Targeted Principal Components Regression

Karl Oskar Ekvall*,1, 2, 3

1Applied Statistics Research Unit, Institute of Statistics and Mathematical Methods in Economics, Faculty of Mathematics and Geoinformation, TU Wien
2Department of Economics, University of Gothenburg
3Division of Biostatistics, Institute of Environmental Medicine Karolinska Institute Nobels väg 13, 171 77 Stockholm, Sweden
karl.oskar.ekvall@ki.se

Abstract

We propose a principal components regression method based on maximizing a joint pseudo-likelihood for responses and predictors. Our method uses both responses and predictors to select linear combinations of the predictors relevant for the regression, thereby addressing an oft-cited deficiency of conventional principal components regression. The proposed estimator is shown to be consistent in a wide range of settings, including ones with non-normal and dependent observations; conditions on the first and second moments suffice if the number of predictors ($p$) is fixed and the number of observations ($n$) tends to infinity and dependence is weak, while stronger distributional assumptions are needed when $p \to \infty$ with $n$. We obtain the estimator’s asymptotic distribution as the projection of a multivariate normal random vector onto a tangent cone of the parameter set at the true parameter, and find the estimator is asymptotically more efficient than competing ones. In simulations our method is substantially more accurate than conventional principal components regression and compares favorably to partial least squares and predictor envelopes. The method’s practical usefulness is illustrated in a data example with cross-sectional prediction of stock returns.

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1 Introduction

In conventional principal components regression (PCR), \( r \geq 1 \) responses are regressed on principal components of \( p \) predictors by least squares (e.g. Jolliffe 2002, Chapter 8). Typically, \( k < p \) components with large sample variances are included as regressors. It is well known this practice can be unreliable (e.g. Cox 1968; Jolliffe 1982; Cook 2018b), essentially because the fit of the regression is ignored when selecting regressors. To be more precise it is useful to distinguish between sample and population principal components: the former are linear combinations of the predictors whose weight vectors are eigenvectors the predictors’ sample covariance matrix; the latter are defined similarly but with eigenvectors of the population covariance matrix. When conventional principal components regression is unreliable, it may be that population principal components with small variances are relevant, that is, have an effect on the responses. Many methods appropriate for such settings have been proposed (e.g. Helland 1992; Cook et al. 2010; Kelly and Pruitt 2015; Lang and Zou 2020). However, it may also be that only \( k < p \) population principal components with large variances are relevant but that they are substantially different from their sample counterparts. Intuitively, this happens when eigenvectors of the predictors’ sample covariance matrix are substantially different from those of the population covariance matrix. Bair et al. (2006) and Yu et al. (2006) showed that in many such settings prediction and classification can be improved by using information in an outcome variable to get relevant linear combinations of the predictors. However, despite the practical relevance of models where only a few population principal components with large variances affect the responses (e.g. Stock and Watson 2002; Bai and Wang 2016; Singer et al. 2016), a unified method for efficient inference and prediction has not been proposed. We address this with a method based on a joint multivariate normal pseudo-likelihood of responses and predictors. Our method uses both responses and predictors to select linear combinations of the predictors relevant for modeling the responses. To contrast with the conventional method, we say our method
targets the responses and, hence, we call it targeted principal components regression (TPCR).

To formalize, consider a model for the first two moments of $Z_i = [Y_i^T, X_i^T]^T \in \mathbb{R}^{r+p}$ ($i = 1, \ldots, n$) which assumes $\mathbb{E}(Z_i) = 0$, $\mathbb{E}(Y_i \mid X_i) = \beta^T X_i$, $\beta \in \mathbb{R}^{p \times r}$, $\text{cov}(Y_i \mid X_i) = \Omega^{-1}$, and $\text{cov}(X_i) = \Sigma_X$. That $\mathbb{E}(Z_i) = 0$ is not needed in practice but simplifies the exposition. To get a principal components structure, suppose also, for $\tau > 0$ and $\Psi \in \mathbb{R}^{p \times p}$, a symmetric and positive semi-definite matrix of rank $k$, $\Sigma_X = \Psi + \tau I_p$; $P_\Psi \beta = \beta$, \hspace{1cm} (1)

where $P_\Psi$ is the orthogonal projection onto the column space of $\Psi$ and $I_p$ the $p \times p$ identity matrix. The first equality in (1) implies eigenvectors of $\Psi$ with non-zero eigenvalues are leading eigenvectors of $\Sigma_X$, that is, eigenvectors corresponding to large eigenvalues. Consequently, the second equality says the columns of $\beta$ lie in the span of $k$ leading eigenvectors of $\Sigma_X$. Equivalently, if $U \in \mathbb{R}^{p \times k}$ has those eigenvectors as columns, the model says $\beta = U \gamma$ for some $\gamma \in \mathbb{R}^{k \times r}$ and hence $\mathbb{E}(Y_i \mid X_i) = \gamma^T U^T X_i$. In particular, the elements of $U^T X_i$ are the $k$ (population) principal components relevant for $Y_i$. The classical (multivariate) linear regression model is a special case with $k = p$. When $k < p$, substantial efficiency gains can often be realized by exploiting the parametric connection between $\beta$ and $\Sigma_X$.

The first condition in (1) also implies the $p - k$ smallest eigenvalues of $\Sigma_X$ are all equal to $\tau$, so $\Sigma_X$ is spiked \cite{Johnstone2001}. A spiked $\Sigma_X$ is not necessary to define a principal components regression model but it facilitates our theory and implementation. Spiked covariance matrices are common in the literature \cite{Johnstone2001, Cai2014, Wang2017, Donoho2018}, and arise naturally in latent variable and factor models. For example, one popular latent variable model, which is also
motivated in our data example (see Section 5), assumes

\[ X_i = \Gamma^T W_i + \sqrt{\tau} E_i, \tag{2} \]

where \( \Gamma \in \mathbb{R}^{k \times p} \) is a parameter and elements of the latent variables \( W_i \in \mathbb{R}^k \) and \( E_i \in \mathbb{R}^p \) are independent with mean zero and unit variance. Then \( \text{cov}(X_i) = \Gamma^T \Gamma + \tau I_p \), which with \( \Psi = \Gamma^T \Gamma \) is consistent with our setting.

To estimate \( \theta = (\beta, \Omega, \tau, \Psi) \) we minimize minus two times a multivariate normal joint likelihood for \( n \) independent observations. However, we assume neither normality nor independence of the \( Z_i \) and hence our estimator is in general a maximum pseudo-likelihood estimator. For an arbitrary realization \( z_i = [y_i^T, x_i^T]^T \in \mathbb{R}^{r+p} \), minus two times the log-pseudo-likelihood is

\[
g(\theta; z_i) = -\log |\Omega| + (y_i - \beta^T x_i)^T \Omega (y_i - \beta^T x_i) + \log |\tau I_p + \Psi| + x_i^T (\tau I_p + \Psi)^{-1} x_i, \tag{3} \]

where \( |\cdot| \) is the determinant. The first two terms of \( g \) correspond to a conditional multivariate likelihood for the responses given the predictors and the remaining two terms to a marginal multivariate normal likelihood for the predictors. To summarize, we consider estimators \( \hat{\theta} = (\hat{\beta}, \hat{\Omega}, \hat{\tau}, \hat{\Psi}) \) that minimize \( G_n(\cdot) = n^{-1} \sum_{i=1}^n g(\cdot; Z_i) \).

To get some intuition for how the proposed method relates to conventional principal components regression, note the connection between \( \beta \) and \( \Sigma_X \) in (1) requires \( \hat{\beta} \) be in the column space of \( \hat{\Psi} \). Thus, when minimizing \( G_n \) one gets a \( \hat{\Psi} \) which balances having a column space leading to a small weighted sum of squared residuals for the regression and increasing the marginal pseudo-likelihood for the predictors. By contrast, the conventional method is equivalent to a two-step procedure where in the first step one obtains minimizers \( (\hat{\tau}, \hat{\Psi}) \) of the partial objective function \( (\tau, \Psi) \mapsto n^{-1} \sum_{i=1}^n \{ \log |\tau I_p + \Psi| + X_i^T (\tau I_p + \Psi)^{-1} X_i \} \) corresponding to the marginal pseudo-likelihood of the predictors (Tipping and Bishop, 1999). Then in a second step \( \beta \) is
estimated by least squares regression of the $Y_i$ on the $\tilde{U}^\top X_i$, where the columns of $\tilde{U}$ are orthonormal eigenvectors of $\tilde{\Psi}$ with non-zero eigenvalues. Importantly, the first step of the conventional method effectively ignores the role of $\Psi$ in the regression, and that is essentially why our estimator is, as we will see, often substantially more accurate. Moreover, because ours is a joint $M$-estimator for all the parameters, we are able establish its asymptotic distribution (see Section 2.2), enabling principled uncertainty quantification and inference.

Other methods postulating connections between the regression coefficient and the covariance matrix of the predictors include partial least squares (PLS) and predictor envelopes (XENV) \cite{Cook2010}. Predictor envelopes assume the columns of $\beta$ lie in the span of a subset of the eigenvectors of $\Sigma_X$, but not necessarily the leading ones. Thus, the predictor envelope model is more flexible and less parsimonious than our model. Partial least squares can be viewed as a moment-based estimator of a predictor envelope \cite{Cook2013}. Loosely speaking, those methods attempt to both infer which eigenvectors are relevant and estimate them. Since our method assumes it is the leading ones that are relevant, we expect it to perform better in settings where that is either true or a reasonable approximation. Our simulations largely confirm this intuition (Section 4). Additionally, our theory in Section 2 shows our estimator of $\beta$ is consistent in settings where it is unknown whether the predictor envelope estimator is, specifically when $p$ grows with $n$, and that ours is asymptotically more efficient when (1) holds.

2 Asymptotic properties

2.1 Consistency

This section gives conditions for consistency of the proposed estimators. The number of predictors $p = p(n)$ can change with $n$, but we focus on settings where $p/n \to 0$ as
Asymptotic theory for related likelihood-based methods typically assumes \( p \) is fixed, but it has been noted that it may be more appropriate to let \( p \) grow with \( n \) (Cook et al., 2007). Since \( p \) can change with \( n \), the parameters can too; for simplicity we suppress this in the notation. The results are for fixed and known \( r \) and \( k \); how to select \( k \) in practice is discussed in Section 3.2. Proofs are in Appendix A.

Let \( S \) be the set of \( p \times p \) symmetric and positive semi-definite matrices with rank at most \( k \) and \( \Theta \) the set of \( \theta = (\beta, \Omega, \tau, \Psi) \in \mathbb{R}^{p \times r} \times \mathbb{R}^{r \times r} \times [0, \infty) \times S \) such that \( P_{\Psi} \beta = \beta \), \( \Omega = \Omega^{T} \), and \( \lambda_{\min}(\Omega) \geq 0 \), where \( \lambda_{\min}(\cdot) \) denotes the smallest eigenvalue; we will denote the largest by \( \lambda_{\max}(\cdot) \) and the \( j \)th in decreasing order by \( \lambda_{j}(\cdot) \). We consider

\[
\hat{\theta} = \arg \min_{\theta \in \Theta} G_{n}(\theta),
\]

where, as in the Introduction, \( G_{n}(\theta) = n^{-1} \sum_{i=1}^{n} g(\theta; Z_{i}) \) for the \( g \) defined in (3). How to compute a \( \hat{\theta} \) in practice is discussed in Section 3.1 for now we focus on theoretical properties, starting with some fixed-sample ones in the following proposition.

Let \( Y = [Y_{1}, \ldots, Y_{n}]^{T} \in \mathbb{R}^{n \times r}, X = [X_{1}, \ldots, X_{n}]^{T} \in \mathbb{R}^{n \times p}, Z = [Y, X] \in \mathbb{R}^{n \times (r+p)} \), and superscript + denote the Moore–Penrose pseudo-inverse.

**Proposition 2.1.** If \( Z \) has full column rank and \( \lambda_{k+1}(X^{T}X) > \lambda_{p}(X^{T}X) \) then \( \hat{\theta} = (\hat{\beta}, \hat{\Omega}, \hat{\tau}, \hat{\Psi}) \) exists and satisfies \( \hat{\beta} = \hat{\Psi} \hat{\gamma} \) with \( \hat{\gamma} = (\hat{\Psi}X^{T}X\hat{\Psi})^{+}\hat{\Psi}X^{T}Y; \; \hat{\Omega}^{-1} = (Y - X\hat{\beta})^{T}(Y - X\hat{\beta})/n; \; \text{tr}\{X^{T}X(\hat{\tau}I_{p} + \hat{\Psi})(\hat{\Psi}X^{T}X)^{-1}\} = np; \; \hat{\tau} > \lambda_{\min}(X^{T}X/n); \; \hat{\Psi} \) has rank \( k \); and \( \hat{\tau} + \lambda_{\max}(\hat{\Psi}) \leq \lambda_{\max}(X^{T}X/n) \).

It is clear from Proposition 2.1 that estimating \( \Psi \) is key: once \( \hat{\Psi} \) is available, obtaining estimates of the other components of \( \theta \) is straightforward. The bounds on \( \hat{\tau} \) and \( \hat{\tau} + \lambda_{\max}(\hat{\Psi}) \) say the eigenvalues of \( \hat{\Sigma}_{X} = \hat{\Psi} + \hat{\tau}I_{p} \) are bounded between the smallest and largest eigenvalues of the sample covariance matrix \( S_{X} = X^{T}X/n \). These bounds are used repeatedly in our proofs of the results to follow.
Now, to examine asymptotic properties of $\hat{\theta}$ define

$$G(\theta) = G(\theta; \theta_*) = -\log |\Omega| + \text{tr}\{(\beta - \beta_*)^T(\tau_* I_p + \Psi_*)(\beta - \beta_*)\Omega\} + \text{tr}(\Omega\Omega_*^{-1})$$

$$+ \log |\tau I_p + \Psi| + \text{tr}\{(\tau I_p + \Psi)^{-1}(\tau_* I_p + \Psi_*)\},$$

where $\theta_* \in \Theta$ is fixed and unknown. If the model is correctly specified, then $\theta_*$ is the true parameter and $\mathbb{E}\{G_n(\theta)\} = G(\theta)$ for every $\theta \in \Theta$. Either way, $\theta_*$ is the unique minimizer of $G$ over $\Theta$; that is, $\theta_* = \text{arg min}_{\theta \in \Theta} G(\theta)$.

Intuitively, we expect $\hat{\theta}$ to be close to $\theta_*$ when $G_n$ is close to $G$. This intuition is formalized in the proof of the next result, which is the main result of the section.

Let $\| \cdot \|_M$ denote the max-norm defined for $(B, O, t, C) \in \mathbb{R}^{p \times r} \times \mathbb{R}^{r \times r} \times \mathbb{R} \times \mathbb{R}^{p \times p}$ by $\|(B, O, t, C)\|_M = \max\{\|B\|, \|O\|, |t|, \|C\|\}$, where $\| \cdot \|$ is the spectral norm for matrices and the Euclidean norm for vectors. Let also

$$\Sigma = \begin{bmatrix} \Omega^{-1} + \beta^T \Sigma \beta & \beta^T \Sigma X \\ \Sigma X \beta & \Sigma_X \end{bmatrix},$$

so that $\Sigma_*$ is the common covariance matrix of the $Z_i$ if the model is correctly specified.

**Theorem 2.2.** Suppose (i) there exists a $c \in (0, \infty)$ not depending on $n$ or $p$ such that $c^{-1} < \lambda_{\min}(\Sigma_*) \leq \lambda_{\max}(\Sigma_*) < c$, (ii) $\|Z^T Z/n - \Sigma_*\| = o_p(1)$ and (iii) $\text{tr}(Z^T Z/n - \Sigma_*) = o_p(1)$; then with probability tending to one a $\hat{\theta}$ exists and $\|\hat{\theta} - \theta_*\|_M = o_p(1)$.

We emphasize that no conditions other than those explicitly stated in the theorem are needed for the conclusion. In particular, the model can be misspecified, including the possibility that $\mathbb{E}(Z_i) \neq 0$ or $\text{cov}(Z_i) \neq \Sigma_*$. Similarly, no particular type of dependence or lack thereof is assumed. However, (ii) effectively requires $p = p(n) < n$ and that the difference between $\mathbb{E}(Z^T Z/n) = n^{-1} \sum_{i=1}^n \mathbb{E}(Z_i Z_i^T)$ and $\Sigma_*$ is asymptotically negligible.

Our proof of Theorem 2.2 is based on showing (i) $G_n$ tends to $G$ uniformly on suitable bounded subsets of $\Theta$, (ii) estimators are in those bounded subsets with probability
tending to one; and (iii) on those subsets, $G(\theta) - G(\theta_*) \geq \delta \|\theta - \theta_*\|_M^2$ for a $\delta > 0$ not depending on $p$ or $n$. Most of the work is due to the parameters and $G$ being allowed to depend on $p$, and hence $n$.

To get some intuition for the types of settings covered by Theorem \ref{thm:main}, note that if $p$ is fixed and the $Z_i$ are independent and identically distributed with mean zero and covariance matrix $\Sigma_*$, so that the model is correctly specified, then conditions (ii) and (iii) hold by the law of large numbers. Of course, many more general stochastic processes have ergodic theorems and hence satisfy (ii) and (iii) if they have the appropriate covariance matrix asymptotically. Condition (ii) can also hold when $p \to \infty$. For example, it holds if $p \to \infty$, $p/n \to 0$, the $Z_i$ are independent with bounded sub-Gaussian norms, and $\text{cov}(Z_i) = \Sigma_*$ for every $i$ (e.g. Vershynin 2018, Theorem 4.6.1).

Condition (iii) is only needed when $p \to \infty$. Specifically, if $p$ is bounded condition (iii) follows from condition (ii). Moreover, because $r$ is fixed, when condition (ii) holds condition (iii) is equivalent to $\text{tr}(S_X - \Sigma_X) = o_p(1)$. The condition ensures terms of $G_n$ depending on $\tau$ concentrate around their expectation. To illuminate in which settings this condition can be expected to hold, the following result outlines some sufficient conditions.

**Proposition 2.3.** If conditions (i) and (ii) of Theorem \ref{thm:main} hold, then condition (iii) of that theorem also holds if any of the following hold: (i) $p$ is bounded as $n \to \infty$, (ii) $p/n \to 0$ and the $X_i$ satisfy \cite{2} with $E(\|W_i\|^4 + \|E_i\|^4) \leq c$ for every $i$ and some $c < \infty$ not depending on $n$, or (iii) $p^2/n \to 0$ and $E\|X_i\|^4 \leq c$ for every $i$ and some $c < \infty$ not depending on $n$.

Setting (ii) of Proposition \ref{prop:cond} includes multivariate normal predictors as a special case, obtained by taking the elements of $W_i$ and $E_i$ in \cite{2} to be standard normal.
2.2 Asymptotic distribution

We next establish the asymptotic distribution of \( \hat{\theta} \) in settings where \( p \) is fixed. To state our result, we require some more notation and a definition of tangent cones. The following definition is equivalent to other common ones (Aubin and Frankowska 2009, pp. 122, 128).

**Definition 2.1.** The (ordinary) tangent cone of a set \( \mathcal{R} \subseteq \mathbb{R}^d \) at \( s \in \mathcal{R} \) is the set of \( t \in \mathbb{R}^d \) for which there exist sequences \( \{t_m\} \in \mathbb{R}^d \) and \( \{a_m\} \in (0, \infty) \) such that \( t_m \to t \), \( a_m \downarrow 0 \), and \( s + a(mt_m) \in \mathcal{R} \) for all \( m \). The derivable tangent cone \( \tilde{T}_R(x) \) is the set of \( t \in \mathbb{R}^d \) for which, for every \( a_m \downarrow 0 \), there exists \( t_m \to t \) such that \( s + a(mt_m) \in \mathcal{R} \) for all \( m \).

Here the relevant cones are for sets of matrices, which to work with Definition 2.1 we implicitly identify with vectors by stacking the columns. Similarly, we identify \( \Theta \) with a subset of \( \mathbb{R}^d \), \( d = pr + r^2 + 1 + p^2 \), by setting \( \theta = [\text{vec}(\beta)^T, \text{vec}(\Omega)^T, \tau, \text{vec}(\Psi)^T]^T \), where \( \text{vec}(\cdot) \) is the vectorization operator. Accordingly, we write \( \|\theta\| \) for the Euclidean norm of \( \theta \).

To state the main result of the section, define for \( i = 1, \ldots, n \)

\[
\varepsilon_i = Y_i - \beta_\ast^T X_i \in \mathbb{R}^r; \quad \xi_i = [\text{vec}(X_iX_i^T)^T, \text{vec}(X_i\varepsilon_i^T)^T, \text{vec}(\varepsilon_i\varepsilon_i^T)^T] \in \mathbb{R}^{p^2 + pr + r^2}.
\]

Let \( V = V(\theta_\ast) \in \mathbb{R}^{d \times d} \) be the Hessian of the function \( G \) defined in (5), evaluated at \( \theta_\ast \). If the likelihood is correctly specified, that is, if \( \theta_\ast \) is the true parameter and the \( \text{vec}(Z_i) \) are multivariate normal; then \( V/2 \) is the Fisher information matrix. Let also \( W \sim \mathcal{N}(0, I_d) \) and \( \mathcal{P}_{T(V)} \) denote the projection onto \( T_\Theta(\theta_\ast) \) in the inner product defined by \( V \). Specifically, for any \( u \in \mathbb{R}^d \),

\[
\mathcal{P}_{T(V)}(u) = \arg \min_{v \in T_\Theta(\theta_\ast)} (u - v)^T V (u - v).
\]

This minimizer exists and is unique for Lebesgue-almost every \( u \) (Geyer 1994).
Theorem 2.4. If (i) \( p \) is fixed as \( n \to \infty \), (ii) \( \tau_\ast > 0 \), \( \lambda_{\text{min}}(\Omega_\ast) > 0 \), and the rank of \( \Psi_\ast \) is \( k \); (iii) \( \mathbb{E}(Z_i) = 0 \) and \( \text{cov}(Z_i) = \Sigma_\ast \) for all \( i \); (iv) \( \|S_Z - \Sigma_\ast\| = o_p(1) \); and (v) \( n^{-1/2} \sum_{i=1}^n \{\xi_i - \mathbb{E}(\xi_i)\} \) tends in distribution to a multivariate normal vector with mean zero; then (a) \( \sqrt{n} \nabla G_n(\theta_\ast) \) tends in distribution to \( H^{1/2}W \) for a covariance matrix \( H \) to be specified and (b) \( \sqrt{n}(\hat{\theta} - \theta_\ast) \) tends in distribution to \( \mathcal{P}_{T(V)}(V^{-1}H^{1/2}W) \).

In addition to \( p \) being fixed, a fundamental difference between the assumptions required for Theorem 2.4 and Theorem 2.2 is the central limit theorem in (v). To get some intuition for the key conclusion in (b), note that if observations are independent and the model is correctly specified, then the covariance matrix \( H \) in Theorem 2.4 is 4 times the Fisher information, or \( 2V \). Thus, if it were also the case that \( T_\Theta(\theta_\ast) = \mathbb{R}^d \), (b) would specialize to the classical statement that maximum likelihood estimators are asymptotically normal with covariance given by the inverse Fisher information.

Before discussing the general case where observations are possibly dependent, we state a corollary for independent observations which helps put Theorem 2.4 in context.

Corollary 2.1. If (i) \( p \) is fixed as \( n \to \infty \), (ii) \( r = 1 \); (iii) \( \tau_\ast > 0 \), \( \Omega_\ast > 0 \), and the rank of \( \Psi_\ast \) is \( k \); and (iv) the \( Z_i \) are independent and multivariate normally distributed with \( \mathbb{E}(Z_i) = 0 \) and \( \text{cov}(Z_i) = \Sigma_\ast \); then \( \sqrt{n}(\hat{\beta} - \beta_\ast) \) tends in distribution to a multivariate normal vector with mean zero and covariance matrix \( \Omega_\ast^{-1}\Psi_\ast(\Psi_\ast\Sigma_X\Psi_\ast)^+\Psi_\ast = \Omega_\ast^{-1}P_{\Psi_\ast}\Sigma_X^{-1}P_{\Psi_\ast} \).

The multivariate normality in Corollary 2.1 is for convenience and can be replaced by conditions on the second to fourth moments of the \( Z_i \). Note, if \( \Psi_\ast \) were known, \( \beta_\ast \) could be estimated by \( \Psi_\ast(X^T X \Psi_\ast)^+ \Psi_\ast X^T Y \) which under regularity conditions has the same asymptotic distribution as that of \( \hat{\beta} \) in Corollary 2.1. In this sense our estimator has an oracle property: asymptotically, it does as well as if \( \Psi_\ast \) were known. We note that, for example, the predictor envelope estimator in general does not have this oracle
property (Cook, 2018a, Proposition 4.5). Intuitively, that and similar estimators pay a price for inferring which eigenvectors of the predictors’ covariance matrix gives linear combinations relevant for the regression.

The fact that Theorem 2.4 covers settings with dependent data distinguishes it from otherwise similar results in the literature. The effect of dependence on the asymptotic distribution is reflected in the matrix $H$. To clarify the role of $H$, suppose for example the process \( \{Z_i\} \) is stationary and strongly mixing in the sense of [Rosenblatt, 1956], and let us focus on the asymptotic distribution of \( \hat{\beta} \). Suppose also \( r = 1 \) for simplicity. The leading $p \times p$ block of $H$, say $H_1$, is then the asymptotic covariance matrix of

$$n^{-1/2} \sum_{i=1}^{n} \nabla \beta g(\theta^*_s; Z_i) = -2n^{-1/2} \sum_{i=1}^{n} X_i \Omega_s \varepsilon_i.$$ 

Thus, assuming $\mathbb{E}\|X_i \varepsilon_i\|^{2+\delta} < \infty$ for some $\delta > 0$ and the mixing coefficients decay sufficiently fast, that is, dependence is not too strong (e.g. [Ibragimov, 1962, Theorem 1.7]);

$$H_1 = \lim_{n \to \infty} \text{cov} \left( -2n^{-1/2} \sum_{i=1}^{n} X_i \Omega_s \varepsilon_i \right) = 4\Omega_s \left\{ \Sigma_{X_s} + 2 \sum_{i=1}^{\infty} \mathbb{E}(X_1 X_{1+i}^T) \right\}. \quad (6)$$

Moreover, it is straightforward to verify $V$ is block-diagonal with leading $p \times p$ block equal to $V_1 = 2\Omega_s \Sigma_{X_s}$. Thus, with $W_1 \sim \mathcal{N}(0, I_p)$, the asymptotic distribution of $\sqrt{n}(\hat{\beta} - \beta^*_s)$ given by Theorem 2.4 is that of the minimizer of $(V_1^{-1/2}W_1 - v)^T V_1 (V_1^{-1/2}W_1 - v)$ over $v$ in the column space of $\Psi_s$; the last assertion follows from the tangent cone in Theorem 2.6 which we will discuss shortly. The minimizing $v$ is $\Psi_s (\Psi_s V_1 \Psi_s)^+ \Psi_s H_1^{1/2} W_1$. It follows that the asymptotic distribution of $\sqrt{n}(\hat{\beta} - \beta^*_s)$ is a singular multivariate normal, concentrated on the column space of $\Psi_s$. In particular, the asymptotic covariance matrix is $\Psi_s (\Psi_s V_1 \Psi_s)^+ \Psi_s H_1 \Psi_s (\Psi_s V_1 \Psi_s)^+ \Psi_s$.

Most of the work in the proof of Theorem 2.4 is deriving the tangent cone and showing the remainder in a linear approximation of $G_n$ around $\theta_s$ is stochastically
equicontinuous (see e.g. Pollard [1984] Section VII). We state two results on tangent cones used in the proof, which may be illuminating and relevant for other work. Recall \( S \) is the set of \( p \times p \) symmetric and positive semi-definite matrices with rank at most \( k \).

**Lemma 2.5.** For any \( \Psi \in S \) with rank \( k \), \( T_S(\Psi) = \tilde{T}_S(\Psi) = \{ C \in \mathbb{R}^{p \times p} : C = C^T, Q_\Psi C Q_\Psi = 0 \} \).

A set is sometimes said to be Chernoff-regular at points where its ordinary and derivable tangent cones agree (Geyer [1994]), in reference to Chernoff [1954]. Lemma 2.5 thus says \( S \) is Chernoff-regular at every \( \Psi \) with rank \( k \). Chernoff regularity is needed to establish the asymptotic distribution of our estimators, and it carries over to \( \Theta \) in the sense made precise in the following theorem.

**Theorem 2.6.** For any \( \theta \in \Theta \) with \( \tau > 0 \), \( \lambda_{\text{min}}(\Omega) > 0 \), and \( \Psi \) with rank \( k \), the tangent cone \( T_{\Theta}(\theta) \) is the set of \((B, O, t, C) \in \mathbb{R}^{p \times r} \times \mathbb{R}^{r \times r} \times \mathbb{R} \times \mathbb{R}^{p \times p} \) such that \( B = P_\Psi B \), \( O = O^T \), \( C = C^T \), and \( Q_\Psi C Q_\Psi = 0 \). Moreover, \( \tilde{T}_{\Theta}(\theta) = T_{\Theta}(\theta) \).

The tangent cones at \( \theta \) with \( \tau = 0 \) or \( \lambda_{\text{min}}(\Omega) = 0 \) could be derived by techniques similar to those used to prove Theorem 2.6. We do not pursue that since we only need the cones at \( \theta_* \), and other conditions require \( \tau_* > 0 \) and \( \lambda_{\text{min}}(\Omega_*) > 0 \).

### 3 Implementation

#### 3.1 Maximizing the pseudo-likelihood

Recall the definition of \( G_n(\theta) = G_n(\beta, \Omega, \tau, \Psi) \) in (5). To minimize \( G_n \) we consider a change of variables, or reparameterization: \( \Sigma_X = \tau(I_p + LL^T) \), that is, \( \Psi = \tau LL^T \), where \( L \in \mathbb{R}^{p \times k} \). Then the column space of \( \Psi \) is the column space of \( L \), and hence the key condition \( P_\Psi \beta = \beta \) in (1) is equivalent to \( P_L \beta = \beta \). That is, there is a \( \gamma \in \mathbb{R}^{k \times r} \) such that \( \beta = L \gamma \). This parameterization is identifiable if \( L \) is constrained to be a lower-echelon matrix (Cantó et al. [2015]). Now, the goal is minimization
of $(\gamma, \Omega, L, \tau) \mapsto G_n(L\gamma, \Omega, \tau, \tau LL^T)$. Routine calculations show this function can be partially minimized analytically in all arguments but $L$, giving that the partially minimized objective $\min_{\gamma, \Omega, \tau} G_n(L\gamma, \Omega, \tau, \tau LL^T)$ is equal to a constant plus

$$H_n(L) = \log |Y^TQ_{XL}Y/n| + \log |I_p + LL^T| + p\log \left\{S_X(I_p + LL^T)^{-1}\right\},$$

where $Q_{XL} = I_n - P_{XL}$. In our software, available at https://github.com/koekvall/tpcr, we use off-the-shelf solvers to minimize $H_n$ over the set of $p \times k$ matrices with elements $L_{ij} = 0$ if $i < j$ and $L_{ij} \geq 0$ if $i = j$. Calculating the gradient necessary to implement a first order method is straightforward but tedious (Appendix A). Given a minimizer $\hat{L}$, the proposed estimators are $\hat{\beta} = \hat{L}\hat{\gamma}$, where $\hat{\gamma} = (\hat{L}^T X^T X \hat{L}) + \hat{L}^T X^T Y$, $\hat{\tau} = \text{tr}\{S_X(I_p + \hat{L}\hat{L}^T)^{-1}\}/p$, and $\hat{\Psi} = \hat{\tau}\hat{L}\hat{L}^T$.

### 3.2 Selecting the number of components

Information criteria are a principled way to select $k$ in practice. Fix $p$ and $r$, and, for any $k \in \{0, \ldots, p\}$, let $d(k)$ denote the number of parameters and $\hat{\theta}(k)$ a minimizer of $G_n$. Then, up to additive constants, many popular information criteria can be written as $\ln(p)(k) = nG_n\{\hat{\theta}(k)\} + \rho d(k)$, where different $\rho > 0$ give different criteria. Akaike’s information criterion (AIC) (Akaike, 1998) and Schwarz’s Bayesian information criterion (BIC) (Schwarz, 1978) set, respectively, $\rho = 2$ and $\rho = \log(n)$. For a given $\rho$, $k$ is selected as $\hat{k} \in \text{arg min}_{k=0,\ldots,p} \ln(p)(k)$. We examine the performance of AIC and BIC in our model using simulations in Section 4. The following proposition establishes $d(k)$.

**Proposition 3.1.** For a given $p$, $r$, and $k$, the number of parameters in our model is $d(k) = r(r+1)/2 + k\{r + 1 + p - (k+1)/2\} + 1$ if $k < p$, and $d(k) = r(r+1)/2 + rk + p(p+1)/2$ if $k = p$. 

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We compare the proposed method (TPCR) to conventional principal components regression (PCR), partial least squares (PLS) using the SIMPLS algorithm in the \texttt{pls} package [Mevik and Wehrens 2007], predictor envelopes (XENV) using the \texttt{Renvlp} package [Lee and Su 2019], and ordinary least squares (OLS). The reported results focus on the root mean squared error (RMSE) for estimating $\beta^*$ and out-of-sample predictions. These are defined, respectively, for a generic estimate $\hat{\beta}$ and independent test set $(X_{\text{new}}, Y_{\text{new}}) \in \mathbb{R}^{n \times p} \times \mathbb{R}^{n \times r}$, as

$$
\| \hat{\beta} - \beta^* \|_F / \sqrt{rp}; \quad \| X_{\text{new}} \hat{\beta} - Y_{\text{new}} \|_F / \sqrt{rn},
$$

where $\| \cdot \|_F$ denotes the Frobenius norm. We consider results both for $k$ known and $k$ treated as unknown. In simulations where $k$ is treated as unknown, we select $k$ using BIC for the likelihood-based methods (TPCR, XENV) and the built-in leave-one-out cross-validation functionality in the \texttt{pls} package for the moment-based methods (PCR, PLS). In simulations not reported here for brevity we selected $k$ using AIC in place of BIC and results were similar. Code for reproducing the results is available at [https://github.com/koekvall/tpcr-suppl/](https://github.com/koekvall/tpcr-suppl/)

In all simulations, both the training set $(X, Y) \in \mathbb{R}^{n \times p} \times \mathbb{R}^{n \times r}$ and the test set are generated as $n$ independent observations from our model with multivariate normal responses and predictors. We fix $r = 2$ and $\Sigma_* = I_2$ and examine performance as $n, p, k, \beta_*$, and the eigenvalues of $\Sigma_{X*}$ vary. More specifically, we set $\Sigma_{X*} = \tau_* (I_p + U_* D_* U_*^T)$ where $U_*$ is a realization from the uniform distribution on the $p \times k$ semi-orthogonal matrices and $D_* = \text{diag}(1.1d_*, \ldots, 0.9d_*)$ for some $d_* > 0$ which we call the average spiked eigenvalue. Thus, $\Psi_* = \tau_* U_* D_* U_*^T$. We pick $\tau_*$ so that $p^{-1} \text{tr}(\Sigma_{X*}) = 1$, which ensures the predictors have approximately the same variance and are on roughly the same scale in all simulations. The coefficient matrix $\beta_*$ is set to $U_* \gamma_*$, where $\gamma_* \in \mathbb{R}^{k \times r}$.
is constructed by drawing its elements as independent realizations of the uniform distribution on \((-1, 1)\) and then normalizing each column to have a Euclidean norm that can change between simulations; we refer to this as the coefficient column norm or the coefficient size. Because \(U_\ast\) is semi-orthogonal, \(\|\beta_{\ast j}\| = \|U_\ast \gamma_{\ast j}\| = \|\gamma_{\ast j}\|\) for any column \(j = 1, \ldots, r\). We take as a baseline

\[(\|\beta_{\ast j}\|, d_\ast, p, k, n) = (1, 5, 30, 3, 120)\]

and vary the settings one parameter at a time around this baseline. The numbers \(n = 120, p = 20,\) and \(k = 3\) to correspond roughly to our data example in Section 5.

The first column in Figure 1 shows estimation results with \(k\) treated as unknown and in the second column \(k\) is known. In the first row, we see the proposed method performs best regardless of the coefficient size. PCR can perform as well if \(k\) is known and the coefficient size is small; this is consistent with TPCR and PCR exploiting the fact that the leading eigenvectors of \(\Sigma_{X_\ast}\) give relevant linear combinations. That is, exploiting the fact that the leading eigenvectors are relevant is particularly useful when the effect of the predictors on the responses is weak. XENV can perform as well as our method if \(k\) is known and the coefficient size is large, while PLS is generally second-best when \(k\) is unknown. The upward slopes show dimension reduction tends to be decreasingly useful relative to OLS when the coefficient size increases.

The second row shows all methods benefit from larger spiked eigenvalues, which is intuitive. Our method generally performs best, but PLS can perform as well or even slightly better when the average spiked eigenvalue is small. Comparing the first and second column shows the performance of XENV is good when \(k\) is known but is substantially worse when \(k\) is unknown, seemingly due to BIC selecting too many components on average.

Results in the third row indicates the likelihood-based methods (TPCR, XENV) perform better relative to the moment-based (PCR, PLS) when there are few predictors.
More generally, the proposed method performs best in all settings when \( k \) is unknown while predictor envelopes can perform better when there are very few predictors and \( k \) is known.

Row four reinforces the impression that in general our method performs best followed by PLS. Notably, PLS and XENV tend to select too few and PCR too many components when there are many relevant components.

The patterns in row five are similar to those observed in other rows, with one notable exception: XENV can perform best of all methods when \( n \) is very large and \( k \) is known.

Figure 2 in Appendix B shows the prediction results, using the same settings as in Figure 1 are qualitatively similar to the estimation results.

5 Data example

5.1 Out-of-sample prediction

We illustrate our method using data on \( n = 123 \) monthly returns, from January 2010 to March 2020, on 29 stocks in the Dow Jones Industrial Average index (one out of the 30 comprising the index is omitted because it was introduced in 2019). Specifically, we consider cross-sectional prediction and modeling of the return on one stock using contemporaneous returns of the other \( p = 28 \) stocks.

It is often hypothesized that stock returns can be decomposed into a stock-specific component, which is independent of the returns on other stocks, and a few common components, or factors [Fama and French 2015, Bai and Wang 2016]. The latter can include, for example, a risk-free interest rate and a market return, and they can be observable or unobservable. Let \( W_t = [W_{t,1}, \ldots, W_{t,k}]^T \in \mathbb{R}^k \) denote a vector of such components at time \( t \in \{1, \ldots, n\} \), and suppose the return on stock \( j \in \{1, \ldots, p + 1\} \) is

\[
R_{t,j} = \mu_j + \Gamma_j^T W_t + \sqrt{\eta} E_{t,j}, \tag{7}
\]
Figure 1: Monte Carlo results for estimating $\beta*$.  

NOTE: Average estimation root mean squared errors and bias in selecting $k$ over 1000 Monte Carlo replications. Reported RMSEs are divided by the RMSE of ordinary least squares with all predictors. In the first column, $k$ is selected by BIC (TPCR, XENV) or leave-one-out cross-validation (PCR, PLS). Plots in the same row use the same settings. When not varying as indicated on the horizontal axes, $n = 120$, $p = 30$, $k = 3$, $r = 2$, $\Sigma_* = I_2$, $d_* = 5$, $\tau_*$ is set to ensure $p = \text{tr}(\Sigma_X\Sigma)$, and $\|\beta_j\| = 1$, $j = 1, \ldots, r$. 

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where $\mu_j \in \mathbb{R}$ and $\Gamma_j \in \mathbb{R}^k$ are parameters and $E_{t,j}$ an unobservable error term. For every $t$, the elements of $W_t$ and $E_{t,j}$ are independent with mean zero and unit variance. The common components are latent variables inducing dependence between contemporaneous returns of different stocks. To see how (7) relates to our model, let $Y_t = R_{t,1}$ be the return to be predicted using the vector of predictors $X_t = [R_{t,2}, \ldots, R_{t,p+1}]^T \in \mathbb{R}^p$. Then with $\Gamma = [\Gamma_2, \ldots, \Gamma_{p+1}]^T \in \mathbb{R}^{p \times k}$ and $\Sigma_W = \text{cov}(W_t)$, $\Sigma_X = \text{cov}(X_t) = \Gamma \Sigma_W \Gamma^T + \tau I_p$, which is compatible with our model by arguments following (2). Moreover, assuming (7) and normality of the returns leads to

$$\mathbb{E}(Y_t | X_t) = \mathbb{E}(Y_t) + \Sigma_X^{-1} \text{cov}(X_t, Y_t)(X_t - \mathbb{E}(X_t)) = \mathbb{E}(Y_t) + \beta^T [X_t - \mathbb{E}(X_t)]$$

where $\beta = (\Gamma \Sigma_W \Gamma^T + \tau I_p)^{-1} \Gamma \Sigma_W \Gamma_1$. It follows that $\beta$ lies in the span of $k$ leading left singular vectors of $\Gamma \Sigma_W^{1/2}$; that is, the column space of $\Gamma \Sigma_W \Gamma^T$.

We split the 123 observations so that the first 70 are training data and the remaining 53 are test data, fit each method to the training data, and compute the root mean square error of prediction on the test data. The number of components ($k$) is selected using BIC (TPCR, XENV) or leave-one-out cross validation (PCR, PLS). We also tried selecting the number of components for TPCR and XENV using AIC but found that BIC generally lead to better predictions for both methods. For TPCR and PCR, which are sensitive to the scales of the predictors, we center and scale the predictors. We focus on prediction of Home Depot’s stock return but to highlight which results are particular to this choice of response, and which hold more generally, we also present summary statistics from repeating the same analysis with the other returns as responses.

Table 1 shows the prediction results. The presented root mean squared errors are divided by that of a model without predictors, that is, the model which predicts all response realizations in the test set are equal to the training data sample mean. Our method has the lowest out-of-sample prediction RMSE for Home Depot’s stock return, followed in turn by PLS, PCR, XENV, and OLS. Our method uses $k = 2$; PLS selects
\begin{table}
\begin{tabular}{lccccc}
\hline
Statistic & TPCR & PCR & PLS & XENV & OLS \\
\hline
Home Depot & & & & & \\
RMSE & 0.748 & 0.787 & 0.765 & 0.844 & 1.047 \\
\hat{k} & 2 & 3 & 1 & 3 & - \\
All stocks & & & & & \\
\# best & 15 & 3 & 9 & 2 & 0 \\
Ave. RMSE & 0.800 & 0.839 & 0.808 & 0.947 & 1.006 \\
Max. RMSE & 0.991 & 1.145 & 0.994 & 1.310 & 1.343 \\
Ave. \hat{k} & 2.000 & 8.345 & 1.552 & 3.793 & - \\
\hline
\end{tabular}
\caption{Our of sample prediction results}
\end{table}

NOTE: Root mean squared errors (RMSEs) are for the last 53 observations and are divided by the RMSE of the training data sample mean. Number of components (\(\hat{k}\)) is selected using BIC (TPCR, XENV) or leave-one-out cross-validation (PCR, PLS). Numbers for "All stocks" are summary statistics of the 29 root mean square error obtained by applying the methods once with every stock return as response. \\

\(k = 1\) while PCR and XENV selects \(k = 3\). These results are generally consistent with the simulations, though PCR performs surprisingly well. As we will see shortly, this can be explained by the fact that, in this example, our method indicates the leading eigenvector of \(\Sigma_{X^g}\) gives the only linear combination relevant for predicting the response, and the eigenvalue corresponding to that eigenvector is much larger than the other eigenvalues.

Summarizing the results from repeating the same analysis with the other 28 stock returns as responses one by one, our method performs best (has the lowest out of sample prediction RMSE) in 15 out of the 29 analyses. It also has the lowest average and maximum RMSE over the 29 analyses. Comparing our method to PCR we see our method uses information in the responses to select a smaller \(k\) on average.

\subsection{5.2 Inference on regression parameters}

We illustrate inference using the proposed method in the model with Home Depot’s return as response and returns on the remaining 28 stocks as predictors, using the full sample. Both responses and predictors are centered and scaled.

Results in Table\ref{table2} include our method and, for context, ordinary least squares. For
our method, the reported standard errors were computed using Theorem 2.4 with the long run covariance of the predictors appearing in (6) estimated using methods by Andrews (1991), implemented in the R package sandwich (Zeileis, 2004; Zeileis et al., 2020). The standard errors for the least squares estimates were also computed using that package. According to our method, several of the estimated coefficients are statistically significantly different from zero at conventional significance levels, and of those coefficients most are estimated to be approximately equal to 0.05. That is, our method indicates several stock returns are associated with that of Home Depot, and the strength of that association is roughly the same for different stocks. By contrast, only one of the least squares estimates is statistically significantly different from zero at the 5% level. This is primarily because the standard errors of the least squares estimates are often 5–10 times those of our estimates, indicating our method leads to substantially more precise inference. To appreciate the difference, one may note this decrease in standard errors is roughly equivalent to increasing the sample size for the least squares estimates 25–100 times; that is, from the current $n = 123$ to about $n \in [2500, 12000]$.

The last column in Table 2 shows the estimated first eigenvector of the predictors’ covariance matrix gives a principal component which is roughly a scaled average of the 28 returns used as predictors. This could be interpreted as representing a market component common to all returns. We only present the first eigenvector because the others give principal components whose effects on the response seem weak; this is shown in Table 3 where we present results from regressing the response on the 5 principal components given by our method by least squares. These results indicate that $k = 5$ is selected by BIC because a lower $k$ gives a poor model for the marginal distribution of the predictors, not because 5 components are important for modeling the conditional distribution of the response given the predictors.
| Predictor | $\beta$  | se($\beta$) | p-val | $\beta_{OLS}$ | se($\beta_{OLS}$) | p-val | se-ratio | $\hat{u}_1$ |
|-----------|---------|-------------|-------|--------------|-----------------|-------|----------|----------|
| UNH       | 0.025   | 0.027       | 0.362 | 0.018        | 0.088           | 0.843 | 3.254    | 0.128    |
| AAPL      | 0.031   | 0.017       | 0.063 | 0.030        | 0.072           | 0.680 | 4.327    | 0.144    |
| MCD       | 0.024   | 0.028       | 0.403 | 0.000        | 0.113           | 0.999 | 4.022    | 0.166    |
| GS        | 0.053   | 0.014       | 0.000 | -0.109       | 0.128           | 0.395 | 8.900    | 0.209    |
| V         | 0.040   | 0.009       | 0.000 | 0.174        | 0.104           | 0.094 | 10.943   | 0.209    |
| MSFT      | 0.029   | 0.024       | 0.242 | 0.050        | 0.127           | 0.697 | 5.220    | 0.183    |
| MMM       | 0.050   | 0.016       | 0.002 | 0.098        | 0.107           | 0.360 | 6.595    | 0.233    |
| BA        | 0.051   | 0.017       | 0.003 | -0.037       | 0.097           | 0.700 | 5.720    | 0.198    |
| JNJ       | 0.022   | 0.017       | 0.184 | -0.227       | 0.105           | 0.030 | 6.227    | 0.198    |
| CAT       | 0.043   | 0.022       | 0.054 | 0.011        | 0.125           | 0.932 | 5.583    | 0.203    |
| WMT       | 0.004   | 0.023       | 0.845 | 0.107        | 0.072           | 0.135 | 3.083    | 0.100    |
| IBM       | 0.043   | 0.013       | 0.001 | 0.126        | 0.099           | 0.203 | 7.679    | 0.188    |
| PG        | 0.009   | 0.018       | 0.641 | 0.066        | 0.095           | 0.487 | 5.198    | 0.131    |
| TRV       | 0.045   | 0.015       | 0.003 | 0.059        | 0.118           | 0.619 | 7.674    | 0.221    |
| DIS       | 0.050   | 0.010       | 0.000 | -0.003       | 0.104           | 0.978 | 10.186   | 0.219    |
| JPM       | 0.053   | 0.016       | 0.001 | 0.164        | 0.156           | 0.291 | 9.765    | 0.230    |
| AXP       | 0.053   | 0.010       | 0.000 | -0.075       | 0.124           | 0.547 | 12.024   | 0.224    |
| CVX       | 0.041   | 0.022       | 0.060 | 0.192        | 0.176           | 0.274 | 8.134    | 0.236    |
| NKE       | 0.052   | 0.042       | 0.214 | 0.140        | 0.093           | 0.132 | 2.215    | 0.153    |
| MRK       | -0.002  | 0.029       | 0.949 | -0.026       | 0.091           | 0.778 | 3.191    | 0.119    |
| RTX       | 0.059   | 0.012       | 0.000 | 0.145        | 0.145           | 0.319 | 12.445   | 0.244    |
| INTC      | 0.030   | 0.020       | 0.138 | -0.056       | 0.108           | 0.605 | 5.411    | 0.167    |
| VZ        | -0.004  | 0.027       | 0.891 | -0.022       | 0.138           | 0.875 | 5.117    | 0.128    |
| KO        | 0.018   | 0.030       | 0.538 | 0.039        | 0.106           | 0.717 | 3.591    | 0.176    |
| XOM       | 0.045   | 0.014       | 0.002 | 0.007        | 0.177           | 0.969 | 12.420   | 0.237    |
| WBA       | 0.035   | 0.030       | 0.246 | -0.087       | 0.126           | 0.489 | 4.199    | 0.170    |
| CSCO      | 0.042   | 0.019       | 0.027 | 0.042        | 0.114           | 0.714 | 6.082    | 0.191    |
| PFE       | 0.023   | 0.026       | 0.373 | 0.165        | 0.131           | 0.209 | 5.025    | 0.179    |

Table 2: Full regression results

NOTE: Results from regressing the centered and scaled stock return of Home Depot on the other 28 centered and scaled stock returns using our method with $k = 5$ and ordinary least squares. The se-ratio is $se(\hat{\beta}_{OLS})$ divided by $se(\hat{\beta})$ and $\hat{u}_1$ is the estimated leading eigenvector of the predictors’ covariance matrix. The standard errors and $p$-values are based on the asymptotic normal distribution in Theorem 2.4 and allow temporal dependence in the predictors. Long run variance of predictors is estimated using methods in Andrews (1991).
Response: HD

\begin{tabular}{lcccc}
  Direction & $\hat{\gamma}$ & se($\hat{\gamma}$) & p-val & $\lambda(\Psi)/\hat{\tau}$ \\
  \hline
  $\hat{u}_1$ & 0.194 & 0.019 & 0.000 & 22.584 \\
  $\hat{u}_2$ & -0.054 & 0.058 & 0.357 & 4.379 \\
  $\hat{u}_3$ & 0.014 & 0.039 & 0.714 & 2.333 \\
  $\hat{u}_4$ & -0.002 & 0.057 & 0.966 & 1.947 \\
  $\hat{u}_5$ & 0.031 & 0.067 & 0.643 & 1.257 \\
\end{tabular}

Table 3: Reduced regression and eigenvalues

NOTE: Results from regressing the stock return of Home Depot on the 5 principal components estimated by our method with $k = 5$, using centered and scaled data (columns 1–4). Relative estimated size of eigenvalues (column 5). Standard errors and computed using methods using methods in Andrews (1991).

6 Final remarks

We have proposed a method for principal components regressions which uses information in the responses to select relevant linear combinations of the predictors. When the leading eigenvalues of the predictors’ covariance matrix are much larger than the trailing, conventional PCR can work well, and our method in general does no worse. When the difference in magnitude between leading and trailing eigenvalues is small, however, conventional PCR often struggles to identify the relevant linear combinations. Then, our method often performs substantially better. In light of this, we also expect that, if a principal components regression model does not hold, then our method will do better than conventional PCR because it takes the fit of the regression into account. That is, we expect our method to be more robust to misspecification of the dimension reducing subspace than conventional PCR.

Our data example indicates $k$ may sometimes need to be larger than the number of relevant linear combinations of the predictors. This can happen when the spiked covariance matrix needs a larger $k$ to fit well or because the $k$th eigenvector gives a relevant linear combination of the predictors but not all preceding eigenvectors do. For example, it may be that the third eigenvector gives a relevant linear combination but the first or second do not. Both of these scenarios suggest it may be useful to extend our method to allow for penalization. For example, by letting $\Psi = UDU^T$ by
spectral decomposition with $D \in \mathbb{R}^{k \times k}$ and parameterizing $\beta = U\gamma$ for some $\gamma \in \mathbb{R}^{k \times r}$, one could select a relatively large $k$ and use an $L_1$ penalty to encourage rows of $\hat{\gamma}$ corresponding to irrelevant components to vanish. With an $L_2$-penalty on $\beta$ our method can be viewed as a pseudo-likelihood alternative to the method proposed by Lang and Zou (2020). Penalizing $\beta$ or $\gamma$ could also make the method operational when $p > n$.

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A Technical details

It will be useful to have analytical expressions for some derivatives of key functions. Recall the $g$ defined in [3]. Its gradient $\nabla g(\theta; z) = \nabla \varphi g(\theta; z)$ is characterized by

$$
\nabla \beta g(\theta; z) = -2x(y - \beta^T x)\Omega;
$$
$$
\nabla \Omega g(\theta; z) = -\Omega^{-1} + (y - \beta^T x)(y - \beta^T x)^T;
$$
$$
\nabla \tau g(\theta; z) = \text{tr}(\Sigma^{-1}_X - \Sigma^{-1}_X xx^T \Sigma^{-1}_X);
$$
$$
\nabla \psi g(\theta; z) = \Sigma^{-1}_X - \Sigma^{-1}_X xx^T \Sigma^{-1}_X.
$$

Putting these together and evaluating at $\theta = \theta^*$ leads to

$$
\nabla g(\theta^*; z) = \begin{bmatrix}
0 \\
-\text{vec}(\Omega^{-1}) \\
\text{tr}(\Sigma^{-1}_X) \\
\text{vec}(\Sigma^{-1}_X)
\end{bmatrix} + \begin{bmatrix}
-2(I_p \otimes \Omega^*) \text{vec}(\varepsilon^T) \\
\text{vec}(\varepsilon^T) \\
-\text{vec}(\Sigma^{-2}_X^*) \text{vec}(xx^T) \\
-(\Sigma^{-1}_X \otimes \Sigma^{-1}_X) \text{vec}(xx^T)
\end{bmatrix} = a^* + B^* \xi,
$$

where $\xi = [\text{vec}(xx^T)^T, \text{vec}(x\varepsilon^T)^T, \text{vec}(\varepsilon^T)^T]^T$, and $a^*$ and $B^* \in \mathbb{R}$ are defined by the last equality. Differentiating again one gets that the non-zero blocks of the Hessian $\nabla^2 g$ are given by

$$
\nabla^2 \beta g(\theta; z) = 2\Omega \otimes xx^T;
$$
$$
\nabla^2 \Omega g(\theta; z) = -2I_r \otimes x(y - \beta^T x)^T;
$$
$$
\nabla^2 \tau g(\theta; z) = \text{tr}\{\Sigma^{-2}_X + \Sigma^{-2}_X xx^T \Sigma^{-1}_X + \Sigma^{-2}_X xx^T \Sigma^{-2}_X\};
$$
$$
\nabla^2 \psi g(\theta; z) = -\Sigma^{-2}_X + \Sigma^{-2}_X xx^T \Sigma^{-1}_X + \Sigma^{-2}_X xx^T \Sigma^{-2}_X;
$$
$$
\nabla^2 \varphi g(\theta; z) = -\Sigma^{-1}_X \otimes \Sigma^{-1}_X + \Sigma^{-1}_X \otimes \Sigma^{-1}_X xx^T \Sigma^{-1}_X + \Sigma^{-1}_X xx^T \Sigma^{-1}_X \otimes \Sigma^{-1}_X.
$$

The derivatives of $G_n = n^{-1} \sum_{i=1}^n g(\theta; Z_i)$ are immediate from those of $g$. 

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Recall the function $G$ in (5). Its gradient is characterized by

$$
\nabla \beta G(\theta; \theta_*) = 2\Sigma_X^*(\beta - \beta_*)\Omega;
$$
$$
\nabla \Omega G(\theta; \theta_*) = -\Omega^{-1} + (\beta - \beta_*)^T\Sigma_X^*(\beta - \beta_*) + \Omega^{-1};
$$
$$
\nabla \tau G(\theta; \theta_*) = \text{tr}\{\Sigma_X^{-1} - \Sigma_X^{-1}\Sigma_X^*\Sigma_X^{-1}\};
$$
$$
\nabla \Psi G(\theta; \theta_*) = \Sigma_X^{-1} - \Sigma_X^{-1}\Sigma_X^*\Sigma_X^{-1}.
$$

Differentiating again one gets that the non-zero blocks of the Hessian $\nabla^2 G$ are given by

$$
\nabla^2 \beta G(\theta; \theta_*) = 2\Omega \otimes \Sigma_X^*;
$$
$$
\nabla^2 \Omega G(\theta; \theta_*) = 2I_r \otimes \Sigma_X^*(\beta - \beta_*));
$$
$$
\nabla^2 \tau G(\theta; \theta_*) = \text{tr}\{-\Sigma_X^{-2} + \Sigma_X^{-2}\Sigma_X^*\Sigma_X^{-1} + \Sigma_X^{-1}\Sigma_X^*\Sigma_X^{-2}\};
$$
$$
\nabla^2 \Psi G(\theta; \theta_*) = -\Sigma_X^{-2} + \Sigma_X^{-2}\Sigma_X^*\Sigma_X^{-1} + \Sigma_X^{-1}\Sigma_X^*\Sigma_X^{-2};
$$
$$
\nabla^2 \Psi G(\theta; \theta_*) = -\Sigma_X^{-1} \otimes \Sigma_X^{-1} + \Sigma_X^{-1} \otimes \Sigma_X^{-1}\Sigma_X^*\Sigma_X^{-1} + \Sigma_X^{-1}\Sigma_X^*\Sigma_X^{-1} \otimes \Sigma_X^{-1}.
$$

Finally before stating proofs, it will be useful to note $G_n$ can also be written

$$
G_n(\theta; Z) = -\log |\Omega| + n^{-1} \text{tr}\{(Y - X\beta)^T(Y - X\beta)\Omega\} + \log |\Sigma_X| + n^{-1} \text{tr}(X^TX\Sigma_X^{-1}),
$$

where $\Sigma_X = \Psi + \tau I_p$ and $Z = [Y, X] \in \mathbb{R}^{n \times (r + p)}$.

Proof of Proposition 2.1. Consider an enlarged parameter set $\Theta_1$ where $\Psi$ is of rank at most $k$ and has a spectral decomposition $UDU^T$, $D \in \mathbb{R}^{k \times k}$, such that $\beta = U\gamma$ for some $\gamma \in \mathbb{R}^{k \times r}$, that is, $\beta$ is in the column space of $U$, but not necessarily in that of $\Psi$ if some diagonal elements of $D$ are equal to zero. Clearly, $G_n$ can be defined the same way on $\Theta_1$ as on $\Theta$. The enlarged parameter set is useful because it is closed. To see this, pick a convergent sequence $\{\theta_m\} \in \Theta_1$; we need to show the limit point
$\theta \in \Theta_1$. It straightforward to show $\Omega$, $\tau$, and $\Psi$ must be symmetric and positive semi-definite, so we omit the details. To see the rank of $\Psi$ is at most $k$, suppose for contradiction it has $k + 1$ strictly positive eigenvalues. Then by Weyl's perturbation theorem ([Bhatia 2012] Corollary III.2.6), so does $\Psi_m$ for all large enough $m$, which is a contradiction to $\Psi_m \in S$. Because $\Psi \in S$, we can write $\Psi = UDU^T$ and it remains to show $P_U \beta = \beta$. To that end, write $\Psi_m = U_mD_mD_m^T$ and $\beta_m = U_m\gamma_m$ for every $m$. Since $\|\beta_m\| = \|\gamma_m\|$ and $\beta_m$ converges, $\{\gamma_m\}$ is bounded. Similarly, $\{D_m\}$ is bounded and $\{U_m\}$ is a sequence in the compact set of $p \times k$ semi-orthogonal matrices. Thus, we can pick out a subsequence along which $\gamma_m$, $D_m$, and $U_m$ converge to some limits $\gamma$, $D$, and $U$. The diagonal elements of $D$ are non-negative since those of $D_m$ are and $U$ is a semi-orthogonal matrix by closedness. Thus, along this subsequence we get by taking limits on both sides of the identities $\beta_m = U_m\gamma_m$ and $\Psi_m = U_mD_mD_m^T$ that $\beta = U\gamma$ and $\Psi = UDU^T$, which proves $\Theta_1$ is closed.

Next, we show there exists a compact $A \subseteq \Theta_1$ such that $G_n(\theta) > G_n(\theta_0)$ for all $\theta \in \Theta_1 \setminus A$ and some arbitrary but fixed $\theta_0 \in \Theta$. Unconstrained partial minimization of $G_n$ in $\beta$ and $\Sigma_X$ shows $G_n(\theta) \geq -\log |\Omega| + \text{tr}(Y^TQ_XY\Omega) + \log |X^T X/n| + \text{tr}(I_p)$, which tends to $\infty$ if $\lambda_{\max}(\Omega) \to \infty$ or $\lambda_{\min}(\Omega) \to 0$; this is so because $Y^TQ_XY$ is positive definite when $[Y, X]$ has full column rank. Similarly, unconstrained partial minimization in $\beta$ and $\Omega$ shows $G_n(\theta) \geq \log |Y^TQ_XY/n| + \text{tr}(I_r) + \log |\tau I_p + \Psi| + n^{-1} \text{tr}\{X^T X(\tau I_p + \Psi)^{-1}\}$, which, since $X^T X$ is positive definite when $X$ has full column rank, tends to $\infty$ if $\tau \to \infty$, $\tau \to 0$, or $\lambda_{\max}(\Psi) \to \infty$. Unconstrained partial minimization in $\Omega$ and $\Sigma_X$ gives $G_n(\theta) \geq \log |(Y - X\beta)^T(Y - X\beta)/n| + \text{tr}(I_r) + \log |X^T X/n| + \text{tr}(I_p)$, which tends to $\infty$ if $\|\beta\| \to \infty$ since $X^T X$ is positive definite. Thus, we can take $A = \{\theta \in \Theta_1 : \|\beta\| \leq c, c^{-1} \leq \lambda_{\min}(\Omega) \leq \lambda_{\max}(\Omega) \leq c, c^{-1} \leq \tau \leq c, \lambda_{\max}(\Psi) \leq c\}$ for some large enough $c < \infty$. Using that $\Theta_1$ is closed and $A$ is bounded by construction, it is routine to show $A$ is a closed and bounded subset of $\mathbb{R}^d$ and hence compact.

Now, $G_n$ is continuous at points where $\tau > 0$ and $\lambda_{\min}(\Omega) > 0$ and hence attains its minimum over $A$, which must be a minimum over $\Theta_1$ by the above. To show $G_n$
attains its minimum over \( \Theta \) it thus suffices to show that for any minimizer \( \hat{\theta} \) over \( \Theta_1 \), it must hold that \( \hat{\Psi} \) has rank \( k \) so that \( \hat{\theta} \in \Theta \). Consider a point \( \theta \) such that \( \Psi \) has rank \( s < k \). Then for any \( v \neq 0 \) such that \( \Psi v = 0, \Psi + vv^T \) has rank \( s + 1 \leq k \) and \( \Psi + vv^T \in \mathcal{S} \). Moreover, \( \beta \) is in the column space of \([U, v]\) since it is in that of \( U \).

Thus, if we can show setting \( v \neq 0 \) decreases the objective function, no point with the rank of \( \Psi \) equal to \( s < k \) can be a minimizer, and hence we are done. Consider the function of \( v \) defined for a fixed \( \theta \) by

\[
\log|\Sigma_X + vv^T| + n^{-1} \log(1 + v^T \Sigma^{-1} X^T X) = \log|\Sigma_X| + n^{-1} \log(1 + v^T \Sigma^{-1} v) + n^{-1} \log(1 + v^T \Sigma^{-1} X^T X) v(1 + v^T \Sigma^{-1} v)^{-1},
\]

where we used the matrix determinant lemma and the Sherman-Morrison formula. Now observe that if \( v \) is orthogonal to the \( s \) leading eigenvectors of \( \Sigma_X \), then \( v^T \Sigma_X v = \|v\|^2 \) and \( v^T \Sigma^{-1}_X v = \tau^{-1} \|v\|^2 \). Let \( c = \|v\|^2 \). Then, with the spectral decomposition \( \Sigma = \sum_{j=1}^{p} \lambda_j^{-1}(\Sigma_X) u_j u_j^T \), the terms of the objective that depend on \( v \) are

\[
\log(1 + \tau^{-1} c) - \frac{c \tau^{-1} \left( \sum_{j=s+1}^{p} v^T u_j u_j^T \right) (S_X/\tau) \left( \sum_{j=s+1}^{p} u_j u_j^T v \right)}{1 + \tau^{-1} c}
\]

Consider a \( v \propto u_j \) for some \( j \in \{s + 1, \ldots, p\} \). The last display then becomes

\[
\log(1+\tau^{-1} c) - (1+\tau^{-1} c)^{-1} c \tau^{-1} u_j^T (S_X/\tau) u_j.
\]

By making the change of variables \( t = c \tau^{-1} \) and letting \( a = u_j^T S_X u_j / \tau \) one gets \( \log(1+t) - (1+t)^{-1} ta \) which is minimized by \( t = a-1 \), which is feasible and non-zero if \( a > 1 \). To see \( \hat{\tau} > \lambda_{\text{min}}(S_X) \) and hence \( a > 1 \), let \( VHV^T \) be a spectral decomposition of \( \Sigma_X \), where the diagonal elements of \( H \) are the eigenvalues \( h_j = \lambda_j(\Sigma_X) \). It follows that \( h_{k+1} = \cdots = h_p = \tau \) and the first \( k \) columns of \( V \) are those of \( U \). The part of \( G_n \) depending on \( H \) is \( \log|\Sigma_X| + \text{tr}(S_X \Sigma^{-1}_X) = p \log h_j + h_j^{-1} a_j \), where \( a_j = V_j^T X^T X V_j / n \). The derivative of this with respect to \( h_j \) is \( h^{-1} - h^{-2} a_j \) if \( j \geq k \) and \( (p-k)h_j^{-1} - h_j^{-2} \sum_{j=k+1}^{p} a_j \) if \( j = k + 1 \). Suppose that \( h_p < \lambda_{\text{min}}(S_X) \); then since \( \sum_{j=k+1}^{p} a_j \geq (p-k) \lambda_{\text{min}}(S_X) \), the derivative for \( h_p \) is negative. That is, moving \( h_p = \tau \) towards \( h_k \) does not affect the ordering of the eigenvalues but decreases the objective function. The same holds for every \( h_j \), so for a minimizer it must be that \( \hat{h}_1 \geq \cdots \geq \hat{h}_p = \hat{\tau} \geq \lambda_{\text{min}}(S_X) \). A similar argument shows \( \hat{h}_1 \leq \lambda_{\text{max}}(S_X) \). It remains
to show $\hat{\tau} \neq \lambda_{\min}(S_X)$. Suppose $\hat{h}_1 = \lambda_{\min}(S_X)$, then in fact $h_j = \lambda_{\min}(S_X)$ for all $j$ giving $\lambda_{\min}(S_X)$ multiplicity $p$, contradicting $\lambda_{k+1}(S_X) > \lambda_p(S_X)$. But then, by the same argument as when showing $\hat{\tau} \geq \lambda_{\min}(S_X)$, it must be that $\hat{h}_2 > \lambda_{\min}(S_X)$ since otherwise the objective could be decreased by moving $\hat{h}_2$ towards $\hat{h}_1$. Continuing this process shows $\hat{h}_{k+1} > \lambda_{\min}(S_X)$ as desired.

Our next goal is to prove Theorem 2.2. We start with a few lemmas.

**Lemma A.1.** Condition (i) of Theorem 2.2 implies, for a generic $0 < c < \infty$ that may change between claims but does not depend on $r$ or $p$: (a) $c^{-1} \leq \lambda_{\min}(\Omega_*) \leq \lambda_{\max}(\Omega_*)$; (b) $c^{-1} \leq \lambda_{\min}(\Omega_*^{-1} + \beta_*^T \Sigma_X \beta) \leq \lambda_{\max}(\Omega_*^{-1} + \beta_*^T \Sigma_X \beta) \leq c$; (c) $c^{-1} \leq \lambda_{\min}(\Sigma_X) \leq \lambda_{\min}(\Sigma_X) \leq c$, and (d) $\|\beta_*\| \leq c$.

**Proof.** Claim (a) follows from observing that $\Omega_*^{-1} = \Sigma_*/\Sigma_X$ is the Schur-complement of $\Sigma_X$ in $\Sigma_*$ ([Smith 1992, Theorem 5]), while (b) and (c) are by the Cauchy interlacing theorem. Now (d) follows since $c \geq v^T(\Omega_*^{-1} + \beta_*^T \Sigma_X \beta)v \geq \lambda_{\min}(\Omega_*) + \|\beta_*\| \lambda_{\min}(\Sigma_X) \geq c^{-1} + c^{-1} \|\beta_*\|$ so that $\|\beta_*\| \leq c^2 - 1$.

For any $c > 1$ define the set $A = A(c)$ by

$$A = \{\theta \in \Theta : \|\beta\| \leq c, c^{-1} \leq \lambda_{\min}(\Omega) \leq \lambda_{\max}(\Omega) \leq c, c^{-1} \leq \tau \leq c, \lambda_{\max}(\Psi) \leq c\}.$$ (8)

**Lemma A.2.** Under the conditions of Theorem 2.2, for all $c < \infty$ large enough and any $\epsilon > 0$,

$$\mathbb{P}\left(\sup_{\theta \in A(c)} |G_n(\theta) - G(\theta)| \geq \epsilon\right) \to 0.$$

**Proof.** We have

$$G_n(\theta) - G(\theta) = n^{-1} \text{tr}\{(Y - X\beta)^T(Y - X\beta)\Omega\} - \text{tr}\{(\beta - \beta_*)^T \Sigma_X (\beta - \beta_*) \Omega\} - \text{tr}(\Omega \Omega_*^{-1}) + n^{-1} \text{tr}(X^T X \Sigma_X^{-1}) - \text{tr}(\Sigma_X \Sigma_X^{-1}).$$
We show that the suprema of lines one and two over \( A \) are both \( o_p(1) \) and start with the first. Let \( \varepsilon = Y - X\beta_* \), \( \tilde{\beta} = \beta_* - \beta \), and \( S_Y = Y^TY/n. \) Then the first line is

\[
n^{-1} \text{tr}\{(\varepsilon^T\varepsilon + 2\varepsilon^TX\tilde{\beta} + \tilde{\beta}^TX^TX\tilde{\beta})\Omega\} - \text{tr}(\tilde{\beta}^T\Sigma_{X_*}\tilde{\beta}\Omega) - \text{tr}(\Omega\Omega^{-1} )
\]
or

\[
\text{tr}\{(S_{\varepsilon} - \Omega_*^{-1})\Omega\} + 2\text{tr}\{(S_{\varepsilon}X\tilde{\beta})\Omega\} + \text{tr}\{\tilde{\beta}(S_X - \Sigma_{X_*})\tilde{\beta}\Omega\}
\]

Thus, repeatedly using that \( \text{tr}(A) \leq r \|A\| \) for any \( A \in \mathbb{R}^{r \times r} \) and that operator norms are sub-multiplicative, the absolute value of the first line is upper bounded on \( A \) by

\[
rc\|S_{\varepsilon} - \Omega_*^{-1}\| + 4rc\|S_{\varepsilon}X\| + 4rc^2\|S_X - \Sigma_{X_*}\|
\]

where we implicitly assumed that the \( c \) in the definition of \( A \) and condition (i) of Theorem 2.2 are the same, which can always be arranged by picking the larger of the two, so that \( \|\beta - \beta_*\| \leq 2c \) on \( A \). But the last display is \( o_p(1) \) by condition (ii) of Theorem 2.2.

Now, the second line whose supremum we need to show is \( o_p(1) \) is, by the Woodbury identity \( \Sigma_X = \tau^{-1}I_p - \tau^{-2}U(D^{-1} + \tau^{-1}I_k)^{-1}U^T \) with spectral decomposition \( \Psi = UDU^T, \)

\[
\text{tr}\{(S_X - \Sigma_{X_*})\Sigma_X^{-1}\} = \tau^{-1} \text{tr}(S_X - \Sigma_{X_*}) - \tau^{-2} \text{tr}\{U^T(S_X - \Sigma_{X_*})U(D^{-1} + \tau^{-1}I_k)^{-1}\}.
\]

The absolute value of first term is, on \( A \), less than \( c\text{tr}(S_X - \Sigma_{X_*}) \) which is \( o_p(1) \) by condition (iii) of Theorem 2.2. Also on \( A \), the absolute value of the second term is, since \( U \in \mathbb{R}^{p \times k} \), less than \( c^2k\|S_X - \Sigma_{X_*}\|(D^{-1} + \tau^{-1}I_k)^{-1}\| \leq c^3k\|S_X - \Sigma_{X_*}\| \), which is \( o_p(1) \) by condition (ii) of Theorem 2.2. \( \Box \)
Lemma A.3. Under the conditions of Theorem 2.2 there exists a $0 < c < \infty$ such that
\[ P\left( \arg \min_{\theta \in \Theta} G_n(\theta) \subseteq A(c) \right) \to 1. \]

Proof. Because $\tau_* \geq c^{-1} > 0$, condition (ii) of Theorem 2.2 implies $S_X = X^T X/n$ is invertible with probability tending to one, so it suffices to consider outcomes with invertible $S_X$. Pick $\hat{\theta} \in \arg \min_{\theta \in \Theta} G_n(\theta)$; if none exists we are done trivially.

Let $\hat{\Psi} = \hat{U} \hat{D} \hat{U}^T$ by spectral decomposition and pick a $\hat{\gamma}$ such that $\hat{\beta} = \hat{U} \hat{\gamma}$. Since $\hat{\theta}$ is a minimizer $\hat{\gamma}$ minimizes $\gamma \mapsto \text{tr}\{(Y - X\hat{U}\gamma)^T(Y - X\hat{U}\gamma)\hat{\Omega}\}$; that is,
\[ \hat{\gamma} = (\hat{U}^T S_X \hat{U})^{-1} \hat{U}^T S_{XY}. \]
Thus, using that the spectral norm is submultiplicative,
\[ \|\hat{\beta}\| = \|\hat{\gamma}\| \leq \|(\hat{U}^T S_X \hat{U})^{-1}\| \|\hat{U}^T S_{XY}\| \leq \lambda_{\text{min}}(S_X)^{-1} \|S_X\|^{1/2} \|S_Y\|^{1/2}, \]
which by condition (ii) of Theorem 2.2 tends in probability to $\tau_*^{-1} \{\tau_* + \lambda_{\text{max}}(\hat{\Psi})\}^{1/2} \|\Omega^{-1} + \beta_* \Sigma X_* \beta_*\|^{1/2} \leq 2^{1/2} c^2$, where the inequality is by condition (i). Thus, with probability tending to one, every minimizer satisfies $\|\hat{\beta}\| \leq c$ for some large enough $c$. Next, since $\hat{\Omega} = (Y^T Q_X Y/n)^{-1}$ and the column space of $X \hat{U}$ is a subset of that of $X$, it follows that
\[ \lambda_{\text{min}}(Y^T Q_X Y/n) \leq \lambda_{\text{min}}(\hat{\Omega}^{-1}) \leq \lambda_{\text{max}}(\hat{\Omega}^{-1}) \leq \lambda_{\text{max}}(Y^T Y/n). \]
By condition (ii), the left-most and right-most expressions tend to, respectively, $0 < \lambda_{\text{min}}(\Omega^{-1})$ and $\lambda_{\text{max}}(\Omega^{-1} + \beta_* \Sigma X_* \beta_* < \infty$, from which it follows, by condition (i), that $c^{-1} \leq \lambda_{\text{min}}(\hat{\Omega}) \leq \lambda_{\text{max}}(\hat{\Omega}) \leq c$ with probability tending to one for some large enough $c$. That $\hat{\tau} \leq c$ and $\lambda_{\text{max}}(\hat{\Psi}) \leq c$ follows similarly from Proposition 2.1 and conditions (i) and (ii).

Lemma A.4. Under condition (i) of Theorem 2.2 there exists a $\delta > 0$, which can depend on $c$ but not $p$, such that, for every $\theta \in A(c)$,
\[ G(\theta) - G(\theta_*) \geq \delta \|\theta - \theta_*\|_M^2. \]
Proof. The inequality is an equality if \( \theta = \theta_* \), so pick a \( \theta \neq \theta_* \) and let \( \epsilon = \| \theta - \theta_* \|_M > 0 \). By definition of \( \| \cdot \|_M \), it must hold that (a) \( \| \beta - \beta_* \| = \epsilon \), (b) \( \| \Omega - \Omega_* \| = \epsilon \), (c) \( |\tau - \tau_*| = \epsilon \), or (d) \( \| \Psi - \Psi_* \| = \epsilon \). Let \( G_1(\theta) = -\log |\Omega| + \text{tr} \{ (\beta - \beta_*)^T (\tau_* I_p + \Psi_*) (\beta - \beta_*) \Omega \} + \text{tr} (\Omega_*^{-1}) \) and \( G_2(\theta) = \log |\Sigma_X| + \text{tr} (\Sigma_*^{-1} \Sigma_*) \). Since both \( G_1 \) and \( G_2 \) are minimized by \( \theta_* \), we have

\[
G(\theta) - G(\theta_*) \geq \max \{ G_1(\theta) - G_1(\theta_*), G_2(\theta) - G_2(\theta_*) \}.
\]

Thus, it suffices to show that if either of (a) – (d) holds, then at least one of the terms in the maximum on the right-hand side are greater than \( \epsilon^2 \delta \) for some \( \delta > 0 \) not depending on \( p \).

Consider first \( G_2 \) and let \( \Omega_X = \Sigma_X^{-1} = (\tau I_p + \Psi)^{-1} \). The map \( \text{vec}(\Omega_X) \mapsto G_2(\theta) \) is convex with gradient vanishing at \( \text{vec}(\Omega_{X_*}) \) and Hessian \( \Sigma_X \otimes \Sigma_X \). Thus, \( G_2(\theta) - G(\theta_*) \geq 2^{-1} \lambda_{\min}(\Sigma_X \otimes \Sigma_X) \| \text{vec}(\Omega_X) - \text{vec}(\Omega) \|^2 \geq 2^{-1} \tau^2 \| \Omega_X - \Omega_{X_*} \|^2 \). Now \( \| \Sigma_X - \Sigma_{X_*} \| = \| \Sigma_X (\Omega_X - \Omega_{X_*}) \Sigma_{X_*} \| \leq \| \Sigma_X \| \| \Sigma_{X_*} \| \| \Omega_X - \Omega_{X_*} \| \), so \( G_2(\theta) - G(\theta_*) \geq 2^{-1} \tau^2 \| \Sigma_X - \Sigma_{X_*} \|^2 / (\| \Sigma_X \| + \| \Sigma_{X_*} \|)^2 \geq 2^{-3} c^{-4} \| \Sigma_X - \Sigma_{X_*} \| \). Now suppose (c) holds, then \( \| \Sigma_X - \Sigma_{X_*} \| \geq \epsilon \) by Weyl’s inequalities, so we can take \( \delta = 2^{-3} c^{-4} \). Next suppose (d) holds. If \( |\tau - \tau_*| \geq \epsilon / 2 \), then we can take \( \delta = 2^{-4} c^{-4} \) by the same argument as before, so suppose \( |\tau - \tau_*| < \epsilon / 2 \). Write \( \Sigma_X - \Sigma_{X_*} = \Psi - \Psi_* + (\tau - \tau_*) I_p \). Then for any unit-length \( v \), \( v^T (\Sigma_X - \Sigma_{X_*}) v = v^T (\Psi - \Psi_* + (\tau - \tau_*)) v \). It follows, since the spectral norm of a symmetric matrix is its largest absolute eigenvalue, that \( \| \Sigma_X - \Sigma_{X_*} \| \geq \epsilon / 2 \), and hence we can take \( \delta = 2^{-4} c^{-4} \).

Consider now \( G_1 \) and suppose (a) holds. Minimize partially in \( \Omega \), which amounts to setting \( \Omega^{-1} = (\beta - \beta_*)^T \Sigma_{X_*} (\beta - \beta_*) + \Omega_*^{-1} \). One obtains that \( G_1(\theta) - G_1(\theta_*) \) is lower bounded by \( \log |(\beta - \beta_*)^T \Sigma_{X_*} (\beta - \beta_*) + \Omega_*^{-1}| - \log |\Omega_*^{-1}| \). By the mean value theorem and using that the gradient of \( \Omega^{-1} \mapsto \log |\Omega^{-1}| \) is \( \text{tr}(\Omega) \), the last display is equal to \( \text{tr} \{ \Omega (\beta - \beta_*)^T \Sigma_{X_*} (\beta - \beta_*) \} \), where \( \tilde{\Omega}^{-1} = \Omega_*^{-1} + s (\beta - \beta_*)^T \Sigma_{X_*} (\beta - \beta_*) \) for some \( s \in [0, 1] \). But the last trace is a quadratic in \( \text{vec}(\beta) \) with Hessian \( \tilde{\Omega} \otimes \Sigma_X \). The eigenvalues of \( \tilde{\Omega}^{-1} \) are less than \( c + c^3 \), so the eigenvalues of the Hessian, which are the

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products of the eigenvalues of the terms, are greater than \( c^{-1}(c + c^3)^{-1} \). Thus, we can take \( \delta = 2^{-1}(c^{-2} + c^{-4}) \).

Finally, suppose (b) holds and minimize partially in \( \beta \); that is, set \( \beta = \beta_s \). One gets \( G_1(\theta) - G(\theta_s) \geq -\log |\Omega| + \text{tr}(\Omega\Omega^{-1}_s) + \log |\Omega_s| - \text{tr}(I_r) \). We already know this is a convex function of \( \text{vec}(\Omega) \) which is minimized at \( \text{vec}(\Omega_s) \) and with Hessian \( \Omega^{-1} \otimes \Omega^{-1} \). Thus, \( G_1(\theta) - G(\theta_s) \geq \|\Omega - \Omega_s\|_F^2 2^{-1}c^{-2} \geq \|\Omega - \Omega_s\|^2 2^{-1}c^{-2} \), so we can take \( \delta = 2^{-1}c^{-2} \). To conclude, we have shown the claim holds with \( \delta = \min\{2^{-4}c^{-4}, 2^{-1}(c^{-2} + c^{-4}), 2^{-1}c^{-2}\} \)

\( \square \)

**Proof of Theorem 2.2** The existence part follows from Proposition 2.1 and conditions (i) and (ii). Pick an \( \epsilon > 0 \) and a \( c \) large enough that Lemma A.2 and A.3 hold on \( A = A(c) \). By increasing \( c \) and decreasing \( \epsilon \) if necessary, we may assume \( B = \{\theta : \|\theta - \theta_s\|_M < \epsilon\} \subset A(c) \). On \( A \setminus B \), \( G(\theta) \geq G(\theta_s) + \delta \epsilon^2 \) by Lemma A.4. Thus, by Lemma A.2 \( G_n(\theta) > G(\theta_s) + \delta \epsilon^2/2 \) with probability tending to one. Also with probability tending to one, \( G_n(\theta_s) < G(\theta_s) + \delta \epsilon^2 \). Thus, with probability tending to one, using Lemma A.3 for the first equality, \( \arg\min_{\theta \in \Theta} G_n(\theta) = \arg\min_{\theta \in A} G_n(\theta) = \arg\min_{\theta \in B} G_n(\theta) \), which completes the proof.

\( \square \)

We next focus on Theorem 2.4 We will use the theory by (Geyer, 1994) and check important conditions of that theory in the following lemmas.

**Lemma A.5.** Under the conditions of Theorem 2.4 \( \sqrt{n}\nabla G_n(\theta_s) \) tends in distribution to a multivariate normal vector with mean zero and positive definite covariance matrix with finite entries.

**Proof.** The gradient of \( g(\cdot ; z) \) at \( \theta_s \), with \( \varepsilon = y - \beta_s^T x \), has subvectors given by the vectorizations of \( \nabla_\beta g(\theta_s; z) = -2x\varepsilon^T\Omega_s \), \( \nabla_\Omega g(\theta_s; z) = -\Omega_s^{-1} + \varepsilon \varepsilon^T \), \( \nabla_\psi g(\theta_s; z) = \Sigma_x^{-1} - \Sigma_x^{-1} x x^T \Sigma_x^{-1} \), and \( \nabla_{\tau} g(\theta_s; z) = \text{tr}\{\nabla_\psi g(\theta_s; z)\} \). Consider, for example, the subvector \( \text{vec}\{\nabla_\beta g(\theta_s; z)\} = -2(\Omega_s \otimes I_p) \text{vec}(x \varepsilon^T) \). Observe \( \mathbb{E}(X_i \varepsilon_i^T) = 0 \) and hence \( n^{-1/2} \sum_{i=1}^n \text{vec}\{\nabla_\beta g(\theta_s; Z_i)\} = -2(\Omega_s \otimes I_p)n^{-1/2} \sum_{i=1}^n \text{vec}(X_i \varepsilon_i^T) \) tends to a multivariate normal vector by assumption (iii). All the other subvectors, and the full vector,
can be treated similarly, using for $\nabla \tau g(\theta_\ast; z)$ that $\text{tr}(\Sigma_{\ast \ast}^{-1} xx^T \Sigma_{\ast \ast}^{-1}) = \text{tr}(\Sigma_{\ast \ast}^{-2} xx^T) = \text{vec}(\Sigma_{\ast \ast}^{-2})^T \text{vec}(xx^T)$. 

**Lemma A.6.** Under the conditions of Theorem 2.4, $g(\theta; z) = g(\theta_\ast; z) + \nabla g(\theta_\ast; z)^T (\theta - \theta_\ast) + \|\theta - \theta_\ast\| r(\theta; z)$ with a $r(\theta; z)$ that is stochastically equicontinuous in the sense that for every $\epsilon > 0$ and $\delta > 0$, there exists a $\rho > 0$ such that

$$
\limsup_{n \to \infty} \mathbb{P}^x \left( \sup_{\|\theta - \theta_\ast\| < \rho} \left| n^{-1/2} \sum_{i=1}^{n} [r(\theta; Z_i) - \mathbb{E}\{r(\theta, Z_i)\}] \right| > \delta \right) < \epsilon,
$$

where the superscript * denotes outer probability.

**Proof.** Consider the function $h(s) = g(\theta_\ast + s(\theta - \theta_\ast); z)$, so that $g(\theta; z) - g(\theta_\ast; z) = h(1) - h(0)$. Taylor expansion with integral-form remainder gives $h(s) = h(0) + h'(0)s + \int_{0}^{s} h''(t)(s-t)dt$, where $h'(s) = \nabla g(\theta_\ast + s(\theta - \theta_\ast); z)^T (\theta - \theta_\ast)$ and $h''(s) = (\theta - \theta_\ast)^T \nabla^2 g(\theta_\ast + s(\theta - \theta_\ast); z)(\theta - \theta_\ast)$. Thus, $r(\theta_\ast; z) = 0$ and for $\theta \neq \theta_\ast$

$$
r(\theta; z) = \frac{\|\theta - \theta_\ast\|^T}{\|\theta - \theta_\ast\|} \int_{0}^{1} \nabla^2 g(\theta_\ast + s(\theta - \theta_\ast); z)(1-s)ds(\theta - \theta_\ast).
$$

Denote the middle term (matrix) by $K(\theta; z)$ so that $r(\theta; z) = \|\theta - \theta_\ast\|^{-1}(\theta - \theta_\ast)^T K(\theta; z)(\theta - \theta_\ast)$. Blocks of the matrix $K$ correspond to blocks of $\nabla^2 g$. For example, the leading $pr \times pr$ block of $K$ is $K_1(\theta; z) = \int \{\Omega_s + s(\Omega - \Omega_s)\}(1-s)ds \otimes xx^T$, and hence

$$
n^{-1} \sum_{i=1}^{n} [K_1(\theta; Z_i) - \mathbb{E}\{K_1(\theta; Z_i)\}] = \int \{\Omega_s + s(\Omega - \Omega_s)\}(1-s)ds \otimes n^{-1/2} \sum_{i=1}^{n} X_i X_i^T - \Sigma_{X_\ast} \}
$$

The elements of the right-hand matrix are $O_p(1)$ since the vectorization satisfies a central limit theorem by condition (iii). The elements of the left-hand matrix are bounded on a neighborhood of $\theta_\ast$. Thus, the elements of $n^{-1} \sum_{i=1}^{n} [K_1(\theta; Z_i) - \mathbb{E}\{K_1(\theta; Z_i)\}]$ are $O_p(1)$ uniformly in $\theta$ near a neighborhood of $\theta_\ast$. Similar arguments for the other blocks, using that the inverse covariance matrices in the Hessian have bounded eigenvalues on small enough neighborhoods of $\theta_\ast$ since $\lambda_{\min}(\Omega_s) > 0$ and $\tau_\ast > 0$, show the elements of $n^{-1/2} \sum_{i=1}^{n} [K(\theta; Z_i) - \mathbb{E}\{K(\theta; Z_i)\}]$ are $O_p(1)$ uniformly in $\theta$ near a neighborhood of $\theta_\ast$; thus, the spectral norm is $O_p(1)$ uniformly in $\theta$ near a neighborhood.
of $\theta_s$. The result follows since $\left| n^{-1/2} \sum_{i=1}^{n} [r(\theta; Z_i) - \mathbb{E}\{r(\theta, Z_i)\}] \right| = \left\| \theta - \theta_s \right\|^{-1} (\theta - \theta_s)^T n^{-1/2} \sum_{i=1}^{n} [K(\theta; Z_i) - \mathbb{E}\{K(\theta, Z_i)\}] (\theta - \theta_s) \leq \left\| \theta - \theta_s \right\| \left| n^{-1/2} \sum_{i=1}^{n} [K(\theta; Z_i) - \mathbb{E}\{K(\theta, Z_i)\}] \right|.$}

Proof of Theorem 2.4. We verify the conditions of Theorem 4.4 from Geyer (1994). Chernoff-regularity is from Theorem 2.6. Assumption A is verified by noting $G$ is minimized at $\theta_s \in \Theta, \nabla G(\theta_s) = 0,$ and that $G$ has a local quadratic approximation with $o(\|\theta - \theta_s\|^2)$ remainder around $\theta_s$ by Taylor’s theorem since the third order derivatives are bounded for $\theta$ close to $\theta_s$. The last statement follows from differentiating the expressions for $\nabla^2 G(\theta)$ and observing that powers of $\Omega$ and $\Sigma_X$ are bounded around $\theta_s$ since $\lambda_{\text{min}}(\Omega_s) > 0$ and $\tau_s > 0$. Assumptions B and C are verified in Lemmas A.6 and A.5 respectively. Assumption D holds since $\hat{\theta}$ is a minimizer by assumption.

To establish the results on tangent cones, we will use the following lemma from Li et al. (2019).

Lemma A.7. Let $\mathcal{R} \subseteq \mathbb{R}^{p \times p}$ be the set of $p \times p$ matrices of rank $k$ and $A$ an arbitrary point in $\mathcal{R}$ with singular value decomposition $A = U D V^T, D \in \mathbb{R}^{k \times k}$; then $T_\mathcal{R}(A) = \{ B \in \mathbb{R}^{p \times p} : Q U B Q V = 0 \}$.

Proof of Lemma 2.5. Using the definition, if $C_m \to C$, $a_m \downarrow 0$, and $\Psi + a_mC_m \in S$ for all $n$, then $C_m$ and hence $C$ must be symmetric. Next, let $\mathcal{R}$ be the set of $p \times p$ matrices of rank $k$. Since $\Psi \in S \subseteq \mathcal{R}$, it is immediate from the definition that $T_S(\Psi) \subseteq T_\mathcal{R}(\Psi) \subseteq T_\mathcal{R}(\Psi)$. But Lemma A.7 says $T_\mathcal{R}(\Psi) = \{ C \in \mathbb{R}^{p \times p} : Q U C Q U = 0 \}$, so we have proved $T_S(\Psi) \subseteq T_\mathcal{R}(\Psi) \subseteq \{ C \in \mathbb{R}^{p \times p} : C = C^T, Q U C Q U = 0 \}$. To prove the reverse inclusions, pick arbitrary symmetric $C$ such that $Q U C Q U = 0$ and $a_m \downarrow 0$. We must find $C_m \to C$ satisfying $\Psi + a_mC_m \in S$ for all $m$. To that end, consider $C_m = C$ and $\Psi_m = \Psi + a_mC$. For any $v$ such that $P_U v = 0$, $v^T \Psi_m v = v^T Q_U (\Psi + a_mC) Q_U v = 0$, while for any $v$ such that $P_U v \neq 0$, $v^T \Psi_m v \geq \|P_U v\| \lambda_k(\Psi) - a_m \|C\|$, which is strictly positive for small enough $a_m$. It follows that the null spaces of $\Psi_n$ and $\Psi$ agree and
that $v^T \Psi_m v > 0$ for any $v$ not in that null space. Thus, as desired, $\Psi_m$ is positive semi-definite with rank $k$. For the at most finitely many $m$ where $a_m$ is not small enough, we may take $C_m = 0$ without affecting the conclusion, and this completes the proof.

**Proof of Theorem 2.6.** The claims that $O = O^T$ and $t \in \mathbb{R}$ are straightforward to verify using the definition so we omit the details. That $C = C^T$ and $Q \Psi C \Psi = 0$ is by Lemma 2.5. To see that $P \Psi B = B$, consider arbitrary sequences $a_m \downarrow 0$ and $(B_m, O_m, t_m, C_m) \to (B, O, t, C)$ satisfying Definition 2.1, that is, $\theta_m = \theta + a_m(B_m, O_m, t_m, C_m)$ is in the parameter set for all (large enough) $m$. Since $\Psi$ has $k$ strictly positive eigenvalues, so does $\Psi_m = \Psi + a_m C_m$ for all large enough $m$, and hence $\Psi_m$ has rank at least $k$; thus, it in fact has rank $k$ since $\theta_m$ is in the parameter set. Let $\Psi = U D U^T$ and consider $Q U \beta_m = Q U (\beta + a_m B_m) = a_m Q U B_m$. Since $\theta_m$ is in the parameter set, we can also write $\beta_m = (\Psi + a_m C_m) \gamma_m$ for some $\gamma_m$ and get $Q U \beta_m = a_m Q U C_m \gamma_m$. Thus, dividing by $a_m$ we get $Q U B_m = Q U C_m \gamma_m$. If we can ensure $\{\gamma_m\}$ is bounded so that it has a convergent subsequence, then we are done upon taking limits along that subsequence to get $Q U B = Q U C \gamma = 0$ since $Q U C = 0$. To see that $\{\gamma_m\}$ can be selected to be bounded, note that we may restrict attention to $\gamma_m$ in the row space of $\Psi_m$, which is also its column space. Thus, $\gamma_m = U_m \alpha_m = \sum_{j=1}^k \alpha_{mj} u_{mj}$ and $\beta_m = \Psi_m \gamma_m = \sum_{j=1}^k \lambda_j (\Psi_m) \alpha_{mj} u_j$. The norm $\| \beta_m \|$ is bounded since $\beta_m$ converges and its square is equal to $\| \sum_{j=1}^k \lambda_j (\Psi_m) \alpha_{mj} u_j \|^2 = \sum_{j=1}^k \lambda_j (\Psi_m)^2 \alpha_{mj}^2 \geq \lambda_k (\Psi_m)^2 \sum_{j=1}^k \alpha_{mj}^2 = \lambda_k (\Psi_m)^2 \| \gamma_m \|$, so $\| \gamma_m \| \leq \lambda_k (\Psi_m)^{-1} \| \beta_m \|$, which for all large enough $m$ is bounded by, say, $2 \| \beta \| \lambda_k (\Psi)^{-1} < \infty$. □

Lastly in this section we derive the gradient needed for the implementation suggest in Section 3.1. We derive the gradient assuming the argument $L$ is an unconstrained matrix; the gradient under the restriction that $L_{ij} = 0$ for $j > i$ is obtained by setting the corresponding elements of the unconstrained gradient to zero. The differential of
\[ Q_{XL} = I_n - XL(L^T X^T XL)^{-1}L^T X \]
is

\[
dQ_{XL} = -X(dL)(L^T X^T XL)^{-1}L^T X^T \\
+ XL(L^T X^T XL)^{-1}[(dL)^T X^T XL + L^T X^T X dL](L^T X^T XL)^{-1}L^T X^T \\
- XL(L^T X^T XL)^{-1}(dL)^T X^T.
\]

Thus, the differential of \( \log |Y^T Q_{XL} Y| \) is, with \( S = Y^T Q_{XL} Y \),

\[
d\log |Y^T Q_{XL} Y| = - \text{tr} \left[ S^{-1}Y^T X (dL)(L^T X^T XL)^{-1}L^T X^T Y \right] \\
+ \text{tr} \left[ S^{-1}Y^T XL(L^T X^T XL)^{-1}[(dL)^T X^T XL + L^T X^T X dL](L^T X^T XL)^{-1}L^T X^T Y \right] \\
- \text{tr} \left[ S^{-1}Y^T XL(L^T X^T XL)^{-1}(dL)^T X^T Y \right] \\
= - \text{tr} \left[ (L^T X^T XL)^{-1}L^T X^T Y S^{-1}Y^T X dL \right] \\
+ \text{tr} \left[ (dL)^T X^T XL(L^T X^T XL)^{-1}L^T X^T Y S^{-1}Y^T XL(L^T X^T XL)^{-1} \right] \\
+ \text{tr} \left[ (L^T X^T XL)^{-1}L^T X^T Y S^{-1}Y^T XL(L^T X^T XL)^{-1}L^T X^T X dL \right] \\
- \text{tr} \left[ (dL)^T X^T Y S^{-1}Y^T XL(L^T X^T XL)^{-1} \right].
\]

Thus, \( \nabla \log |Y^T Q_{XL} Y| \) is

\[
\nabla \log |Y^T Q_{XL} Y| = -2X^T Y S^{-1}Y^T XL(L^T X^T XL)^{-1} \\
+ 2X^T XL(L^T X^T XL)^{-1}L^T X^T Y S^{-1}Y^T XL(L^T X^T XL)^{-1}
\]

Finally,

\[
\nabla \log |I_p + LL^T| = 2(I_p + LL^T)^{-1}L,
\]

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and

$$\nabla \log \text{tr} \left[ X^T X (I_p + LL^T)^{-1} \right] = -\frac{2}{\text{tr} [X^T X (I_p + LL^T)^{-1}]} (I_p + LL^T)^{-1} X^T X (I_p + LL^T)^{-1} L.$$

## B Additional results

Figure 2 shows Monte Carlo average root mean squared prediction errors under the same settings as in Figure 1.
Figure 2: Monte Carlo results for prediction

NOTE: Average prediction root mean squared errors over 1000 Monte Carlo replications. Reported numbers are divided by the RMSE of ordinary least squares with all predictors. The number of components $k$ is selected by BIC (TPCR, XENV) or leave-one-out cross-validation (PCR, PLS). Plots in the same row use the same settings. When not varying as indicated on the horizontal axes, $n = 120$, $p = 30$, $k = 3$, $r = 2$, $\Sigma_* = I_2$, $d_* = 5$, $\tau_*$ is set to ensure $p = \text{tr}(\Sigma_X)$, and $\|\beta_{*j}\| = 1$, $j = 1, \ldots, r$. 

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