt{n} - \frac{\boldsymbol{z}_{j}^{\top}\boldsymbol{F}(\tilde{\boldsymbol{z}}_{j})}{\sqrt{n}} - \frac{\operatorname{Rem}_{j}}{\sqrt{n}}\right\|^{2}\right]$$
$$\leq \frac{2}{n} \mathbb{E}\left[\sum_{j=1}^{p} \|\operatorname{Rem}_{j}\|^{2}\right] + \frac{6}{n} \mathbb{E}\left[\sum_{i=1}^{n}\sum_{j=1}^{p} \left\|\frac{\partial\boldsymbol{F}(\boldsymbol{z}_{j})}{\partial\boldsymbol{z}_{ij}}\right\|_{\mathrm{F}}^{2}\right].$$

We now bound the two terms in the last line. For the first term, it is bounded from above by $C(\zeta, T, \kappa, \gamma) \operatorname{var}(y_1)$ thanks to Lemma I.1. For the second term, we first rewrite the derivative with respect to z_{ij} using chain rule of differentiation. Recall $\boldsymbol{X} = \boldsymbol{X} \boldsymbol{\Pi}_j + \boldsymbol{z}_j \frac{\boldsymbol{e}_j^\top}{\|\boldsymbol{\Sigma}^{-1/2} \boldsymbol{e}_j\|}$. Conditional on $\boldsymbol{X} \boldsymbol{\Pi}_j$, we have $\frac{\partial \boldsymbol{F}}{\partial z_{ij}} = \frac{\partial \boldsymbol{F}}{\partial x_{ij}} \frac{1}{\|\boldsymbol{\Sigma}^{-1/2} \boldsymbol{e}_j\|}$. Thus,

$$\frac{1}{n}\mathbb{E}\Big[\sum_{i=1}^{n}\sum_{j=1}^{p}\left\|\frac{\partial \boldsymbol{F}(\boldsymbol{z}_{j})}{\partial z_{ij}}\right\|_{\mathrm{F}}^{2}\Big] = \frac{1}{n}\mathbb{E}\Big[\sum_{t=1}^{T}\sum_{i=1}^{n}\sum_{j=1}^{p}(\boldsymbol{e}_{j}^{\top}\boldsymbol{\Sigma}^{-1}\boldsymbol{e}_{j})^{-1}\left\|\frac{\partial \boldsymbol{F}\boldsymbol{e}_{t}}{\partial x_{ij}}\right\|_{\mathrm{F}}^{2}\Big].$$

According to Lemma I.2, the last line is bounded by $C(\zeta, T, \kappa, \gamma)(\|\mathbf{\Sigma}^{1/2}b^*\| + \sigma^2)$. In summary, $\sum_{j=1}^p \mathbb{E}[\|\mathbf{w}_j^{\top}\|^2] \leq C(\zeta, T, \kappa, \gamma) \operatorname{var}(y_1)$. Let

$$\boldsymbol{L}_n = (\boldsymbol{I}_T - \boldsymbol{A}/n)^{-1}.$$

Left multiplying $(I_T - \widehat{\mathbf{A}}/n)^{-1}$ inside the ℓ_2 norm of w_j , we have

$$\sum_{j=1}^{p} \mathbb{E}\Big[\Big\|\frac{\boldsymbol{L}_{n}(\boldsymbol{Y}-\boldsymbol{X}\widehat{\boldsymbol{B}})^{\top}\boldsymbol{X}\boldsymbol{\Sigma}^{-1}\boldsymbol{e}_{j}+n(\widehat{\boldsymbol{B}}-\boldsymbol{B}^{*})^{\top}\boldsymbol{e}_{j}}{\sqrt{n}\|\boldsymbol{\Sigma}^{-1/2}\boldsymbol{e}_{j}\|}-\frac{\boldsymbol{L}_{n}\boldsymbol{F}(\widetilde{\boldsymbol{z}}_{j})^{\top}\boldsymbol{z}_{j}}{\sqrt{n}}\Big\|^{2}\Big]=\sum_{j=1}^{p} \mathbb{E}\Big[\Big\|\boldsymbol{L}_{n}\boldsymbol{w}_{j}\Big\|^{2}\Big].$$

Since $\|(\boldsymbol{I}_T - \widehat{\boldsymbol{A}}/n)^{-1}\|_{\text{op}} \leq C(\zeta, T)(1 + \|\boldsymbol{X}\|_{\text{op}}^2/n)^{T^2}$ from Lemma E.3, define the event $\Omega = \{\boldsymbol{X} \in \mathbb{R}^{n \times p} : \|\boldsymbol{X}\|_{\text{op}}/\sqrt{n} \leq 2 + \sqrt{\gamma}\}$ as before, so that

$$\sum_{j=1}^{p} \mathbb{E}[\|\boldsymbol{L}_{n}\boldsymbol{w}_{j}\|^{2}] \leq \sum_{j=1}^{p} C(\zeta, T, \gamma) \mathbb{E}\Big[\|\mathbb{I}\{\Omega\}\boldsymbol{w}_{j}\|^{2}\Big] + \sum_{j=1}^{p} \mathbb{E}\Big[\|\mathbb{I}\{\Omega^{c}\}\boldsymbol{L}_{n}\boldsymbol{w}_{j}\|^{2}\Big].$$

For the first term with $\mathbb{I}\{\Omega\}$, the previously established bound $\sum_{j=1}^{p} \mathbb{E}[\|\boldsymbol{w}_{j}\|^{2}] \leq C(\zeta, T, \kappa, \gamma) \operatorname{var}(y_{1})$ bounds from above the first term. Each summand in the second term is exponentially small, using $\mathbb{E}[\mathbb{I}\{\Omega^{c}\}\|\boldsymbol{w}_{j}\|^{2}] \leq \mathbb{P}(\Omega^{c})^{1/2}\mathbb{E}[\|\boldsymbol{w}_{j}\|^{4}]^{1/2}$ with $\mathbb{P}(\Omega^{c})^{1/2} \leq e^{-n/4}$, while $\mathbb{E}[\|\boldsymbol{w}_{j}\|^{4}]^{1/2}/\operatorname{var}(y_{1})$ is at most polynomial in (n, p) with multiplicate constant $C(\zeta, T, \kappa, \gamma)$ thanks to several applications of the Cauchy-Schwarz inequality to combine the moment bounds in Lemmas E.8 and E.10 and the equality in distribution $F(\tilde{\boldsymbol{z}}_{j}) =^{d} \boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{B}}$.

We wish to show that for the 2-Wasserstein distance,

(I.3)
$$\max_{j \in [p]} W_2\left(\mathsf{Law}\left(\frac{\boldsymbol{L}_n \boldsymbol{F}(\boldsymbol{\widetilde{z}}_j)^\top \boldsymbol{z}_j}{\sqrt{n}}\right), \ \mathsf{N}\left(\boldsymbol{0}_T, \boldsymbol{S} + \mathbb{E}[\boldsymbol{H}^\top \boldsymbol{\Sigma} \boldsymbol{H}]\right)\right) \to 0.$$

By Lemma E.10, we may extract a subsequence of regression problems such that there exists psd matrices $K, \bar{K} \in \mathbb{R}^{T \times T}$ such that (E.14) holds. We will not adapt a particular notation for the extracted subsequence, but keep in mind that we are now working along this subsequence and that $n \to +\infty$ with n being restricted to this subsequence.

By (E.16) and (E.17),

(I.4)
$$\mathbb{E}[\|\boldsymbol{F}^{\top}\boldsymbol{F}/n-\boldsymbol{K}\|_{\mathrm{F}}^{2}] \to 0, \qquad \mathbb{E}[\|\boldsymbol{H}^{\top}\boldsymbol{\Sigma}\boldsymbol{H}+\boldsymbol{S}-\bar{\boldsymbol{K}}\|_{\mathrm{F}}^{2}] \to 0.$$

Note that Theorem 2.2 further shows that

(I.5)
$$\mathbb{E}[\|\boldsymbol{L}_n(\boldsymbol{F}^{\top}\boldsymbol{F}/n)\boldsymbol{L}_n^{\top} - \bar{\boldsymbol{K}}\|_{\mathrm{F}}] \to 0.$$

Consider the LDLT decompositions $\mathbf{K} = \mathbf{L}\mathbf{D}\mathbf{L}^{\top}$ and $\bar{\mathbf{K}} = \bar{\mathbf{L}}\bar{\mathbf{D}}\bar{\mathbf{L}}^{\top}$ for the psd matrices \mathbf{K} and $\bar{\mathbf{K}}$, so that $\mathbf{D}, \bar{\mathbf{D}}$ are diagonal with non-negative entries and $\mathbf{L}, \bar{\mathbf{L}}$ are lower triangular with all diagonal entries equal to 1. Since Lemma E.3 gives $\|\mathbf{L}_n\|_{\text{op}} = O_P(1)$,

(I.6)
$$\boldsymbol{L}_{n}\boldsymbol{K}\boldsymbol{L}_{n}^{\top}-\bar{\boldsymbol{K}}\overset{\mathrm{p}}{\longrightarrow}0, \quad \bar{\boldsymbol{L}}^{-1}\boldsymbol{L}_{n}\boldsymbol{L}\boldsymbol{D}-\bar{\boldsymbol{D}}\bar{\boldsymbol{L}}^{\top}(\boldsymbol{L}_{n}^{\top})^{-1}(\boldsymbol{L}^{\top})^{-1}\overset{\mathrm{p}}{\longrightarrow}0.$$

On the right, we have the difference of a lower triangular matrix with diagonal D and an upper triangular matrix with diagonal \overline{D} . Thus the convergence to 0 in probability gives $D = \overline{D}$ and $\overline{L}^{-1}L_nLD \xrightarrow{P} D$.

We also have $\bar{L}^{-1}L_nL\sqrt{D} \xrightarrow{p} \sqrt{D}$ by multiplying on the right by the pseudo-inverse of \sqrt{D} . Now let $L_{\infty} = \bar{L}L^{-1}$, so that

$$(\boldsymbol{L}_n - \boldsymbol{L}_\infty)\boldsymbol{L}\sqrt{\boldsymbol{D}} = \bar{\boldsymbol{L}}\bar{\boldsymbol{L}}^{-1}(\boldsymbol{L}_n - \boldsymbol{L}_\infty)\boldsymbol{L}\sqrt{\boldsymbol{D}}$$
$$= \bar{\boldsymbol{L}}(\bar{\boldsymbol{L}}^{-1}\boldsymbol{L}_n\boldsymbol{L}\sqrt{\boldsymbol{D}} - \sqrt{\boldsymbol{D}})\overset{\mathrm{p}}{\longrightarrow} 0.$$

By the continuous mapping theorem, $(\boldsymbol{L}_n - \boldsymbol{L}_\infty)\boldsymbol{K}(\boldsymbol{L}_n - \boldsymbol{L}_\infty)^\top \xrightarrow{\mathrm{p}} 0$, and since Lemma E.3 gives $\|\boldsymbol{L}_n\|_{\mathrm{op}} = O_P(1)$,

(I.7)
$$(\boldsymbol{L}_n - \boldsymbol{L}_\infty)(\boldsymbol{F}^\top \boldsymbol{F}/n)(\boldsymbol{L}_n - \boldsymbol{L}_\infty)^\top \xrightarrow{\mathbf{p}} 0, \qquad \|(\boldsymbol{L}_n - \boldsymbol{L}_\infty)\boldsymbol{F}^\top/\sqrt{n}\| \xrightarrow{\mathbf{p}} 0.$$

Although we have not shown that $L_n \xrightarrow{p} L_\infty$, this means that we can still replace L_n by the deterministic L_∞ up to when multiplied on the right by F^{\top}/\sqrt{n} . The previous display also holds with F replaced by $F(\tilde{z}_j)$, uniformly over $j \in [p]$ since

(I.8)
$$\mathbb{E}\|(\boldsymbol{L}_{n}-\boldsymbol{L}_{\infty})\frac{\boldsymbol{F}^{\top}\boldsymbol{F}}{n}(\boldsymbol{L}_{n}-\boldsymbol{L}_{\infty})^{\top}-(\boldsymbol{L}_{n}-\boldsymbol{L}_{\infty})\frac{\boldsymbol{F}(\tilde{\boldsymbol{z}}_{j})^{\top}\boldsymbol{F}(\tilde{\boldsymbol{z}}_{j})}{n}(\boldsymbol{L}_{n}-\boldsymbol{L}_{\infty})^{\top}\|_{\mathrm{op}}$$
$$\leq \mathbb{E}[\|\boldsymbol{L}_{n}-\boldsymbol{L}_{\infty}\|_{\mathrm{op}}^{2}\|\boldsymbol{F}^{\top}\boldsymbol{F}/n-\boldsymbol{F}(\tilde{\boldsymbol{z}}_{j})^{\top}\boldsymbol{F}(\tilde{\boldsymbol{z}}_{j})/n\|_{\mathrm{op}}]$$
$$\leq \mathbb{E}[\|\boldsymbol{L}_{n}-\boldsymbol{L}_{\infty}\|_{\mathrm{op}}^{4}]^{1/2}2\mathbb{E}[\|\boldsymbol{F}^{\top}\boldsymbol{F}/n-\mathbb{E}[\boldsymbol{F}^{\top}\boldsymbol{F}/n]\|_{\mathrm{op}}^{2}] \to 0$$

thanks to the Cauchy-Schwarz inequality and the equality in distribution $\boldsymbol{F} = \boldsymbol{F}(\tilde{\boldsymbol{z}}_j)$ for the last inequality. The last line converges to 0 thanks to Lemma E.3 to show that $\mathbb{E}[\|\boldsymbol{L}_n - \boldsymbol{L}_{\infty}\|_{\text{op}}^4]^{1/2}$ is bounded, and thanks to (E.16) which gives $\mathbb{E}[\|\boldsymbol{F}^{\top}\boldsymbol{F}/n - \mathbb{E}[\boldsymbol{F}^{\top}\boldsymbol{F}/n]\|_{\text{op}}^2] \to 0$. This gives that $\|\boldsymbol{L}_n\boldsymbol{F}(\tilde{\boldsymbol{z}}_j)/\sqrt{n}\|_{\text{op}} \xrightarrow{\mathrm{p}} 0$ uniformly over $j \in [p]$, so that

$$\boldsymbol{L}_{n}\boldsymbol{F}(\widetilde{\boldsymbol{z}}_{j})^{\top}\boldsymbol{z}_{j}/\sqrt{n} = \boldsymbol{L}_{\infty}\boldsymbol{F}(\widetilde{\boldsymbol{z}}_{j})^{\top}\boldsymbol{z}_{j}/\sqrt{n} + o_{P}(1)$$

Since L_{∞} is deterministic, the distribution $L_{\infty}F(\tilde{z}_j)^{\top}z_j/\sqrt{n}$ is independent of j and is the same as the distribution of $L_{\infty}F^{\top}g/\sqrt{n}$ where $g \sim N(0, I_n)$ is independent of F. For any $w \in \mathbb{R}^T$, the characteristic function of $L_{\infty}F^{\top}g/\sqrt{n}$ evaluated at w is

$$\mathbb{E}[\exp(\sqrt{-1}\boldsymbol{w}^{\top}\boldsymbol{F}^{\top}\boldsymbol{g}/\sqrt{n})] = \mathbb{E}\left[\mathbb{E}[\exp(\sqrt{-1}\boldsymbol{w}^{\top}\boldsymbol{L}_{\infty}\boldsymbol{F}^{\top}\boldsymbol{g}/\sqrt{n}) \mid \boldsymbol{g}]\right]$$
$$= \mathbb{E}\left[\exp(-\frac{1}{2n}\boldsymbol{w}^{\top}\boldsymbol{L}_{\infty}\boldsymbol{F}^{\top}\boldsymbol{F}\boldsymbol{L}_{\infty}^{\top}\boldsymbol{w})\right].$$

This converges to $\exp(-\frac{1}{2}\boldsymbol{w}^{\top}\bar{\boldsymbol{K}}\boldsymbol{w})$ by (I.7) and (I.5). We have established the weak convergence $\boldsymbol{L}_{n}\boldsymbol{F}(\boldsymbol{\tilde{z}}_{j})^{\top}\boldsymbol{z}_{j}/\sqrt{n} \xrightarrow{d} \mathsf{N}(\boldsymbol{0}, \bar{\boldsymbol{K}})$ uniformly over $j \in [p]$.

To prove convergence in 2-Wasserstein distance to N(0, K), it is enough to establish convergence in distribution and convergence in the second moment (Villani et al., 2009, Def. 6.8 and Theorem 6.9). Since we have already established convergence in distribution, it is enough to prove

(I.9)
$$\mathbb{E}[\|\boldsymbol{L}_n \boldsymbol{F}(\boldsymbol{\widetilde{z}}_j)^\top \boldsymbol{z}_j / \sqrt{n}\|^2] \to \operatorname{Tr} \boldsymbol{\bar{K}} = \mathbb{E}[\|\mathsf{N}(\mathbf{0}, \boldsymbol{\bar{K}})\|^2]$$

Since **F** is equal in distribution to $F(\tilde{z}_j)$, and \tilde{z}_j is independent of $F(\tilde{z}_j)$, we have

$$\mathbb{E}[\|\boldsymbol{L}_{\infty}\boldsymbol{F}(\widetilde{\boldsymbol{z}}_{j})^{\top}\boldsymbol{z}_{j}/\sqrt{n}\|^{2}] = \mathrm{Tr}[\boldsymbol{L}_{\infty}\mathbb{E}[\boldsymbol{F}^{\top}\boldsymbol{F}/n]\boldsymbol{L}_{\infty}^{\top}] \to \mathrm{Tr}[\boldsymbol{L}_{\infty}\boldsymbol{K}\boldsymbol{L}_{\infty}^{\top}] = \mathrm{Tr}\,\bar{\boldsymbol{K}}.$$

where we used that $D = \overline{D}$ and $L_{\infty} = \overline{L}L^{-1}$ for the last inequality. By the triangle inequality in $L^2(\mathbb{R}^T)$,

$$\left| \mathbb{E} \Big[\| \boldsymbol{L}_{\infty} \boldsymbol{F}(\widetilde{\boldsymbol{z}}_{j})^{\top} \boldsymbol{z}_{j} / \sqrt{n} \|^{2} \Big]^{\frac{1}{2}} - \mathbb{E} \Big[\| \boldsymbol{L}_{n} \boldsymbol{F}(\widetilde{\boldsymbol{z}}_{j})^{\top} \boldsymbol{z}_{j} / \sqrt{n} \|^{2} \Big]^{\frac{1}{2}} \right| \leq \mathbb{E} \Big[\| (\boldsymbol{L}_{n} - \boldsymbol{L}_{\infty}) \boldsymbol{F}(\widetilde{\boldsymbol{z}}_{j})^{\top} \boldsymbol{z}_{j} / \sqrt{n} \|^{2} \Big]^{\frac{1}{2}}.$$

Let $\widetilde{\mathbf{Q}} \in \mathbb{R}^{n \times n}$ be the orthogonal projector on the image of $\mathbf{F}(\widetilde{\mathbf{z}}_j)$, which is of rank at most T and such that $\mathbf{F}(\widetilde{\mathbf{z}}_j)^{\top}\widetilde{\mathbf{Q}} = \mathbf{F}(\widetilde{\mathbf{z}}_j)$. Let $\chi_T^2 = \|\widetilde{\mathbf{Q}}\mathbf{z}_j\|^2$ which has chi-square distribution with at most T degrees of freedom. We may bound from above the integrand in the right-hand side by $\|\mathbf{L}_n - \mathbf{L}_{\infty}\mathbf{F}(\widetilde{\mathbf{z}}_j)/\sqrt{n}\|^2\chi_T^2$. Since T is bounded, $\chi_T^2 = O_P(1)$ and $\|\mathbf{L}_n - \mathbf{L}_{\infty}\mathbf{F}(\widetilde{\mathbf{z}}_j)/\sqrt{n}\| \xrightarrow{\mathrm{p}} 0$ by (I.8). Since the integrand has finite second moment by Lemmas E.3 and E.10 and $\mathbb{E}[(\chi_T^2)^4] < \infty$, it is uniformly integrable so the last display converges to 0.

We have established convergence in distribution and in the second moment, hence by (Villani et al., 2009, Def. 6.8 and Theorem 6.9),

(I.10)
$$\max_{j \in [p]} W_2\left(\mathsf{Law}\left(\frac{\boldsymbol{L}_n \boldsymbol{F}(\widetilde{\boldsymbol{z}}_j)^\top \boldsymbol{z}_j}{\sqrt{n}}\right), \ \mathsf{N}(0, \overline{\boldsymbol{K}})\right) \to 0.$$

Since $S + \mathbb{E}[H^{\top}\Sigma H] \rightarrow \bar{K}$ and $C \mapsto \mathsf{N}(\mathbf{0}, C)$ is continuous in 2-Wasserstein distance, so that $W_2(\mathsf{N}(\mathbf{0}, \bar{K}), S + \mathbb{E}[H^{\top}\Sigma H]) \rightarrow 0$. Combined with (I.10) and (Villani et al., 2009, Corollary 6.11), we obtain (I.3) along any subsequence such that (E.14) holds.

Actually, the convergence (I.3) holds without extracting a subsequence for the following reason. Since both distributions inside W_2 in (I.3) have uniformly bounded second (thanks to Lemmas E.3 and E.10), the W_2 distance in (I.3) is uniformly bounded. To prove (I.3), it is sufficient to prove that 0 is the only limit point of the sequence in the left-hand side of (I.3). For any subsequence such that the left-hand side of (I.3) converges to a limit ν , we may extract further a subsequence such that (E.14) and the above argument holds, showing that the limit point must be $\nu = 0$. Since the bounded sequence in the left-hand side of (I.3) has a unique limit point equal to 0, the convergence (I.3) holds.

Appendix J: Proof of Corollary 2.5

Proof of Corollary 2.5. Let $J_{n,p} \subset [p]$ be the set of $j \in [p]$ such that

(J.1)
$$\mathbb{E}\left[\left(\sqrt{\frac{n}{\|\boldsymbol{\Sigma}^{-1/2}\boldsymbol{e}_j\|^2}} \left(\widehat{\boldsymbol{b}}_j^{t,\text{debias}} - \boldsymbol{b}_j^*\right) - \boldsymbol{\zeta}_{jt}\right)^2\right] \le \frac{1}{a_p} C(\boldsymbol{\zeta}, T, \kappa, \gamma) \text{var}(y_1)$$

for the same constant $C(\zeta, T, \kappa, \gamma)$ as in (2.23). Bounding the left-hand side of (2.23) from below by the sum indexed over $[p] \setminus J_{n,p}$, we get $\frac{1}{a_p} |[p] \setminus J_{n,p}| \leq 1$. On the one hand, $W_2(\text{Law}(\zeta_{jt}), \mathsf{N}(0, \mathbb{E}[r_t])) \to 0$ by (2.22), uniformly over $j \in [p]$. On the other hand, (J.1) provides a vanishing upper bound on the W_2 distance between the law of ζ_{jt} and the law of $\frac{\sqrt{n}}{\|\boldsymbol{\Sigma}^{-1/2}\boldsymbol{e}_j\|} (\hat{\boldsymbol{b}}_j^{t,\text{debias}} - \boldsymbol{b}_j^*)$, uniformly over $j \in J_{n,p}$. The triangle inequality for the 2-Wasserstein distance completes the proof of (2.24).

Appendix K: Asymptotic normality and state evolution in the separable case

Theorem K.1. Let Assumptions 2.1 to 2.4 be fulfilled with $\Sigma = I_p$, assume $var(y_1) \leq v_0$, and assume that T, v_0 are fixed constant as $n, p \to +\infty$. Then there exists deterministic weights $\bar{w}_{s,t}$ (possibly depending on n, p) such that

(K.1)
$$\max_{t=1,\ldots,T} \left(\frac{1}{n} \|\sum_{s=1}^{t} (\hat{w}_{t,s} - \bar{w}_{t,s}) (\boldsymbol{y} - \boldsymbol{X} \widehat{\boldsymbol{b}}^s) \|^2 \right) \xrightarrow{\mathbf{p}} 0.$$

Given these deterministic weights $\bar{w}_{t,s}$, define the debiased estimate $\bar{\boldsymbol{b}}^{T,\text{debias}} \in \mathbb{R}^p$ by $\bar{\boldsymbol{b}}_j^{T,\text{debias}} = \hat{\boldsymbol{b}}_j^T + n^{-1}(\boldsymbol{X}\boldsymbol{e}_j)^\top \sum_{s=1}^T \bar{w}_{T,s}(\boldsymbol{y} - \boldsymbol{X}\hat{\boldsymbol{b}}^s).$

Let $(\eta_j)_{j \in [p]}$ be ζ -Lipschitz functions. Choose the T+1-th nonlinear function g_{T+1} in (2.8) at t = T+1 by applying the functions η_j componentwise to $\bar{\mathbf{b}}_j^{T,\text{debias}}$, i.e., $\hat{\mathbf{b}}_j^{T+1} = \eta_j(\bar{\mathbf{b}}_j^{T,\text{debias}})$. Then the following asymptotic recursion holds between $\mathbb{E}[r_T]$ and $\mathbb{E}[r_{T+1}]$,

(K.2)
$$\left(\sigma^2 + \mathbb{E}_{Z_j \sim \mathsf{N}(0,\mathbb{E}[r_t])} \left[\sum_{j=1}^p \left\{ \eta_j \left(\boldsymbol{b}_j^* + \frac{Z_j}{\sqrt{n}} \right) - \boldsymbol{b}_j^* \right\}^2 \right] \right)^{1/2} - \mathbb{E} \left[r_{T+1} \right]^{1/2} \to 0$$

as $n, p \to +\infty$, as well as $(\sigma^2 + \mathbb{E}[\sum_{j=1}^p \{\eta_j(\widehat{b}_j^{t, \text{debias}}) - b_j^*\}^2])^{1/2} - \mathbb{E}[r_{T+1}]^{1/2} \to 0.$

Proof of Theorem K.1. Without loss of generality, assume that the sequence of regression problems and data (\mathbf{X}, \mathbf{y}) is defined on the same probability space $(\Omega, \mathcal{A}, \mathbb{P})$. We have already proved in Lemmas E.3, E.10 and E.13 and Theorem 2.2 that the event Ω_n defined as

(K.3)
$$\|(\boldsymbol{I}_T - \widehat{\mathbf{A}}/n)^{-1}\|_{\mathrm{op}} + \|\boldsymbol{I}_T - \widehat{\mathbf{A}}/n\|_{\mathrm{op}} \le C(\zeta, T, \gamma, v_0),$$

(K.4)
$$\|(\boldsymbol{I}_T - \widehat{\mathbf{A}}/n)^{-1} \boldsymbol{F}^\top \boldsymbol{F}/n(\boldsymbol{I}_T - \widehat{\mathbf{A}}/n)^{-1} - (\sigma^2 \mathbf{1}_T \mathbf{1}_T^\top + \boldsymbol{H}^\top \boldsymbol{H})\|_{\mathrm{F}} \le n^{-0.49}$$

(K.5)
$$\|\boldsymbol{F}^{\top}\boldsymbol{F}/n - \mathbb{E}[\boldsymbol{F}^{\top}\boldsymbol{F}/n]\|_{\mathrm{F}} + \|\boldsymbol{H}^{\top}\boldsymbol{H} - \mathbb{E}[\boldsymbol{H}^{\top}\boldsymbol{H}]\|_{\mathrm{F}} \le n^{-0.49}$$

for a large enough constant $C(\zeta, T, \gamma, v_0)$ has probability approaching one. In particular, this event $\Omega_n \in \mathcal{A}$ is non-empty and contains some outcome ω_n . For each $s, t \leq T$, for a given regression problem in the sequence (indexed by n), we may define the weight $\bar{w}_{t,s}$ as the random variable $\hat{w}_{t,s} = \mathbf{e}_t^{\top} (\mathbf{I}_T - \hat{\mathbf{A}}/n)^{-1} \mathbf{e}_s$ taken as the outcome ω_n , so that $\bar{w}_{t,s}$ is deterministic. Let us emphasize that this weight implicitly depends on n, i.e., it depends on $n, p, \mathbf{b}^*, (\mathbf{g}_t)_{t \leq T}$ and all other parameters that are allowed to change as $n, p \to +\infty$. Since ω_n is an outcome in Ω_n , the above inequalities give that $\bar{\mathbf{W}} = (\bar{w}_{t,s})_{t \in T, s \in [T]}$ satisfies

(K.6)
$$\|\bar{\boldsymbol{W}}\mathbb{E}[\boldsymbol{F}^{\top}\boldsymbol{F}/n]\bar{\boldsymbol{W}}^{\top} - (\sigma^{2}\boldsymbol{1}_{T}\boldsymbol{1}_{T}^{\top} + \mathbb{E}[\boldsymbol{H}^{\top}\boldsymbol{H}])\|_{\mathrm{F}} \leq C(\zeta, T, \gamma, v_{0})n^{-0.49}$$

in the sense of convergence of a deterministic sequence. Let us now show that (K.1) holds. Denote by $\widehat{W} = (I_T - \widehat{\mathbf{A}}/n)^{-1}$ so that (K.1) is equivalent to $\|(\overline{W} - \widehat{W})\mathbf{F}^\top/\sqrt{n}\|_{\mathrm{F}}^2 \xrightarrow{\mathrm{P}} 0$. Since convergence in probability to 0 for the sequence U_n is equivalent to convergence of $\mathbb{E}[1 \wedge |U_n|] \to 0$, the convergence in probability (K.1) is equivalent to $u_n \stackrel{\text{def}}{=} \mathbb{E}[1 \wedge \|(\overline{W} - \widehat{W})\mathbf{F}^\top/\sqrt{n}\|_{\mathrm{F}}^2] \to 0$. Consider a converging subsequence (u_{n_k}) of $(u_n)_{n\geq 1}$ with limit point $u_\infty \in [0, 1]$. By (E.14), we may further extract a subsequence $(u_{n_{k_m}})$, such that in this nested subsequence $u_{n_{k_m}} \to u_\infty$ and $\mathbb{E}[\mathbf{F}^\top \mathbf{F}/n] \to \mathbf{K}$ both holds. In the event Ω_n , (K.6) is also satisfied for \widehat{W} , hence in this subsequence and in Ω_n ,

(K.7)
$$\|\bar{\boldsymbol{W}}\boldsymbol{K}\bar{\boldsymbol{W}}^{\top} - \widehat{\boldsymbol{W}}\boldsymbol{K}\widehat{\boldsymbol{W}}^{\top}\|_{\mathrm{F}} \leq C(\zeta, T, \gamma, v_0)(n^{-0.49} + \|\boldsymbol{K} - \mathbb{E}[\boldsymbol{F}^{\top}\boldsymbol{F}/n]\|_{\mathrm{F}}).$$

Let $\mathbf{K} = \mathbf{L}\mathbf{D}\mathbf{L}^{\top}$ be the LDLT decomposition of \mathbf{K} with \mathbf{L} triangular with diagonal elements all equal to 1 and \mathbf{D} diagonal with non-negative entries. Since the operator norms of $\mathbf{\bar{W}}$ and $\mathbf{\widehat{W}}$ are bounded by $C(\zeta, T, \gamma, v_0)$ in Ω_n , multiplying on the left by $\mathbf{L}^{-1}\mathbf{\widehat{W}}^{-1}$ and on the right by $(\mathbf{L}^{\top}\mathbf{\bar{W}}^{\top})^{-1}$, we get

$$\begin{aligned} \|(\widehat{\boldsymbol{W}}\boldsymbol{L})^{-1}\bar{\boldsymbol{W}}\boldsymbol{L}\boldsymbol{D} - \boldsymbol{D}\boldsymbol{L}^{\top}\widehat{\boldsymbol{W}}^{\top}(\boldsymbol{L}^{\top}\bar{\boldsymbol{W}}^{\top})^{-1}\|_{\mathrm{F}} \\ &\leq C(\zeta,T,\gamma,v_{0},\|\boldsymbol{L}\|_{\mathrm{op}})(n^{-0.49} + \|\boldsymbol{K} - \mathbb{E}[\boldsymbol{F}^{\top}\boldsymbol{F}/n]\|_{\mathrm{F}}). \end{aligned}$$

Now $(\widehat{\boldsymbol{W}}\boldsymbol{L})^{-1}\overline{\boldsymbol{W}}\boldsymbol{L}\boldsymbol{D}$ is lower triangular while $\boldsymbol{D}\boldsymbol{L}^{\top}\widehat{\boldsymbol{W}}^{\top}(\boldsymbol{L}^{\top}\overline{\boldsymbol{W}}^{\top})^{-1}$ is upper triangular, so the left-hand side is bounded from below by $\|(\widehat{\boldsymbol{W}}\boldsymbol{L})^{-1}\overline{\boldsymbol{W}}\boldsymbol{L}\boldsymbol{D}-\boldsymbol{D}\|_{\mathrm{F}}$ (we may bound from below the full Frobenius norm by the Frobenius norm of the lower triangular part only). Thus on Ω_n ,

$$\|(\widehat{\boldsymbol{W}}\boldsymbol{L})^{-1}\bar{\boldsymbol{W}}\boldsymbol{L}\boldsymbol{D}-\boldsymbol{D}\|_{\mathrm{F}} \leq C(\zeta,T,\gamma,v_0,\|\boldsymbol{L}\|_{\mathrm{op}})(n^{-0.49}+\|\boldsymbol{K}-\mathbb{E}[\boldsymbol{F}^{\top}\boldsymbol{F}/n]\|_{\mathrm{F}}).$$

Multiplying by $\widehat{W}L$ on the left again, and by $L^{\top}(\widehat{W} - \overline{W})^{\top}$ on the right, we have proved that on Ω_n ,

$$\|(\bar{\boldsymbol{W}}\boldsymbol{L}\boldsymbol{D} - \widehat{\boldsymbol{W}}\boldsymbol{L}\boldsymbol{D})\boldsymbol{L}^{\top}(\widehat{\boldsymbol{W}} - \bar{\boldsymbol{W}})^{\top}\|_{\mathrm{F}} \leq C(\zeta, T, \gamma, v_0, \|\boldsymbol{L}\|_{\mathrm{op}})(n^{-0.49} + \|\boldsymbol{K} - \mathbb{E}[\boldsymbol{F}^{\top}\boldsymbol{F}/n]\|_{\mathrm{F}}).$$

Finally, we may replace $\mathbf{K} = \mathbf{L}\mathbf{D}\mathbf{L}^{\top}$ by $\mathbf{F}^{\top}\mathbf{F}/n$ on Ω_n in the left-hand side by enlarging the right-hand side by a constant if necessary. This implies that in Ω_n ,

$$\|(\bar{\boldsymbol{W}} - \widehat{\boldsymbol{W}})(\boldsymbol{F}^{\top}\boldsymbol{F}/n)(\widehat{\boldsymbol{W}} - \bar{\boldsymbol{W}})^{\top}\|_{\mathrm{F}} \le C(\zeta, T, \gamma, v_0, \|\boldsymbol{L}\|_{\mathrm{op}})(n^{-0.49} + \|\boldsymbol{K} - \mathbb{E}[\boldsymbol{F}^{\top}\boldsymbol{F}/n]\|_{\mathrm{F}})$$

and since $\mathbb{P}(\Omega_n) \to 1$, this shows that $u_{\infty} = 0$ is the unique limit point of the sequence $(u_n)_{n \ge 1}$. Since 0 is the unique limit point, $(u_n)_{n \ge 1} \to 0$ and (K.1) holds.

Recall that $\mathbb{E}[r_{T+1}] = \sigma^2 + \mathbb{E}[\|\boldsymbol{g}_{T+1}(\bar{\boldsymbol{b}}^{T,\text{debias}}) - \boldsymbol{b}^*\|^2]$ by definition of $\hat{\boldsymbol{b}}^{T+1}$. By the triangle inequality for $\mathbb{E}[\sigma^2 + \|\cdot\|^2]^{1/2}$ we have

$$\begin{aligned} \left| \left(\sigma^{2} + \mathbb{E}[\|\boldsymbol{g}_{T+1}(\widehat{\boldsymbol{b}}^{T,\text{debias}}) - \boldsymbol{b}^{*}\|^{2}] \right)^{1/2} - \mathbb{E}[r_{T+1}]^{1/2} \right| \\ &\leq \mathbb{E}[\|\boldsymbol{g}_{T+1}(\widehat{\boldsymbol{b}}^{T,\text{debias}}) - \boldsymbol{g}_{T+1}(\overline{\boldsymbol{b}}^{T,\text{debias}})\|^{2}]^{1/2} \\ &\leq \zeta \mathbb{E}[\|\widehat{\boldsymbol{b}}^{T,\text{debias}} - \overline{\boldsymbol{b}}^{T,\text{debias}}\|^{2}]^{1/2} \\ &= \zeta \mathbb{E}[\|\boldsymbol{n}^{-1}\boldsymbol{X}^{\top}\boldsymbol{F}(\bar{\boldsymbol{W}} - \widehat{\boldsymbol{W}})\|_{\text{F}}^{2}]^{1/2} \\ &\leq \zeta \mathbb{E}[\|\boldsymbol{X}^{\top}\boldsymbol{X}/n\|_{\text{op}}\|n^{-1/2}\boldsymbol{F}(\bar{\boldsymbol{W}} - \widehat{\boldsymbol{W}})\|_{\text{F}}^{2}]^{1/2} \end{aligned}$$

since $\hat{\boldsymbol{b}}^{T,\text{debias}}$ and $\bar{\boldsymbol{b}}^{T,\text{debias}}$ only differ in the weights used for the columns of \boldsymbol{F} . The random variable inside the final expectation converges to 0 in probability by the previous argument, and has uniformly bounded fourth moment by Lemmas E.3, E.8 and E.10. By dominated convergence, the left-hand side converges to 0. Similarly, Theorem 2.4 gives

$$\mathbb{E}[\|\widehat{\boldsymbol{b}}^{T,\text{debias}} - (\boldsymbol{b}^* + n^{-1/2}\boldsymbol{\zeta}_{\cdot,T})\|^2] \le C(\zeta, \gamma, T, v_0)/n$$

where $\boldsymbol{\zeta}_{,T} \in \mathbb{R}^p$ is the random vector with components $(\boldsymbol{\zeta}_{j,T}) j \in [p]$ from Theorem 2.4. By the triangle inequality, similarly to the above display,

(K.9)
$$\begin{aligned} & \left| \left(\sigma^2 + \mathbb{E}[\|\boldsymbol{g}_{T+1}(\hat{\boldsymbol{b}}^{T,\text{debias}}) - \boldsymbol{b}^*\|^2] \right)^{1/2} - \left(\sigma^2 + \mathbb{E}[\|\boldsymbol{g}_{T+1}(\boldsymbol{b}^* + n^{-1/2}\boldsymbol{\zeta}_{\cdot,T}) - \boldsymbol{b}^*\|^2] \right)^{1/2} \right| \\ & \leq \zeta \mathbb{E}[\|\hat{\boldsymbol{b}}^{T,\text{debias}} - (\boldsymbol{b}^* + n^{-1/2}\boldsymbol{\zeta}_{\cdot,T})\|^2]^{1/2} \\ & \leq C(\zeta, T, \gamma, v_0) / \sqrt{n}. \end{aligned}$$

Finally, by (2.22), for each $j \in [p]$ there exists a coupling $(Z_j, \zeta_{j,T})$ with $Z_j \sim \mathsf{N}(0, \mathbb{E}[\mathsf{r}_t])$ such that $\mathbb{E}[(Z_j - \zeta_{j,T})^2]^{1/2} \leq (2.22) \to 0$ where (2.22) the maximum over $j \in [p]$ of the 2-Wasserstein distance in the left-hand side of (2.22). Since $g_{T+1} : \mathbb{R}^p \to \mathbb{R}^p$ is separable, acting componentwise with the ζ -Lipschitz functions $\eta_j : \mathbb{R} \to \mathbb{R}$,

(K.10)
$$\left\| \left(\sigma^{2} + \sum_{j=1}^{p} \mathbb{E} \left[\left(\eta_{j} \left(b_{j}^{*} + \frac{Z_{j}}{\sqrt{n}} \right) - b_{j}^{*} \right)^{2} \right] \right)^{1/2} - \left(\sigma^{2} + \mathbb{E} \left[\left\| \boldsymbol{g}_{T+1} \left(\boldsymbol{b}^{*} + \frac{\boldsymbol{\zeta}_{\cdot,T}}{\sqrt{n}} \right) - \boldsymbol{b}^{*} \right\|^{2} \right] \right)^{1/2} \right\|$$
$$\leq \zeta \mathbb{E} \left[\sum_{j=1}^{p} \left(\frac{Z_{j}}{\sqrt{n}} - \frac{\zeta_{jT}}{\sqrt{n}} \right)^{2} \right]^{1/2} \leq \zeta \sqrt{\frac{p}{n}} (2.22) \to 0.$$

Combining the inequalities (K.8)-(K.10) gives (K.2).

The result $(\sigma^2 + \mathbb{E}[\sum_{j=1}^p \{\eta_j(\hat{b}_j^{t,\text{debias}}) - b_j^*\}^2])^{1/2} - \mathbb{E}[r_{T+1}]^{1/2} \to 0$ is a direct consequence of (K.2) and the triangle inequality. This concludes the proof of Theorem K.1.