Cross-Validated Loss-Based Covariance Matrix Estimator Selection in High Dimensions

Philippe Boileau  
Graduate Group in Biostatistics and Center for Computational Biology, UC Berkeley  

Nima S. Hejazi  
Division of Biostatistics, Department of Population Health Sciences, Weill Cornell Medicine  

Mark J. van der Laan  
Division of Biostatistics, Department of Statistics, and Center for Computational Biology, UC Berkeley  

Sandrine Dudoit*  
Department of Statistics, Division of Biostatistics, and Center for Computational Biology, UC Berkeley  

May 10, 2022  

Abstract  

The covariance matrix plays a fundamental role in many modern exploratory and inferential statistical procedures, including dimensionality reduction, hypothesis testing, and regression. In low-dimensional regimes, where the number of observations far exceeds the number of variables, the optimality of the sample covariance matrix as an estimator of this parameter is well-established. High-dimensional regimes do not admit such a convenience. Thus, a variety of estimators have been derived to overcome the shortcomings of the canonical estimator in such settings. Yet, selecting an optimal estimator from among the plethora available remains an open challenge. Using the framework of cross-validated loss-based estimation, we develop the theoretical underpinnings of just such an estimator selection procedure. We propose a general class of loss functions for covariance matrix estimation and establish accompanying finite-sample risk bounds and conditions for the asymptotic optimality of the cross-validation selector. In numerical experiments, we demonstrate the optimality of our proposed selector in moderate sample sizes and across diverse data-generating processes. The practical benefits of our procedure are highlighted in a dimension reduction application to single-cell transcriptome sequencing data.  

Keywords: covariance matrix estimation; cross-validation; dimension reduction; high-dimensional statistics; loss-based estimation  

*To whom correspondence should be addressed: sandrine@stat.berkeley.edu
1 Introduction

The covariance matrix underlies numerous exploratory and inferential statistical procedures central to analyses regularly performed in diverse fields. For instance, in computational biology, this statistical parameter serves as a key ingredient in many popular dimensionality reduction, clustering, and classification methods which are regularly relied upon in quality control assessments, exploratory data analysis, and, recently, the discovery and characterization of novel types of cells. Other important areas in which the covariance matrix is critical include financial economics, climate modeling and weather forecasting, imaging data processing and analysis, probabilistic graphical modeling, and text corpora compression and retrieval. Even more fundamentally, the covariance matrix plays a key role in assessing the strengths of linear relationships within multivariate data, in generating simultaneous confidence bands and regions, and in the construction and evaluation of hypothesis tests. Accurate estimation of this parameter is therefore essential.

When the number of observations in a data set far exceeds the number of features, the estimator of choice for the covariance matrix is the sample covariance matrix: it is an efficient estimator under minimal regularity assumptions on the data-generating distribution (Anderson, 2003; Smith, 2005). In high-dimensional regimes, however, this simple estimator has undesirable properties. When the number of features outstrips the number of observations, the sample covariance matrix is singular. Even when the number of observations slightly exceeds the number of features, the sample covariance matrix is numerically unstable on account of an overly large condition number (Golub and Van Loan, 1996). Its eigenvalues are also generally over-dispersed when compared to those of the population covariance matrix (Johnstone, 2001; Ledoit and Wolf, 2004): the leading eigenvalues are positively biased, while the trailing eigenvalues are negatively biased (Marčenko and Pastur, 1967).

High-dimensional data have become increasingly widespread in myriad scientific domains, with many examples arising from challenges posed by cutting-edge biological sequencing technologies. Accordingly, researchers have turned to developing novel covariance matrix estimators to remediate the deficiencies of the sample covariance matrix. Under certain sparsity assumptions, Bickel and Levina (2008b,a); Rothman et al. (2009); Lam and Fan
Cai et al. (2010), and Cai and Liu (2011), among others, demonstrated that the true covariance matrix can be estimated consistently under specific losses by applying element-wise thresholding or tapering functions to the sample covariance matrix. Another thread of the literature, which includes notable contributions by Stock and Watson (2002); Bai (2003); Fan et al. (2008, 2013, 2016, 2019), and Onatski (2012), has championed methods employing factor models in covariance matrix estimation. Other popular proposals include the families of estimators inspired by the empirical Bayes framework (Robbins, 1964; Efron, 2012), formulated by Schäfer and Strimmer (2005) and Ledoit and Wolf (2004, 2012, 2015, 2018). We briefly review several of these estimator families in Section 4 of the Online Supplement.

Despite the flexibility afforded by the apparent wealth of candidate estimators, this variety poses many practical issues. Namely, identifying the most appropriate estimator from among a collection of candidates is itself a significant challenge. A partial answer to this problem has come in the form of data-adaptive approaches designed to select the optimal estimator within a particular class (for example, Bickel and Levina, 2008b,a; Cai and Liu, 2011; Fan et al., 2013; Fang et al., 2016; Bartz, 2016). Such approaches, however, are inherently limited by their focus on relatively narrow families of covariance matrix estimators. The successful application of such estimator selection frameworks requires, as a preliminary step, that the practitioner make a successful choice among estimator families, injecting a degree of subjectivity in their deployment. The broader question of selecting an optimal estimator from among a diverse library of candidates has remained unaddressed. We offer a general loss-based framework building upon the seminal work of van der Laan and Dudoit (2003); Dudoit and van der Laan (2005); van der Vaart et al. (2006) for asymptotically optimal covariance matrix estimator selection based upon cross-validation.

In the cross-validated loss-based estimation framework, the parameter of interest is defined as the risk minimizer, with respect to the data-generating distribution, based on a loss function chosen to reflect the problem at hand. Candidate estimators may be generated in a variety of manners, including as empirical risk minimizers with respect to an empirical distribution over parameter subspaces corresponding to models for the data-generating distribution. One would ideally select as optimal estimator that which minimizes the “true”
risk with respect to the data-generating distribution. However, as this distribution is typi-
cally unknown, one turns to cross-validation for risk estimation. van der Laan and Dudoit
(2003); Dudoit and van der Laan (2005); van der Vaart et al. (2006) have shown that, under
general conditions on the data-generating distribution and loss function, the cross-validated
estimator selector is asymptotically optimal in the sense that it performs asymptotically as
well in terms of risk as an optimal oracle selector based on the true, unknown data-generating
distribution. These results extend prior work summarized by Györfi et al. (2002, Ch. 7–8).

Focusing specifically on the covariance matrix as the parameter of interest, we address
the choice of loss function and candidate estimators, and derive new, high-dimensional
asymptotic optimality results for multivariate cross-validated estimator selection procedures.
Requiring generally nonrestrictive assumptions about the structure of the true covariance
matrix, the proposed framework accommodates arbitrary families of covariance matrix esti-
mators. The method therefore enables the objective selection of an optimal estimator while
fully taking advantage of the plethora of available estimators. As such, it generalizes ex-
isting, but more limited, data-adaptive estimator selection frameworks where the library of
candidate estimators is narrowed based on available subject matter knowledge, or, as is more
commonly the case, for convenience’s sake.

2 Problem Formulation and Background

Consider a data set \( X_{n 	imes J} = \{X_1, \ldots, X_n : X_i \in \mathbb{R}^J \} \), comprising \( n \) independent and identi-
cally distributed (i.i.d.) random vectors, where \( n \approx J \) or \( n < J \). Let \( X_i \sim P_0 \in \mathcal{M} \), where
\( P_0 \) denotes the true data-generating distribution and \( \mathcal{M} \) the statistical model, that is, a
collection of possible data-generating distributions \( P \) for \( X_i \). We assume a nonparametric
statistical model \( \mathcal{M} \) for \( P_0 \), minimizing assumptions on the form of \( P_0 \). We denote by \( P_n \) the
empirical distribution of the \( n \) random vectors forming \( X_{n \times J} \). Letting \( \mathbb{E}[X_i] = 0 \) without loss
of generality and defining \( \psi_0 := \text{Var}[X_i] \), we take as our goal the estimation of the covariance
matrix \( \psi_0 \). This is accomplished by identifying the “optimal” estimator of \( \psi_0 \) from among
a collection of candidates, where, as detailed below, optimality is defined in terms of risk.

For any distribution \( P \in \mathcal{M} \), define its covariance matrix as \( \psi = \Psi(P) \), where \( \Psi \) is a
mapping from the model \( \mathcal{M} \) to the set of \( J \times J \) symmetric, positive semi-definite matrices. Furthermore, candidate estimators of the covariance matrix are defined as \( \hat{\psi}_k := \hat{\Psi}_k(P_n) \) for \( k = 1, \ldots, K \) in terms of mappings \( \hat{\Psi}_k \) from the empirical distribution \( P_n \) to \( \Psi := \{ \psi \in \mathbb{R}^{J \times J} | \psi = \psi^\top \} \). While this notation suggests that the number of candidate estimators \( K \) is fixed, and we treat it as such throughout, this framework may be extended such that \( K \) grows as a function of \( n \) and \( J \). It also follows that \( \{ \psi = \Psi(P) : P \in \mathcal{M} \} \subset \Psi \); that is, the set of all covariance matrices corresponding to the data-generating distributions \( P \) belonging to the model \( \mathcal{M} \) is a subset of \( \Psi \).

In order to assess the optimality of estimators in the set \( \Psi \), we introduce a generic loss function \( L(X; \psi, \eta) \) characterizing a cost applicable to any \( \psi \in \Psi \) and \( X \sim P \in \mathcal{M} \), and where \( \eta \) is a (possibly empty) nuisance parameter. Specific examples of loss functions for the covariance estimation setting are proposed in Section 3.1. Define \( H \) as the mapping from the model \( \mathcal{M} \) to the nuisance parameter space \( \mathcal{H} := \{ \eta = H(P) : P \in \mathcal{M} \} \) and let \( \hat{\eta} := \hat{H}(P_n) \) denote a generic nuisance parameter estimator, where \( \hat{H} \) is a mapping from \( P_n \) to \( \mathcal{H} \). Given any \( \eta \in \mathcal{H} \), the risk under \( P \in \mathcal{M} \) for any \( \psi \in \Psi \) is defined as the expected value of \( L(X; \psi, \eta) \) with respect to \( P \):

\[
\Theta(\psi, \eta, P) := \int L(x; \psi, \eta) dP(x) = \mathbb{E}_P [L(X; \psi, \eta)].
\]

Under the additional constraint on the loss function that a risk minimizer exists under the true data-generating distribution \( P_0 \), the minimizer is given by the parameter of interest

\[
\psi_0 := \arg\min_{\psi \in \Psi} \Theta(\psi, \eta_0, P_0), \tag{1}
\]

where \( \eta_0 := H(P_0) \). The risk minimizer need not be unique. The optimal risk under \( P_0 \) is

\[
\theta_0 := \min_{\psi \in \Psi} \Theta(\psi, \eta_0, P_0),
\]

which is to say that a risk minimizer \( \psi_0 \) attains risk \( \theta_0 \).

For any given estimator \( \hat{\psi}_k \) of \( \psi_0 \), its conditional risk given \( P_n \) with respect to the true
data-generating distribution $P_0$ is
\[
\tilde{\theta}_n(k, \eta_0) := \mathbb{E}_{P_0}[L(X; \hat{\Psi}_k(P_n), \eta_0) | P_n] = \Theta(\hat{\psi}_k, \eta_0, P_0).
\]
Defining the risk difference of the $k^{th}$ estimator as $\tilde{\theta}_n(k, \eta_0) - \theta_0$, the index of the estimator that achieves the minimal risk difference is
\[
\tilde{k}_n := \arg\min_{k \in \{1, \ldots, K\}} \tilde{\theta}_n(k, \eta_0) - \theta_0.
\]
The subscript $n$ emphasizes that the risk and optimal estimator index are conditional on the empirical distribution $P_n$. They are therefore random variables.

Given the high-dimensional nature of the data, it is generally most convenient to study the performance of estimators of $\psi_0$ using *Kolmogorov asymptotics*, that is, in the setting in which both $n \to \infty$ and $J \to \infty$ such that $J/n \to m < \infty$. Historically, estimators have been derived within this high-dimensional asymptotic regime to improve upon the finite sample results of estimators brought about by traditional asymptotic arguments. After all, the sample covariance matrix retains its asymptotic optimality properties when $J$ is fixed, even though it is known to perform poorly in high-dimensional settings.

Naturally, it would be desirable for an estimator selection procedure to select the estimator indexed by $\tilde{k}_n$; however, this quantity depends on the true, unknown data-generating distribution $P_0$. As a substitute for the candidates’ true conditional risks, we employ instead the cross-validated estimators of these same conditional risks.

Cross-validation (CV) consists of randomly, and possibly repeatedly, partitioning a data set into a training set and a validation set. The observations in the training set are fed to the candidate estimators and the observations in the validation set are used to evaluate the performance of these estimators (Breiman and Spector, 1992; Friedman et al., 2001). A range of CV schemes have been proposed and investigated, both theoretically and computationally; Dudoit and van der Laan (2005) provide a thorough review of popular CV schemes and their properties. Among the variety, $V$-fold stands out as an approach that has gained traction on account of its relative computational feasibility and good performance. Any CV scheme can be expressed in terms of a binary random vector $B_n$, which assigns observations
into either the training or validation set. Observation \( i \) is said to lie in the training set when \( B_n(i) = 0 \) and in the validation set otherwise. The training set therefore contains \( \sum_i (1 - B_n(i)) = n(1 - p_n) \) observations and the validation set \( \sum_i B_n(i) = np_n \) observations, where \( p_n \) is the fixed validation set proportion corresponding to the chosen CV procedure.

The empirical distributions of the training and validation sets are denoted by \( P_{0,n,B_n} \) and \( P_{1,n,B_n} \), respectively, for any given realization of \( B_n \). \( B_n \), we emphasize, is independent of \( P_n \).

Using this general definition, the cross-validated estimator of a candidate \( \hat{\Psi}_k \)'s risk is

\[
\hat{\theta}_{p_n,n}(k, \hat{H}(P_{n,B_n})) := E_{B_n} \left[ \Theta(\hat{\Psi}_k(P_{0,n,B_n}), \hat{H}(P_{n,B_n}), P_{1,n,B_n}) \right]
\]

\[
= E_{B_n} \left[ \frac{1}{np_n} \sum_{i=1}^{n} I(B_n(i) = 1)L(X_i; \hat{\Psi}_k(P_{0,n,B_n}), \hat{H}(P_{n,B_n})) \right],
\]

for a nuisance parameter estimator mapping \( \hat{H} \). Here, \( E_{B_n}[\cdot] \) denotes the expectation with respect to \( B_n \). The corresponding cross-validated selector is

\[
\hat{k}_{p_n,n} := \arg\min_{k \in \{1, \ldots, K\}} \hat{\theta}_{p_n,n}(k, \hat{H}(P_{n,B_n})).
\]

As a benchmark, the unknown cross-validated conditional risk of the \( k \)th estimator is

\[
\tilde{\theta}_{p_n,n}(k, \eta_0) := E_{B_n} \left[ \Theta(\hat{\Psi}_k(P_{0,n,B_n}), \eta_0, P_0) \right].
\]

The cross-validated oracle selector is then

\[
\tilde{k}_{p_n,n} := \arg\min_{k \in \{1, \ldots, K\}} \tilde{\theta}_{p_n,n}(k, \eta_0).
\]

As before, the \( p_n \) and \( n \) subscripts highlight the dependence of these objects on the CV procedure and the empirical distribution \( P_n \), respectively, thus making them random variables.

Ideally, the cross-validated estimator selection procedure should identify a \( \hat{k}_{p_n,n} \) that is asymptotically (in \( n, J, \) and possibly \( K \)) equivalent in terms of risk to the oracle \( \tilde{k}_{p_n,n} \), under a set of nonrestrictive assumptions based on the choice of loss function, target parameter space, estimator ranges, and, if applicable, nuisance parameter space, in the sense that

\[
\frac{\hat{\theta}_{p_n,n}(\hat{k}_{p_n,n}, \eta_0) - \theta_0}{\tilde{\theta}_{p_n,n}(\tilde{k}_{p_n,n}, \eta_0) - \theta_0} \overset{P}{\to} 1 \text{ as } n, J \to \infty.
\]

That is, the estimator selected via CV is equivalent in terms of risk to the CV scheme's oracle estimator chosen from among all candidates.
When Equation (2) holds, a further step may be taken by relating the performance of the cross-validated selector to that of the full-dataset oracle selector, $\tilde{k}_n$:

$$\frac{\hat{\theta}_n(\tilde{k}_{p,n}, \eta_0) - \theta_0}{\hat{\theta}_n(\tilde{k}_n, \eta_0) - \theta_0} \xrightarrow{p} 1 \text{ as } n, J \rightarrow \infty. \quad (3)$$

When the cross-validated selection procedure’s full-dataset conditional risk difference converges in probability to that of the full-dataset oracle’s, the chosen estimator is asymptotically optimal. In other words, the data-adaptively selected estimator performs asymptotically as well, with respect to the chosen loss, as the candidate that would be picked from the collection of estimators if the true data-generating distribution were known.

### 3 Loss Functions and Estimator Selection

#### 3.1 Proposed Loss Function

The choice of loss function should reflect the goals of the estimation task. While loss functions based on the sample covariance matrix and either the Frobenius or the spectral norms are often employed in the covariance matrix estimation literature, Dudoit and van der Laan (2005)’s estimator selection framework is more amenable to loss functions that operate over random vectors. Accordingly, we propose the observation-level Frobenius loss:

$$L(X; \psi, \eta_0) := \|XX^\top - \psi\|_{F, \eta_0}^2 = \sum_{j=1}^J \sum_{l=1}^J \eta_0^{(jl)} (X^{(j)} X^{(l)} - \psi^{(jl)})^2, \quad (4)$$

where $X^{(j)}$ is the $j$th element of a random vector $X \sim P \in \mathcal{M}$, $\psi^{(jl)}$ is the entry in the $j$th row and $l$th column of an arbitrary covariance matrix $\psi \in \Psi$, and $\eta_0$ is a $J \times J$ matrix acting as a scaling factor, that is, a potential nuisance parameter. For an estimator $\hat{\eta}$ of $\eta_0$, the cross-validated risk estimator of the $k$th candidate estimator $\hat{\Psi}_k$ under the observation-level Frobenius loss is

$$\hat{\theta}_{p,n}(k, \hat{H}(P_{n,B_n}^0)) = \mathbb{E}_{B_n} \left[ \frac{1}{n \eta_{p,n}} \sum_{i=1}^n \mathbb{I}(B_n(i) = 1) \|X_i X_i^\top - \hat{\Psi}_k(P_{n,B_n}^0)\|_{F, \hat{H}(P_{n,B_n}^0)}^2 \right].$$

Ledoit and Wolf (2004), Bickel and Levina (2008a), and Rothman et al. (2009), among others, have employed analogous (scaled) Frobenius losses to prove various optimality results,
defining $\eta^{(jl)}_0 = 1/J$, $\forall j,l$. This particular choice of scaling factor is such that whatever the value of $J$, $\|I_{J \times J}\|_{F,\eta_0} = 1$. With such a scaling factor, the loss function may be viewed as a relative loss whose yardstick is the $J \times J$ identity matrix. A similarly reasonable option for when the true covariance matrix is assumed to be dense is $\eta^{(jl)}_0 = 1/J^2$. This weighting scheme effectively computes the average squared error across every entry of the covariance matrix; however, when the scaling factor is constant, it only impacts the interpretation of the loss. Constant scaling factors have no impact on our asymptotic analysis. Since it need not be estimated, it is not a nuisance parameter in the conventional sense.

When the scaling factor of Equation (4) is constant, the risk minimizers are identical for the cross-validated observation-level Frobenius risk and the common cross-validated Frobenius risk (used by, for example, Bickel and Levina, 2008a; Rothman et al., 2009; Fan et al., 2013; Fang et al., 2016).

**Proposition 1** Define the cross-validated Frobenius risk for an estimator $\hat{\Psi}_k$ as

$$\hat{R}_n(\hat{\Psi}_k, \eta_0) := \mathbb{E}_{B_n} \left[ \|S_n(P_{n,B_n}^1) - \hat{\Psi}_k(P_{n,B_n}^0)\|_{F,\eta_0}^2 \right], \quad (5)$$

where $S_n(P_{n,B_n}^1)$ is the sample covariance matrix computed over the validation set $P_{n,B_n}^1$, and $\eta_0$ is some constant scaling matrix. Then, $\hat{R}_n(\hat{\Psi}_k, \eta_0) - \hat{\theta}_{p_{n,n}}(k, \eta_0)$ is constant with respect to $\hat{\Psi}_k(P_{n,B_n}^0)$ such that

$$\hat{k}_{p_{n,n}} = \arg\min_{k \in \{1, \ldots, K\}} \hat{\theta}_{p_{n,n}}(k, \eta_0)$$

$$= \arg\min_{k \in \{1, \ldots, K\}} \hat{R}_n(\hat{\Psi}_k, \eta_0).$$

Note that the traditional Frobenius loss corresponds to the sum of the squared eigenvalues of the difference between the sample covariance matrix and the estimate. Proposition 1 therefore implies the existence of a similar relationship for our observation-level Frobenius loss. It may therefore serve as a surrogate for a loss based on the spectral norm.

We are not restricted to a constant scaling factor matrix. One might consider weighting the covariance matrix’s off-diagonal elements’ errors by their corresponding diagonal entries, especially useful when the random variables are of different scales. Such a scaling factor
might offer a more equitable evaluation across all entries of the parameter:

\[
L_{\text{weighted}}(X; \psi, \eta_0) := \sqrt{\sum_{j=1}^{J} \sum_{l=1}^{J} \frac{1}{\psi_0^{(jj)} \psi_0^{(ll)}} (X^{(j)} X^{(l)} - \psi^{(jl)})^2}.
\]

Here, \( \eta_0 = \text{diag}(\psi_0) \) is a genuine nuisance parameter which can be estimated via the diagonal entries of the sample covariance matrix.

Finally, the covariance matrix \( \psi_0 \) is the risk minimizer of the observation-level Frobenius loss if the integral with respect to \( X \) and the partial differential operators with respect to \( \psi \) are interchangeable.

**Proposition 2** Let the integral with respect to \( X \) and the partial differential operators with respect to \( \psi \) be interchangeable, and let \( \eta \) be some fixed \( J \times J \) matrix. Then

\[
\psi_0 = \arg\min_{\psi \in \Psi} \Theta(\psi, \eta, P_0)
\]

for \( \Theta(\cdot) \) defined under the observation-level Frobenius loss.

The proof is provided in the Online Supplement. Our proposed loss therefore satisfies the condition of Equation (1). The main results of the paper, however, relate only to the constant scaling factor case. In a minor abuse of notation, we set \( \eta_0 = 1 \), and suppress dependence of the loss function on the scaling factor wherever possible throughout the remainder of the text.

### 3.2 Optimality of the Cross-validated Estimator Selector

Having defined a suitable loss function, we turn to a discussion of the theoretical properties of the cross-validated estimator selection procedure. Specifically, we present, in Theorem 1, sufficient conditions under which the method is asymptotically equivalent in terms of risk to the commensurate CV oracle selector (as per Equation (2)). This theorem extends the general framework of Dudoit and van der Laan (2005) for use in high-dimensional multivariate estimator selection. Adapting their existing theory to this setting requires a judicious choice of loss function, new assumptions, and updated proofs reflecting the use of high-dimensional asymptotics. Corollary 1 then builds on Theorem 1 and details conditions under which the
procedure produces asymptotically optimal selections in the sense of Equation (3). All proofs are provided in Section 1 of the Online Supplement.

**Theorem 1** Let $X_1, \ldots, X_n$ be a random sample of $n$ i.i.d. random vectors of dimension $J$, such that $X_i \sim P_0 \in \mathcal{M}$, $i = 1, \ldots, n$. Assume, without loss of generality, that $\mathbb{E}[X_i] = 0$, and define $\psi_0 := \text{Var}[X_i]$. Denote the set of $K$ candidate estimators by $\{\bar{\Psi}_k(\cdot) : k = 1, \ldots, K\}$. Next, define the observation-level Frobenius loss function as $L(X; \psi) := \|X^\top X - \psi\|_F^2$. Finally, designate $p_n$ as the proportion of observations in any given cross-validated validation set. Consider the following assumptions:

**Assumption 1** For any $P \in \mathcal{M}$ and $X \sim P$, $\max_{j=1,\ldots,J} (|X^{(j)}|) < \sqrt{M_1} < \infty$ almost surely (a.s.).

**Assumption 2** Define $\Psi := \{\psi \in \mathbb{R}^{J \times J} | \psi = \psi^\top, |\psi^{(j)}| < M_2 < \infty, \forall j, l = 1, \ldots, J\}$, and assume that $\bar{\Psi}_k(P_n), \psi_0 \in \Psi$.

**Finite-Sample Result.** Let $\bar{M}(J) := 4(M_1 + M_2)^2 J^2$ and $c(\delta, \bar{M}(J)) := 2(1 + \delta)^2 \bar{M}(J)(1/3 + 1/\delta)$. Then, for any $\delta > 0$,

$$0 \leq \mathbb{E}_{P_0}[\tilde{\theta}_{p,n}(\hat{k}_{p,n}) - \theta_0] \leq (1 + 2\delta)\mathbb{E}_{P_0}[\tilde{\theta}_{p,n}(\hat{k}_{p,n}) - \theta_0] + 2c(\delta, \bar{M}(J)) \frac{1 + \log(K)}{n p_n}. \quad (6)$$

**High-Dimensional Asymptotic Result.** The finite-sample result in Equation (6) has the following asymptotic implications: If $c(\delta, \bar{M}(J))(1 + \log(K))/(np_n\mathbb{E}_{P_0}[\tilde{\theta}_{p,n}(\hat{k}_{p,n}) - \theta_0]) \to 0$ and $J/n \to m < \infty$ as $n, J \to \infty$, then

$$\frac{\mathbb{E}_{P_0}[\tilde{\theta}_{p,n}(\hat{k}_{p,n}) - \theta_0]}{\mathbb{E}_{P_0}[\bar{\theta}_{p,n}(\hat{k}_{p,n}) - \theta_0]} \to 1. \quad (7)$$

Further, if $c(\delta, \bar{M}(J))(1 + \log(K))/(np_n(\bar{\theta}_{p,n}(\hat{k}_{p,n}) - \theta_0)) \overset{P}{\to} 0$ as $n, J \to \infty$, then

$$\frac{\tilde{\theta}_{p,n}(\hat{k}_{p,n}) - \theta_0}{\bar{\theta}_{p,n}(\hat{k}_{p,n}) - \theta_0} \overset{P}{\to} 1. \quad (8)$$

The proof relies on special properties of the random variable $Z_k := L(X; \bar{\Psi}_k(P_n)) - L(X; \psi_0)$ and on an application of Bernstein’s inequality (Bennett, 1962). Together, they are used to show that $2c(\delta, \bar{M}(J))(1 + \log(K))/(np_n)$ is a finite-sample bound for comparing the performance of the cross-validated selector, $\hat{k}_{p,n}$, against that of the oracle selector over the
training sets, \( \tilde{k}_{p_n,n} \). Once this bound is established, the high-dimensional asymptotic results follow immediately.

Only a few sufficient conditions are required to provide finite-sample bounds on the expected risk difference of the estimator selected via our CV procedure. First, that each element of the random vector \( X \) be bounded, and, second, that the entries of all covariance matrices in the parameter space and the set of possible estimates be bounded. Together, these assumptions allow for the definition of \( \overline{M}(J) \), the object permitting the extension of the loss-based estimation framework to the high-dimensional covariance matrix estimation problem.

The first assumption is technical in nature — it makes the proofs tractable. While it may appear stringent, and, for instance, is not satisfied by Gaussian distributions, we believe it to be generally applicable. We stress that parametric data-generating distributions, like those exhibiting Gaussianity, rarely reflect reality, that is, they are merely mathematical conveniences\(^1\). Most random variables, or transformations thereof, arising in scientific practice are bounded by limitations of the physical, electronic, or biological measurement process; thus, our method remains widely applicable. For example, in microarray and next-generation sequencing experiments, the raw data are images on a 16-bit scale, constraining them to \([0, 2^{16})\). Similarly, the measurement of immunologic markers, of substantial interest in vaccine efficacy trials of HIV-1, COVID-19, and other infectious diseases, are bounded by the limits of detection and/or quantitation imposed by assay biotechnology.

Verifying that the additional assumptions required by Theorem 1’s asymptotic results hold proves to be more challenging. We write \( f(y) = O(g(y)) \) if \( |f| \) is bounded above by \( g \), \( f(y) = o(g(y)) \) if \( f \) is dominated by \( g \), \( f(y) = \Omega(g(y)) \) if \( f \) is bounded below by \( g \), and \( f(y) = \omega(g(y)) \) if \( f \) dominates \( g \), all in asymptotics with respect to \( n \) and \( J \). Further, a subscript “\( P \)” might be added to these bounds, denoting a convergence in probability. Now, note that \( c(\delta, \overline{M}(J))(1 + \log(K))/(np_n) = O(J) \) for fixed \( p_n \) and as \( J/n \to m > 0 \). Then the conditions associated with Equation (7) and Equation (8) hold so long as \( \mathbb{E}_{P_0}[\hat{\theta}_{p_n,n}(\tilde{k}_{p_n,n}) - \theta_0] = \omega(J) \)

\(^1\)Anecdotal, one cannot help but find themself reminded that “Everyone is sure of this [that errors are normally distributed] ... since the experimentalists believe that it is a mathematical theorem, and the mathematicians that it is an experimentally determined fact.” (Poincaré, 1912, p. 171)
and \( \tilde{\theta}_{p,n}(\tilde{k}_{p,n}) - \theta_0 = \omega_P(J) \), respectively.

These requirements do not seem particularly restrictive given that the complexity of the problem generally increases as a function of the number of features. There are many more entries in the covariance matrix requiring estimation than there are observations. This intuition is corroborated by our extensive simulation study in the following section. Consistent estimation in terms of the Frobenius risk is therefore not possible in high-dimensions without additional assumptions about the data-generating process.

Some additional insight might be gained by identifying conditions under which these assumptions are unmet for popular structural beliefs about the true covariance matrix. In particular, we consider the sparse covariance matrices defined in Bickel and Levina (2008a) and accompanying hard-thresholding estimators (see Section 4.1 of the Online Supplement):

**Proposition 3** In addition to Assumptions 1 and 2 of Theorem 1, assume that \( \psi_0 \) is a member of the following set of matrices:

\[
\left\{ \psi : \psi^{(jj)} < M_2; \sum_{l=1}^{J} I(\psi^{(jl)} \neq 0) < s(J) \text{ for all } j = 1, \ldots, J \right\}
\]

where \( s(J) \) is the row sparsity, that the hard-thresholding estimator is in the library of candidates, and that it uses a “sufficiently large” thresholding hyperparameter value in the sense of Bickel and Levina (2008a). Then, by Theorem 2 of Bickel and Levina (2008a), we have

\[
\mathbb{E}_{P_{\psi_0}}[\tilde{\theta}_{p,n}(\tilde{k}_{p,n}) - \theta_0] = o(J) \text{ if } s(J)/J = o(1/\log J) \text{ asymptotically in } n \text{ and } J.
\]

Proposition 3 states that the conditions for achieving the asymptotic results of Theorem 1 are not met if the proportion of non-zero elements in the covariance matrix’s row with the most non-zero elements converges to zero faster than \( 1/\log J \) and the library of candidates possesses a hard-thresholding estimator whose thresholding hyperparameter is reasonable in the sense of Bickel and Levina (2008a)’s Theorem 2 and its subsequent discussion. Plainly, the true covariance matrix cannot be too sparse if the collection of considered estimators contains the hard-thresholding estimator with a correctly specified thresholding hyperparameter value.

This implies that banded covariance matrices whose number of bands are fixed for \( J \) do not meet the criteria for our theory to apply, assuming that one of the candidate estimators
correctly specifies the number of bands. Nevertheless, we observe empirically in Section 4 that our cross-validated procedure selects an optimal estimator when the true covariance matrix is banded or tapered more quickly in terms of $n$ and $J$ than any other type of true covariance matrix.

These results are likely explained by the relatively low complexity of the estimation problem in this setting. High-dimensional asymptotic arguments are perhaps unnecessary when the proportion of entries needing to be estimated in the true covariance matrix quickly converges to zero. These limitations of our theory reflect stringent, and typically unverifiable, structural assumptions about the estimand. We reiterate that the conditions of Theorem 1 are generally satisfied. In situations where the true covariance matrix is known to possess this level sparsity, practitioners might instead appeal to Equation (39) of Bickel and Levina (2008a) to support their use of a cross-validated estimator selection procedure. This result, coupled with that of Proposition 1, likely explains the aforementioned simulation findings of the banded and tapered covariance matrices.

Now, Theorem 1’s high-dimensional asymptotic results relate the performance of the cross-validated selector to that of the oracle selector for the CV scheme. As indicated by the expression in Equation (3), however, we would like our cross-validated procedure to be asymptotically equivalent to the oracle over the entire data set. The conditions to obtain this desired result are provided in Corollary 1, a minor adaptation of previous work by Dudoit and van der Laan (2005). This extension accounts for increasing $J$, thereby permitting its use in high-dimensional asymptotics.

**Corollary 1** Building upon Assumptions 1 and 2 of Theorem 1, we introduce the additional assumptions that, as $n, J \to \infty$ and $J/n \to m < \infty$, $p_n \to 0$, $c(\delta, \overline{M}(J))(1 + \log(K))/(np_n(\hat{\theta}_{pn,n}(\bar{k}_{pn,n}) - \theta_0)) \to 0,$ and

$$\frac{\bar{\theta}_{pn,n}(\bar{k}_{pn,n}) - \theta_0}{\bar{\theta}_n(\bar{k}_n) - \theta_0} \xrightarrow{P} 1.$$ (9)

Under these assumptions, it follows that

$$\frac{\bar{\theta}_{pn,n}(\bar{k}_{pn,n}) - \theta_0}{\bar{\theta}_n(\bar{k}_n) - \theta_0} \xrightarrow{P} 1.$$ (10)
The proof is a direct application of the asymptotic results of Theorem 1.

As before, the assumption that \( c(\delta, M(J))(1 + \log(K))/(np_n(\bar{\theta}_{p_n,n}(\bar{k}_{p_n,n}) - \theta_0)) \xrightarrow{P} 0 \) remains difficult to verify, but essentially requires the estimation error of the oracle to increase quickly as the number of features grows. That is, \( np_n(\bar{\theta}_{p_n,n}(\bar{k}_{p_n,n}) - \theta_0) = o(P(J)) \). We posit that this condition is generally satisfied, similarly to the asymptotic results of Theorem 1.

Now, a sufficient condition for Equation (9) is that there exists a \( \gamma > 0 \) such that

\[
\left(n^{\gamma}(\bar{\theta}_{n}(\bar{k}_n) - \theta_0), (n(1 - p_n))^{\gamma}(\bar{\theta}_{p_n,n}(\bar{k}_{p_n,n}) - \theta_0)\right) \xrightarrow{d} (Z, Z),
\]

for a single random variable \( Z \) with \( P(Z > a) = 1 \) for some \( a > 0 \). For single-split validation, where \( P(B_n = b) = 1 \) for some \( b \in \{0, 1\}^n \), it suffices to assume that there exists a \( \gamma > 0 \) such that \( n^{\gamma}(\bar{\theta}_{n}(\bar{k}_n) - \theta_0) \xrightarrow{d} Z \) for a random variable \( Z \) with \( P(Z > a) = 1 \) for some \( a > 0 \).

Equation (9) essentially requires that the (appropriately scaled) distributions of the cross-validated and full-dataset conditional risk differences of their respective oracle selections converge in distribution as \( p_n \to 0 \). Again, this condition is unrestrictive. As \( p_n \to 0 \), the composition of each training set becomes increasingly similar to that of the full-dataset. The resulting estimates produced by each candidate estimator over the training sets and the full-dataset will correspondingly converge. Naturally, so too will the cross-validated and full-dataset conditional risk difference distributions of their respective selections.

While the number of candidates in the estimator library \( K \) has been assumed to be fixed in this discussion of the proposed method’s asymptotic results, it may be allowed to grow as a function of \( n \) and \( J \). Of course, this will negatively impact the convergence rates of \( c(\delta, \bar{M}(J))(1 + \log(K))/(np_n\mathbb{E}_{P_0}[\bar{\theta}_{p_n,n}(\bar{k}_{p_n,n}) - \theta_0]) \) and \( c(\delta, \bar{M}(J))(1 + \log(K))/(np_n(\bar{\theta}_{p_n,n}(\bar{k}_{p_n,n}) - \theta_0)) \). The sufficient conditions outlined in the asymptotic results of Theorem 1 are achieved so long as the library of candidates does not grow too aggressively. That is, we can make the additional assumptions that \( K = o(\exp(\mathbb{E}_{P_0}[\bar{\theta}_{p_n,n}(\bar{k}_{p_n,n}) - \theta_0]/J)) \) and \( K = o_P(\exp(\{\bar{\theta}_{p_n,n}(\bar{k}_{p_n,n}) - \theta_0] / J\}) \) such that the results of Equations (7) and (8) are achieved, respectively.

Finally, we have assumed thus far that \( \mathbb{E}_{P_0}[X] \) is known. This is generally not the case in practice. In place of a random vector centered at zero, we might instead consider the set of \( n \) demeaned random vectors \( \tilde{X}_{n \times J} \) where \( \tilde{X}_i = X_i - \bar{X} \) and \( \tilde{X}^{(j)} = 1/n \sum X_i^{(j)} \). It follows
from the details given in Remark 1 of the Online Supplement that the asymptotic results of Theorem 1 and Corollary 1 apply to $\tilde{X}_{n \times J}$.

### 4 Simulation Study

#### 4.1 Simulation Study Design

We conducted a series of simulation experiments using prominent covariance models to verify the theoretical results of our cross-validated estimator selection procedure. These models are described below.

**Model 1**: A dense covariance matrix, where

$$\psi^{(jl)} = \begin{cases} 1, & j = l \\ 0.5, & \text{otherwise} \end{cases}$$

**Model 2**: An AR(1) model, where $\psi^{(jl)} = 0.7^{|j-l|}$. This covariance matrix, corresponding to a common timeseries model, is approximately sparse for large $J$, since the off-diagonal elements quickly shrink to zero.

**Model 3**: An MA(1) model, where $\psi^{(jl)} = 0.7^{|j-l|} \cdot 1(|j - l| \leq 1)$. This covariance matrix, corresponding to another common timeseries model, is truly sparse. Only the diagonal, subdiagonal, and superdiagonal contain non-zero elements.

**Model 4**: An MA(2) model, where

$$\psi^{(jl)} = \begin{cases} 1, & j = l \\ 0.6, & |j - l| = 1 \\ 0.3, & |j - l| = 2 \\ 0, & \text{otherwise} \end{cases}$$

This timeseries model is similar to Model 3, but slightly less sparse.
Model 5: A random covariance matrix model. First, a $J \times J$ random matrix whose elements are i.i.d. Uniform(0, 1) is generated. Next, entries below $1/4$ are set to 1, entries between $1/4$ and $1/2$ are set to $-1$, and the remaining entries are set to 0. The square of this matrix is then computed and added to the identity matrix $I_{J\times J}$. Finally, the corresponding correlation matrix is computed and used as the model’s covariance matrix.

Model 6: A Toeplitz covariance matrix, where

$$
\psi^{(jl)} = \begin{cases}
1, & j = l \\
0.6|j - l|^{-1.3}, & \text{otherwise}
\end{cases}.
$$

Like the AR(1) model, this covariance matrix is approximately sparse for large $J$. However, the off-diagonal entries decay less quickly as their distance from the diagonal increases.

Model 7: A Toeplitz covariance matrix with alternating signs, where

$$
\psi^{(jl)} = \begin{cases}
1, & j = l \\
(-1)^{|j-l|}0.6|j - l|^{-1.3}, & \text{otherwise}
\end{cases}.
$$

This model is almost identical to Model 6, though the signs of the covariance matrix’s entries are alternating.

Model 8: A covariance matrix inspired by the latent variable model described in the Online Supplement’s Equation (3). Let $\boldsymbol{\beta}_{J\times 3} = (\beta_1, \ldots, \beta_J)^T$, where $\beta_j$ are randomly generated using a $N(0, I_{3\times 3})$ distribution for $j = 1, \ldots, J$. Then $\psi = \boldsymbol{\beta}\boldsymbol{\beta}^T + I_{J\times J}$ is the covariance matrix of a model with three latent factors.

Each covariance model was used to generate data sets consisting of $n \in \{50, 100, 200, 500\}$ i.i.d. multivariate Gaussian, mean-zero observations. The uniform boundedness condition of Theorem 1’s Assumption 1 is therefore not satisfied; we do this purposefully to further stress that this assumption is not limiting in many practical settings. For each model and sample size, five data dimension ratios were considered: $J/n \in \{0.3, 0.5, 1, 2, 5\}$. Together,
the eight covariance models, four sample sizes, and five dimensionality ratios result in 160
distinct simulation settings. For each such setting, the performance of the cross-validated
selector with respect to the various oracle selectors and several well-established estimators
is evaluated based on aggregation across 200 Monte Carlo repetitions.

We applied our estimator selection procedure, which we refer to as cvCovEst, using a 5-
fold CV scheme. The library of candidate estimators is provided in the Online Supplement’s
Table 1, which includes details on these estimators’ possible hyperparameters. Seventy-
four estimators make up the library of candidates. We note that no penalty is attributed
to estimators generating rank-deficient estimates, like the sample covariance matrix when
\( J > n \), though this limitation is generally of practical importance. When the situation
dictates that the resulting estimate must be positive-definite, the library of candidates should
be assembled accordingly.

### 4.2 Simulation Study Results

To examine empirically the optimality results of Theorem 1, we computed analytically, for
each replication, the cross-validated conditional risk differences of the cross-validated selec-
tion, \( \hat{k}_{p_n,n} \), and the cross-validated oracle selection, \( \tilde{k}_{p_n,n} \). The Monte Carlo expectations of
the risk differences stratified by \( n \), \( J/n \), and the covariance model were computed from the
cross-validated conditional risk differences. The ratios of the expected risk differences are
presented in Figure 1A. These results make clear that, for virtually all models considered,
the estimator chosen by our proposed cross-validated selection procedure has a risk difference
asymptotically identical on average to that of the cross-validated oracle.

A stronger result, corresponding to Equation (8) of Theorem 1, is presented in the Online
Supplement’s Figure 1. For all but Models 1 and 8, we find that our algorithm’s selection is
virtually equivalent to the cross-validated oracle selection for \( n \geq 200 \) and \( J/n \geq 0.5 \). Even
for Model 8, in which the covariance matrices are more difficult to estimate due to their
dense structures, we find that our selector identifies the optimal estimator with probability
tending to 1 for \( n \geq 200 \) and \( J/n = 5 \).

More impressive still are the results presented in Figure 1B that characterize the full-
dataset conditional risk difference ratios. For all covariance matrix models considered, with
Figure 1: (A) Comparison of the cross-validated selection and cross-validated oracle selection’s mean cross-validated conditional risk differences. (B) Comparison of the cross-validated selection and oracle selection’s full-dataset conditional risk differences. Note the differing y-axis scales for the different models.
the exception of Model 1, our procedure’s selections attain near asymptotic optimality for moderate values of $n$ and $J/n$. This suggests that our loss-based estimator selection approach’s theoretical guarantee, as outlined in Corollary 1, is achievable in many practical settings.

In addition to verifying our method’s asymptotic behavior, we compared its estimates against those of competing approaches. We computed the Frobenius and spectral norms of each procedure’s estimate against the corresponding true covariance matrix. The mean norms over all simulations were then computed for each covariance matrix estimation procedure, again stratified by $n$, $J/n$, and the covariance matrix model (Figures 3 and 4 of the Online Supplement). Our data-adaptive procedure is found to perform at least as well as the best alternative estimation strategy across all simulation scenarios under both norms.

## 5 Real Data Examples

Single-cell transcriptome sequencing (scRNA-seq) allows researchers to study the gene expression profiles of individual cells. The fine-grained transcriptomic data that it provides have been used to identify rare cell populations and to elucidate the developmental relationships between diverse cellular states.

Given that a typical scRNA-seq data set possesses tens of thousands of features (genes), most workflows prescribe a dimensionality reduction step. In addition to reducing the amount of computational resources needed to analyze the data, reducing the dimensions mitigates the effect of corrupting noise on interesting biological signal. The lower-dimensional embedding is then used in downstream analyses, like novel cell-type discovery via clustering.

One of the most popular methods used to reduce the dimensionality of scRNA-seq data is uniform manifold approximation and projection (UMAP) (McInnes et al., 2018). This method captures the most salient non-linear relationships among a high-dimensional data set’s features and projects them onto a reduced-dimensional space. Instead of applying UMAP directly, the scRNA-seq data set’s leading principal components (PCs) are often used as an initialization.

This initial dimensionality reduction by PCA is believed to play a helpful role in denoising.
However, PCA typically relies on the sample covariance matrix, and so when the data set is high-dimensional, the resulting principal components are known to be poor estimates of those of the population (Johnstone and Lu, 2009). We hence posit that our cross-validated estimator selection procedure could form a basis for an improved PCA. That is, we hope that the eigenvectors resulting from the eigendecomposition of our estimated covariance matrix could be used to generate a set of estimates closer to the true PCs in terms of risk. These PCs could then be fed to UMAP to produce an enhanced embedding. Indeed, additional simulation results provided in Section 3 of the Online Supplement suggest that cvCovEst produces estimates of the leading eigenvalue at least as well as those produced by the sample covariance matrix, in terms of the spectral norm.

We applied our procedure to two scRNA-seq data sets for which the cell types are known \textit{a priori}. These data were obtained from the scRNAseq Bioconductor R package (Risso and Cole, 2020), and prepared for analysis using a workflow outlined in Amezquita et al. (2020). A 5-fold CV scheme was used; the library of candidate estimators is provided in the Online
Supplement’s Table 2. We expect that cells of the same class will form tight, distinct clusters within the low-dimensional representations. The resulting embeddings, which we refer to as the \textit{cvCovEst-based} embeddings, were then compared to those produced by UMAP using traditional PCA for initialization, which we refer to as the \textit{PCA-based} embeddings. For each embedding, the 20 leading PCs were fed to UMAP. The first data set is a collection of 285 mouse visual cortex cells (Tasic et al., 2016), and the second data set consists of 2,816 mouse brain cells (Zeisel et al., 2015). The 1,000 most variable genes of each data set were used to compute the PCs of both embeddings.

The resulting UMAP plots are presented in Figure 2. Though the two embeddings generated for each data set are qualitatively similar, the low-dimensional representation relying on our loss-based approach is more refined in Figure 2A. A number of cells erroneously clustered in the PCA-based embedding are correctly represented in the cvCovEst-based embedding. This explains the 41% increase in average silhouette width of our method relative to the traditional approach. Further insight is gleaned from the diagnostic plots of Figure 3. Figure 3A indicates that cvCovEst selected the POET estimator (Fan et al., 2013) with 5 latent factors and a thresholding hyperparameter of 0.3. It that the selected estimator significantly improves upon the sample covariance matrix in terms of the cross-validated Frobenius risk. Figure 3B provides further insight into the discrepancies between the UMAP results of Figure 2A: the sample covariance matrix likely over-estimates many of the leading eigenvalues.

The embeddings in Figure 2B qualitatively identical, and so too are their average silhouette widths. This is expected, the Zeisel et al. (2015) is not truly high-dimensional. The sample covariance matrix likely is a reasonable estimator in this setting. Ideally, data-adaptive selection procedures should be cognizant of this. Indeed, cvCovEst, when applied to the Zeisel et al. (2015) data set, selects an estimator whose cross-validated empirical risk is only slightly smaller than that of the sample covariance matrix, and whose leading PCs are virtually identical (Figure 2 of the Online Supplement).
Figure 3: Tasic dataset: Diagnostic plots and tables generated using the cvCovEst R package. (A) The top-left plot presents the cross-validated Frobenius risk of the estimator selected by our method. $k$ represents the number of potential latent factors, and $\lambda$ the thresholding value used. The top-right panel contains a line plot of the selected estimator’s eigenvalues. The bottom-left plot displays the absolute values of the estimated correlation matrix output by the cvCovEst selection, and the bottom-right table lists the best performing estimators from all classes of estimators considered. (B) Side-by-side line plots of the estimated leading eigenvalues of the cvCovEst selection and the sample covariance matrix.
6 Discussion

This work extends Dudoit and van der Laan (2005)’s framework for asymptotically optimal, data-adaptive estimator selection to the problem of covariance matrix estimation in high-dimensional settings. We provide sufficient conditions under which our cross-validated procedure is asymptotically optimal in terms of risk, and show that it generalizes the cross-validated hyperparameter selection procedures employed by existing estimation approaches. Future work might derive analogous results for other loss functions, or perhaps even for other parameters like the precision matrix.

The simulation study provides evidence that near-optimal results are achieved in data sets with relatively modest numbers of observations and many features across models indexed by diverse covariance matrix structures. These results also establish that our cross-validated procedure performs as well as the best bespoke estimation procedure in a variety of settings. Our scRNA-seq data examples further illustrate the utility of our approach in fields where high-dimensional data are collected routinely.

Practitioners need no longer rely upon intuition alone when deciding which candidate estimator is best from among a library of diverse estimators. We expect that a variety of computational procedures relying upon the accurate estimation of the covariance matrix beyond the exploratory analyses considered here, like clustering and latent variable estimation, stand to benefit from the application of this framework.

SUPPLEMENTARY MATERIAL

Online Supplement: All technical proofs and additional simulation results are included in the online supplement. A brief review of popular covariance matrix estimators is also included.

cvCovEst R package: The cross-validated covariance matrix estimator selection procedure is implemented in cvCovEst (Boileau et al., 2021), an open-source R package (R Core Team, 2021). This package is available via the Comprehensive R Archive Network (CRAN) at https://CRAN.R-project.org/package=cvCovEst. Internally, the
cvCovEst package relies upon the generalized CV framework of the origami R package (Coyle and Hejazi, 2018).

Simulation and Analysis Code: Results in Sections 4 and 5 were produced using version 0.1.3 of the cvCovEst R package. The code and data used to produce these analyses are publicly available on GitHub at https://github.com/PhilBoileau/pub_cvCovEst.

Acknowledgements

We thank Brian Collica and Jamarcus Liu for significant contributions to the development of the cvCovEst R package. PB is funded by the Fonds de recherche du Québec - Nature et technologies, and the Natural Sciences and Engineering Research Council of Canada. NSH gratefully acknowledges the support of the National Science Foundation (award no. DMS 2102840).

References

Amezquita, R. A., Lun, A. T. L., Becht, E., Carey, V. J., Carpp, L. N., Geistlinger, L., Marini, F., Rue-Albrecht, K., Risso, D., Soneson, C., Waldron, L., Pagès, H., Smith, M. L., Huber, W., Morgan, M., Gottardo, R., and Hicks, S. C. (2020), “Orchestrating single-cell analysis with Bioconductor,” Nature Methods, 17, 137–145, URL https://doi.org/10.1038/s41592-019-0654-x.

Anderson, T. (2003), An introduction to multivariate statistical analysis, Hoboken, New Jersey: John Wiley & Sons, Inc., third edition.

Bai, J. (2003), “Inferential Theory for Factor Models of Large Dimensions,” Econometrica, 71, 135–171.

Bartz, D. (2016), “Cross-validation based Nonlinear Shrinkage,” URL https://arxiv.org/abs/1611.00798.

Bennett, G. (1962), “Probability inequalities for the sum of independent random variables,” Journal of the American Statistical Association, 57, 33–45.

Bickel, P. J. and Levina, E. (2008a), “Covariance Regularization by Thresholding,” Annals of Statistics, 36, 2577–2604, URL http://www.jstor.org/stable/25464728.

— (2008b), “Regularized Estimation of Large Covariance Matrices,” Annals of Statistics, 36, 199–227, URL http://www.jstor.org/stable/25464621.

Boileau, P., Hejazi, N. S., Collica, B., van der Laan, M. J., and Dudoit, S. (2021), “cvCovEst: Cross-validated covariance matrix estimator selection and evaluation in R,” Journal of Open Source Software, 6, 3273, URL https://doi.org/10.21105/joss.03273.
Breiman, L. and Spector, P. (1992), “Submodel selection and evaluation in regression. The X-random case,” *International Statistical Review*, 291–319.

Cai, T. and Liu, W. (2011), “Adaptive Thresholding for Sparse Covariance Matrix Estimation,” *Journal of the American Statistical Association*, 106, 672–684, URL https://doi.org/10.1198/jasa.2011.tm10560.

Cai, T. T., Zhang, C.-H., and Zhou, H. H. (2010), “Optimal rates of convergence for covariance matrix estimation,” *Annals of Statistics*, 38, 2118–2144.

Coyle, J. and Hejazi, N. (2018), “origami: A Generalized Framework for Cross-Validation in R,” *Journal of Open Source Software*, 3, 512, URL https://doi.org/10.21105/joss.00512.

Dudoit, S. and van der Laan, M. J. (2005), “Asymptotics of cross-validated risk estimation in estimator selection and performance assessment,” *Statistical Methodology*, 2, 131–154.

Efron, B. (2012), *Large-Scale Inference: Empirical Bayes Methods for Estimation, Testing, and Prediction*, Cambridge University Press.

Fan, J., Fan, Y., and Lv, J. (2008), “High dimensional covariance matrix estimation using a factor model,” *Journal of Econometrics*, 147, 186 – 197, URL http://www.sciencedirect.com/science/article/pii/S0304407608001346. Econometric modelling in finance and risk management: An overview.

Fan, J., Liao, Y., and Mincheva, M. (2013), “Large covariance estimation by thresholding principal orthogonal complements,” *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 75, 603–680.

Fan, J., Liao, Y., and Wang, W. (2016), “Projected principal component analysis in factor models,” *Annals of Statistics*, 44, 219–254.

Fan, J., Wang, W., and Zhong, Y. (2019), “Robust covariance estimation for approximate factor models,” *Journal of Econometrics*, 208, 5 – 22. Special Issue on Financial Engineering and Risk Management.

Fang, Y., Wang, B., and Feng, Y. (2016), “Tuning-parameter selection in regularized estimations of large covariance matrices,” *Journal of Statistical Computation and Simulation*, 86, 494–509, URL https://doi.org/10.1080/00949655.2015.1017823.

Friedman, J., Hastie, T., and Tibshirani, R. (2001), *The Elements of Statistical Learning*, volume 1, Springer series in statistics New York.

Golub, G. H. and Van Loan, C. F. (1996), *Matrix Computations*, Johns Hopkins Universtiy Press, 3rd edition.

Györfi, L., Kohler, M., Krzyzak, A., and Walk, H. (2002), *A Distribution-Free Theory of Nonparametric Regression*, Springer series in statistics, Springer.

Johnstone, I. M. (2001), “On the distribution of the largest eigenvalue in principal components analysis,” *Annals of Statistics*, 295–327.

Johnstone, I. M. and Lu, A. Y. (2009), “On Consistency and Sparsity for Principal Components Analysis in High Dimensions,” *Journal of the American Statistical Association*, 104, 682–693. PMID: 20617121.
Lam, C. and Fan, J. (2009), “Sparsistency and rates of convergence in large covariance matrix estimation,” Annals of Statistics, 37, 4254–4278.

Ledoit, O. and Wolf, M. (2004), “A well-conditioned estimator for large-dimensional covariance matrices,” Journal of Multivariate Analysis, 88, 365 – 411.
— (2012), “Nonlinear shrinkage estimation of large-dimensional covariance matrices,” Annals of Statistics, 40, 1024–1060.
— (2015), “Spectrum estimation: A unified framework for covariance matrix estimation and PCA in large dimensions,” Journal of Multivariate Analysis, 139, 360 – 384.
— (2018), “Analytical nonlinear shrinkage of large-dimensional covariance matrices,” ECON - Working Papers 264, Department of Economics - University of Zurich, URL https://EconPapers.repec.org/RePEc:zur:econwp:264.

Marčenko, V. A. and Pastur, L. A. (1967), “DISTRIBUTION OF EIGENVALUES FOR SOME SETS OF RANDOM MATRICES,” Mathematics of the USSR-Sbornik, 1, 457–483.

McInnes, L., Healy, J., and Melville, J. (2018), “UMAP: Uniform Manifold Approximation and Projection for Dimension Reduction,” arXiv, 1802.03426, URL http://arxiv.org/abs/1802.03426.

Onatski, A. (2012), “Asymptotics of the principal components estimator of large factor models with weakly influential factors,” Journal of Econometrics, 168, 244 – 258.

Poincaré, H. (1912), Calcul des probabilités, volume 1, Gauthier-Villars.

R Core Team (2021), R: A Language and Environment for Statistical Computing, R Foundation for Statistical Computing, Vienna, Austria, URL https://www.R-project.org/.

Risso, D. and Cole, M. (2020), scRNAseq: Collection of Public Single-Cell RNA-Seq Datasets. R package version 2.3.17.

Robbins, H. (1964), “The empirical Bayes approach to statistical decision problems,” Annals of Mathematical Statistics, 35, 1–20.

Rothman, A. J., Levina, E., and Zhu, J. (2009), “Generalized Thresholding of Large Covariance Matrices,” Journal of the American Statistical Association, 104, 177–186, URL https://doi.org/10.1198/jasa.2009.0101.

Schäfer, J. and Strimmer, K. (2005), “A Shrinkage Approach to Large-Scale Covariance Matrix Estimation and Implications for Functional Genomics,” Statistical Applications in Genetics and Molecular Biology, 4.

Smith, S. (2005), “Covariance, subspace, and intrinsic Cramér-Rao bounds,” IEEE Transactions on Signal Processing, 53, 1610–1630.

Stock, J. H. and Watson, M. W. (2002), “Forecasting Using Principal Components from a Large Number of Predictors,” Journal of the American Statistical Association, 97, 1167–1179, URL http://www.jstor.org/stable/3085839.

Tasic, B., Menon, V., Nguyen, T. N., Kim, T. K., Jarsky, T., Yao, Z., Levi, B., Gray, L. T., Sorensen,
S. A., Dolbeare, T., Bertagnolli, D., Goldy, J., Shapovalova, N., Parry, S., Lee, C., Smith, K., Bernard, A., Madisen, L., Sunkin, S. M., Hawrylycz, M., Koch, C., and Zeng, H. (2016), “Adult mouse cortical cell taxonomy revealed by single cell transcriptomics,” *Nature Neuroscience*, 19, 335–346, URL https://doi.org/10.1038/nn.4216.

van der Laan, M. J. and Dudoit, S. (2003), “Unified Cross-Validation Methodology For Selection Among Estimators and a General Cross-Validated Adaptive Epsilon-Net Estimator: Finite Sample Oracle Inequalities and Examples,” Working Paper 130, University of California, Berkeley, URL https://biostats.bepress.com/ucbbiostat/paper130/.

van der Vaart, A. W., Dudoit, S., and van der Laan, M. J. (2006), “Oracle inequalities for multi-fold cross validation,” *Statistics and Decisions*, 24, 351–371.

Zeisel, A., Muñoz-Manchado, A. B., Codeluppi, S., Lönnerberg, P., La Manno, G., Juréus, A., Marques, S., Munguba, H., He, L., Betsholtz, C., Rolny, C., Castelo-Branco, G., Hjerling-Leffler, J., and Linnarsson, S. (2015), “Cell types in the mouse cortex and hippocampus revealed by single-cell RNA-seq.” *Science*, 347, 1138–1142.
Supplementary Material for “Cross-Validated Loss-Based Covariance Matrix Estimator Selection in High Dimensions”

Philippe Boileau
Graduate Group in Biostatistics and Center for Computational Biology, UC Berkeley

Nima S. Hejazi
Division of Biostatistics, Department of Population Health Sciences, Weill Cornell Medicine

Mark J. van der Laan
Division of Biostatistics, Department of Statistics, and Center for Computational Biology, UC Berkeley

Sandrine Dudoit*
Department of Statistics, Division of Biostatistics, and Center for Computational Biology, UC Berkeley

May 10, 2022

*To whom correspondence should be addressed: sandrine@stat.berkeley.edu
1 Proofs

Proof. Proposition 1.

Assume without loss of generality that $\mathbb{E}_{P_0}[X] = 0$ and $\eta_0 = 1$. Then,

$$\hat{\theta}_{p,n}(k,1) = \mathbb{E}_{B_n} \left[ \frac{1}{np_n} \sum_{i=1}^{n} \|B_n(i) = 1\| X_i^T - \hat{\Psi}_k(P_{n,B_n}^0)\|_{F,1}^2 \right]$$

$$= \mathbb{E}_{B_n} \left[ \frac{1}{np_n} \sum_{i=1}^{n} \|B_n(i) = 1\| \sum_{j=1}^{J} \sum_{l=1}^{J} \left( X_i^{(j)} X_i^{(l)} - \hat{\Psi}_k(P_{n,B_n}^0)^{(jl)} \right)^2 \right]$$

$$= \mathbb{E}_{B_n} \left[ \frac{1}{np_n} \sum_{j=1}^{J} \sum_{l=1}^{J} \sum_{\{i:B_n(i) = 1\}} \left( X_i^{(j)} X_i^{(l)} - 2X_i^{(j)} X_i^{(l)} \hat{\Psi}_k(P_{n,B_n}^0)^{(jl)} + (\hat{\Psi}_k(P_{n,B_n}^0)^{(jl)})^2 \right) \right]$$

$$= \mathbb{E}_{B_n} \left[ \sum_{j=1}^{J} \sum_{l=1}^{J} \left( (\hat{\Psi}_k(P_{n,B_n}^0)^{(jl)})^2 - 2S(P_{n,B_n}^1)^{(jl)} \hat{\Psi}_k(P_{n,B_n}^0)^{(jl)} + (S(P_{n,B_n}^1)^{(jl)})^2 \right) \right] + C_1,$$

where $C_1$ is constant with respect to $\hat{\Psi}_k(P_{n,B_n}^0)$.

From Equation (5) of the main text, notice that

$$\hat{R}_n(\hat{\Psi}_k, 1) = \mathbb{E}_{B_n} \left[ \|\hat{\Psi}_k(P_{n,B_n}^0) - S_n(P_{n,B_n}^1)\|_{F,1}^2 \right]$$

$$= \mathbb{E}_{B_n} \left[ \sum_{j=1}^{J} \sum_{l=1}^{J} \left( (\hat{\Psi}_k(P_{n,B_n}^0)^{(jl)})^2 - 2S(P_{n,B_n}^1)^{(jl)} \hat{\Psi}_k(P_{n,B_n}^0)^{(jl)} + (S(P_{n,B_n}^1)^{(jl)})^2 \right) \right]$$

$$= \mathbb{E}_{B_n} \left[ \sum_{j=1}^{J} \sum_{l=1}^{J} \left( (\hat{\Psi}_k(P_{n,B_n}^0)^{(jl)})^2 - 2S(P_{n,B_n}^1)^{(jl)} \hat{\Psi}_k(P_{n,B_n}^0)^{(jl)} \right) \right] + C_2,$$

where $C_2$ is constant with respect to $\hat{\Psi}_k(P_{n,B_n}^0)$.

Thus,

$$\hat{k}_{p,n} = \arg \min_{k \in \{1, \ldots, K\}} \hat{\theta}_{p,n}(k, 1)$$

$$= \arg \min_{k \in \{1, \ldots, K\}} \hat{R}_n(\hat{\Psi}_k, 1).$$

\[ \square \]

Proof. Proposition 2.
For any $a = 1, \ldots, J$ and $b = 1, \ldots, J$, we find that
\[
0 = \frac{\delta}{\delta \psi(ab)} \Theta(\psi, \eta, P_0) \\
= \frac{\delta}{\delta \psi(ab)} \mathbb{E}_{P_0} [L(X; \psi, \eta)] \\
= \frac{\delta}{\delta \psi(ab)} \sum_{j=1}^J \sum_{l=1}^J \eta^{(jl)} \left( X^{(j)} X^{(l)} - \psi^{(jl)} \right)^2 \\
= \mathbb{E}_{P_0} \left[ \frac{\delta}{\delta \psi(ab)} \sum_{j=1}^J \sum_{l=1}^J \eta^{(jl)} \left( X^{(j)} X^{(l)} - \psi^{(jl)} \right)^2 \right] \\
\propto \mathbb{E}_{P_0} \left( X^{(a)} X^{(b)} - \psi^{(ab)} \right) \\
= \psi^{(ab)} = \psi_0^{(ab)}.
\]
It follows that $\psi_0$ is a risk minimizer.

**Proof. Proposition 3.**

Let the hard-thresholding estimator minimizing the expected cross-validated conditional risk under $P_0$ be indexed by $k_0$. Then
\[
\mathbb{E}_{P_0} [\hat{\theta}_{p_n,n}(\hat{k}_{p_n,n}) - \theta_0] \leq \mathbb{E}_{P_0} [\hat{\theta}_{p_n,n}(k_0) - \theta_0] \\
= \mathbb{E}_{P_0} \left[ \mathbb{E}_{B_n} \left[ \mathbb{E}_{P_0} \left[ \| \hat{\Psi}_{k_0}(P_{0,n,B_n}) - X X^\top \|_{F,1}^2 \right] \right] \right] \\
= \mathbb{E}_{P_0} \left[ \mathbb{E}_{B_n} \left[ \mathbb{E}_{P_0} \left[ \| \hat{\Psi}_{k_0}(P_{0,n,B_n}) - \psi_0 \|_{F,1}^2 \right] \right] \right] \leq O(s(J) \log J).
\]
The first inequality follows from the definition of the cross-validated conditional risk under $P_0$; the last equality follows from Theorem 2 (and its subsequent discussion) of Bickel and Levina (2008a), since $X$ is sub-Gaussian by the boundedness condition of Assumption 1 and $J/n \to m$ as $n, J \to \infty$. Then,
\[
\frac{c(\delta, \overline{M}(J))(1 + \log(K))}{n p_n \mathbb{E}_{P_0} [\hat{\theta}_{p_n,n}(k_{p_n,n}) - \theta_0]} = \Omega \left( \frac{J}{s(J) \log J} \right).
\]

**Lemma 1.** Let $Z_k := L(X; \hat{\Psi}_k(P_{0,n,B_n}^0)) - L(X; \psi_0)$. Then,
\[
\text{Var}_{P_0} [Z_k \mid P_{0,n,B_n}^0, B_n] \leq \overline{M}(J) \mathbb{E}_{P_0} [Z_k \mid P_{0,n,B_n}^0, B_n],
\]
where $\overline{M}(J) := 4(M_1 + M_2)^2 J^2$.
Proof.

\[ \mathbb{E}_{P_0} [Z_k \mid P_{n,B_n}^0, B_n] = \mathbb{E}_{P_0} \left[ L(X; \hat{\Psi}_k(P_{n,B_n}^0)) - L(X; \psi_0) \right| P_{n,B_n}^0, B_n] \]

\[ = \mathbb{E}_{P_0} \left[ \sum_{j=1}^J \sum_{l=1}^J (X^{(j)} X^{(l)} - \hat{\Psi}_k^{(j)(l)}(P_{n,B_n}^0))^2 - (X^{(j)} X^{(l)} - \psi_0^{(j)(l)})^2 \right| P_{n,B_n}^0, B_n] \]

\[ = \sum_{j=1}^J \sum_{l=1}^J \mathbb{E}_{P_0} \left[ \left( \psi_0^{(j)(l)} - \hat{\Psi}_k^{(j)(l)}(P_{n,B_n}^0) \right)(2X^{(j)} X^{(l)} - \psi_0^{(j)(l)}) \right| P_{n,B_n}^0, B_n] \]

\[ = \sum_{j=1}^J \sum_{l=1}^J \mathbb{E}_{P_0} \left[ 2X^{(j)} X^{(l)} - \psi_0^{(j)(l)} - \hat{\Psi}_k^{(j)(l)}(P_{n,B_n}^0) \right| P_{n,B_n}^0, B_n] \]

\[ = \sum_{j=1}^J \sum_{l=1}^J \mathbb{E}_{P_0} \left[ \left( \psi_0^{(j)(l)} - \hat{\Psi}_k^{(j)(l)}(P_{n,B_n}^0) \right)^2 \right| P_{n,B_n}^0, B_n] , \]

where the second to last equality follows by noting that \( \mathbb{E}_{P_0}[X^{(j)} X^{(l)}|P_{n,B_n}^0, B_n] = \mathbb{E}_{P_0}[X^{(j)} X^{(l)}] \)

and that, by definition, \( \mathbb{E}_{P_0}[X^{(j)} X^{(l)}] = \psi_0^{(j)} \). Then,
\[ \text{Var}_P [Z_k \mid P_{n,B_n}^0, B_n] \leq \text{E}_P [Z_k^2 \mid P_{n,B_n}^0, B_n] \]
\[ = \text{E}_P \left[ \left( \sum_{j=1}^{J} \sum_{l=1}^{J} (\psi_0^{(jl)} - \hat{\psi}_k^{(jl)}(P_{n,B_n}^0))(2X^{(j)}X^{(l)} - \psi_0^{(jl)}) \right)^2 \left| P_{n,B_n}^0, B_n \right| \right] \]
\[ = J^4 \text{E}_P \left[ \left( \frac{1}{J^2} \sum_{j=1}^{J} \sum_{l=1}^{J} (\psi_0^{(jl)} - \hat{\psi}_k^{(jl)}(P_{n,B_n}^0))(2X^{(j)}X^{(l)} - \psi_0^{(jl)}) \right)^2 \left| P_{n,B_n}^0, B_n \right| \right] \]
\[ \leq J^4 \text{E}_P \left[ \frac{1}{J^2} \sum_{j=1}^{J} \sum_{l=1}^{J} (\psi_0^{(jl)} - \hat{\psi}_k^{(jl)}(P_{n,B_n}^0))^2(2X^{(j)}X^{(l)} - \psi_0^{(jl)}) \right. \]
\[ \left. - \hat{\psi}_k^{(jl)}(P_{n,B_n}^0) \right)^2 \left| P_{n,B_n}^0, B_n \right| \]
\[ \leq J^2 4(M_1 + M_2)^2 \text{E}_P \left[ \sum_{j=1}^{J} \sum_{l=1}^{J} (\psi_0^{(jl)} - \hat{\psi}_k^{(jl)}(P_{n,B_n}^0))^2 \right| P_{n,B_n}^0, B_n \right] \]
\[ = 4(M_1 + M_2)^2 J^2 \text{E}_P [Z_k \mid P_{n,B_n}^0, B_n] \]
\[ = \tilde{M}(J) \text{E}_P [Z_k \mid P_{n,B_n}^0, B_n]. \]

Here, the second inequality holds from the application of Jensen’s Inequality to the square of the double sum, which is effectively an expectation of a discrete uniform random variable when scaled by \(J^2\). The final inequality results from Assumptions 1 and 2, and concludes the proof. \(\square\)

The following lemma is a result taken directly from Dudoit and van der Laan (2005). It is restated here for convenience.

**Lemma 2.** Let \(Y_1, Y_2, \ldots\) be a sequence of random variables. If \(\text{E}[|Y_n|] = O(g(n))\) for some positive function \(g(\cdot)\), then \(Y_n = O_P(g(n))\).

**Proof.** We must show that, for each \(\epsilon > 0\), there exists an \(N\) and \(B > 0\) such that \(\mathbb{P}(|Y_n|/g(n) > B) < \epsilon\) for all \(n > N\). By assumption, there exists an \(N\) and a \(C > 0\) such that \(\mathbb{E}[|Y_n|]/g(n) < C\) for all \(n > N\). By defining \(C/B = \epsilon\) and making use of Markov’s Inequality, we find that
\[ \mathbb{P} \left( \frac{|Y_n|}{g(n)} > B \right) \leq \frac{\mathbb{E}[|Y_n|]}{g(n)B} \leq \frac{C}{B} = \epsilon. \]
\(\square\)

Having derived Lemma 1, the remainder of the proof for Theorem 1 closely follows the proof of the first theorem in Dudoit and van der Laan (2005).

**Proof.** Theorem 1, Finite-Sample Result.
0 \leq \hat{\theta}_{p,n}(\hat{k}_{p,n}) - \theta_0
\leq \mathbb{E}_{B_n}\left[\int (L(x; \hat{\Psi}_{k,n}^0(P_{n,B_n}^0)) - L(x; \psi_0))dP_0(x)
- (1 + \delta) \int (L(x; \hat{\Psi}_{k,n}^0(P_{n,B_n}^0)) - L(x; \psi_0))dP_{n,B_n}^1(x)
+ (1 + \delta) \int (L(x; \hat{\Psi}_{k,n}^0(P_{n,B_n}^0)) - L(x; \psi_0))dP_{n,B_n}^1(x)\right]
\leq \mathbb{E}_{B_n}\left[\int (L(x; \hat{\Psi}_{k,n}^0(P_{n,B_n}^0)) - L(x; \psi_0))dP_0(x)
- (1 + \delta) \int (L(x; \hat{\Psi}_{k,n}^0(P_{n,B_n}^0)) - L(x; \psi_0))dP_{n,B_n}^1(x)
+ (1 + \delta) \int (L(x; \hat{\Psi}_{k,n}^0(P_{n,B_n}^0)) - L(x; \psi_0))dP_{n,B_n}^1(x)\right]
= \mathbb{E}_{B_n}\left[\int (L(x; \hat{\Psi}_{k,n}^0(P_{n,B_n}^0)) - L(x; \psi_0))dP_0(x)
- (1 + \delta) \int (L(x; \hat{\Psi}_{k,n}^0(P_{n,B_n}^0)) - L(x; \psi_0))dP_{n,B_n}^1(x)
+ (1 + \delta) \int (L(x; \hat{\Psi}_{k,n}^0(P_{n,B_n}^0)) - L(x; \psi_0))dP_{n,B_n}^1(x)
- (1 + 2\delta) \int (L(x; \hat{\Psi}_{k,n}^0(P_{n,B_n}^0)) - L(x; \psi_0))dP_0(x)
+ (1 + 2\delta) \int (L(x; \hat{\Psi}_{k,n}^0(P_{n,B_n}^0)) - L(x; \psi_0))dP_0(x)\right].

The first inequality is by assumption, and the second is by definition of \( \hat{k}_{p,n} \) such that \( \hat{\theta}_{p,n}(\hat{k}_{p,n}) \leq \hat{\theta}_{p,n}(k) \) \( \forall k \). For simplicity in the remainder of the proof, we replace \( \hat{k}_{p,n} \) and \( \hat{k}_{p,n} \) with \( \hat{k} \) and \( \hat{k} \), respectively, in a slight abuse of notation.

Now, let the first two terms of the last expression in Equation (1) be denoted by \( R_{k,n} \), and the third and fourth terms by \( T_{k,n} \). The last term is the cross-validated oracle’s risk difference: \( (1 + 2\delta)(\hat{\theta}_{p,n}(\hat{k}) - \theta_0) \). Thus,

\[ 0 \leq \hat{\theta}_{p,n}(\hat{k}) - \theta_0 \leq (1 + 2\delta)(\hat{\theta}_{p,n}(\hat{k}) - \theta_0) + R_{k,n} + T_{k,n}. \quad (2) \]

We next show that \( \mathbb{E}_{P_0}[R_{k,n} + T_{k,n}] \leq 2c(\delta, \mathcal{M}(J))(1 + \log(K))/(np_n) \), where \( c(\delta, \mathcal{M}(J)) = 2(1 + \delta)^2\mathcal{M}(J)(1/\delta + 1/3) \) for some \( \delta > 0 \). For convenience, let

\[ \hat{H}_k := \int (L(x; \hat{\Psi}_{k}(P_{n,B_n}^0)) - L(x; \psi_0))dP_{n,B_n}^1(x) \]
\[ \hat{H}_k := \int (L(x; \hat{\Psi}_{k}(P_{n,B_n}^0)) - L(x; \psi_0))dP_0(x) \]

\[ R_{k,n}(B_n) := (1 + \delta)(\hat{H}_k - \hat{H}_k) - \delta \hat{H}_k \]
\[ T_{k,n}(B_n) := (1 + \delta)(\hat{H}_k - \hat{H}_k) - \delta \hat{H}_k, \]

so that \( R_{k,n} = \mathbb{E}_{B_n}[R_{k,n}(B_n)] \) and \( T_{k,n} = \mathbb{E}_{B_n}[T_{k,n}(B_n)] \).
Given $B_n$ and $P^0_{n,B_n}$, let $Z_{k,i}$, $1 \leq i \leq np_n$, denote the $np_n$ i.i.d. copies of $Z_k$ corresponding with the validation set, that is, with $\{X_i : B_n(i) = 1\}$ (as defined in Lemma 1). Then, $\hat{H}_k = \sum_i Z_{k,i}/np_n$ and $\hat{H}_k = \mathbb{E}_{P_0}[Z_{k,i} \mid P^0_{n,B_n}, B_n]$. Hence, $\hat{H}_k - \bar{H}_k$ is an empirical mean of $np_n$ i.i.d. centered random variables. Further, by Assumptions 1 and 2, $|Z_{k,i}| < 2(M_1 + M_2)^2J^2$ a.s.. Next, we apply Bernstein’s Inequality to the centered empirical mean $\hat{H}_k - \bar{H}_k$, using the property of the $Z_{k,i}$’s derived in Lemma 1, to obtain a bound for the tail probabilities of $R_{k,n}(B_n)$ and $T_{k,n}(B_n)$:

$$\sigma_k^2 := \text{Var}_{P_0} \left[ Z_k \mid P^0_{n,B_n}, B_n \right] \leq \overline{M}(J) \mathbb{E} \left[ Z_k \mid P^0_{n,B_n}, B_n \right] = \overline{M}(J) \hat{H}_k.$$ 

Then, for $s > 0$, Bernstein’s Inequality yields

$$\mathbb{P}_0 \left( R_{k,n}(B_n) > s \mid P^0_{n,B_n}, B_n \right) = \mathbb{P}_0 \left( \frac{\hat{H}_k - \hat{H}_k}{1 + \delta} > \frac{s + \delta \hat{H}_k}{1 + \delta} \mid P^0_{n,B_n}, B_n \right) \leq \mathbb{P}_0 \left( \frac{\hat{H}_k - \hat{H}_k}{1 + \delta} > \frac{s + \delta \hat{H}_k}{1 + \delta} \mid P^0_{n,B_n}, B_n \right) \leq \exp \left\{ - \frac{np_n}{2(1 + \delta)^2} \left( \sigma_k^2 + \frac{\overline{M}(J)}{3(1 + \delta)} \right) \left( s + \delta \sigma_k^2 / \overline{M}(J) \right)^2 \right\}.$$ 

Note that

$$\frac{(s + \delta \sigma_k^2 / \overline{M}(J))^2}{\sigma_k^2 + \frac{\overline{M}(J)}{3(1 + \delta)} \left( s + \delta \sigma_k^2 / \overline{M}(J) \right)} = \frac{s + \delta \sigma_k^2 / \overline{M}(J)}{\frac{\sigma_k^2}{s + \delta \sigma_k^2 / \overline{M}(J)} + \frac{\overline{M}(J)}{3(1 + \delta)}} \geq \frac{s + \delta \sigma_k^2 / \overline{M}(J)}{\overline{M}(J) \left( \frac{1}{\overline{M}(J)} + \frac{1}{3} \right)} \geq \frac{s}{\overline{M}(J) \left( \frac{1}{\overline{M}(J)} + \frac{1}{3} \right)}.$$ 

And so, for $s > 0$,

$$\mathbb{P}_0 \left( R_{k,n}(B_n) > s \mid P^0_{n,B_n}, B_n \right) \leq \exp \left\{ - \frac{np_n}{c(\delta, \overline{M}(J))} s \right\} \leq K \exp \left\{ - \frac{np_n}{c(\delta, \overline{M}(J))} s \right\},$$

where $c(\delta, \overline{M}(J)) = 2(1 + \delta)^2 \overline{M}(J) \left( \frac{1}{\overline{M}(J)} + \frac{1}{3} \right)$. The same bound applies for the marginal probabilities of $\mathbb{P}_0(R_{k,n}(B_n) > s)$ since they hold for arbitrary choices of $B_n$ and $P^0_{n,B_n}$. The second inequality follows from $K$ being larger than or equal to 1 by definition.

Finally, for any $u > 0$, we have by the properties of expectations and the previously derived result that

$$\mathbb{E}_{P_0}[R_{k,n}] = \int_0^\infty \mathbb{P}_0(R_{k,n} > s)ds - \int_{-\infty}^0 \mathbb{P}_0(R_{k,n} \leq s)ds \leq \int_0^\infty \mathbb{P}_0(R_{k,n} > s)ds \leq u + \int_u^\infty \mathbb{P}_0(R_{k,n} > s)ds \leq u + \int_u^\infty K \exp \left\{ - \frac{np_n}{c(\delta, \overline{M}(J))} s \right\} ds.$$ 

Since the expression on the right-hand side of the inequality above achieves its minimum value of $c(\delta, \overline{M}(J))(1 + \log(K)/np_n)$ at $u_n = c(\delta, \overline{M}(J))\log(K)/(np_n)$, then

7
\[ 
\mathbb{E}_{\mathbb{P}_0}[R_{k,n}] \leq c(\delta, M(J)) \frac{1 + \log(K)}{np_n}.
\]

The same bound applies to \( \mathbb{E}_{\mathbb{P}_0}[T_{k,n}] \). Therefore, taking the expected values of the inequality in Equation (2), we produce the desired finite-sample result in Equation (6) of the main text.

**Proof. Theorem 1, High-Dimensional Asymptotic Result.**

The expected risk differences ratio’s convergence follows directly from the main text’s Equation (6) for some \( \delta > 0 \), so long as \( c(\delta, M(J))(1 + \log(K))/(np_n \mathbb{E}_{\mathbb{P}_0}[\hat{\theta}_{p,n}(k_{p,n}) - \theta_0]) \to 0 \) as \( n, J \to \infty \). Given the assumption in Kolmogorov asymptotics that \( J/n \to m < \infty \) as \( J, n \to \infty \), an equivalent condition is that \( m(M_1 + M_2)^2J(1 + \log(K))/(np_n \mathbb{E}_{\mathbb{P}_0}[\hat{\theta}_{p,n}(k_{p,n}) - \theta_0]) \to 0 \) as \( n, J \to \infty \). Convergence in probability then follows from Lemma 2.

Though there are minor adaptations to the assumptions to reflect the use of high-dimensional asymptotics, the proof of Corollary 1 follows that of Corollary 1 in Dudoit and van der Laan (2005).

**Proof. Corollary 1.**

The asymptotic statement of the main text’s Equation (10) is an immediate result of Theorem 1’s Equation (8).

\[
\frac{\hat{\theta}_{p,n}(k_{p,n}) - \theta_0 - \hat{\theta}_{p,n}(k_{p,n}) - \theta_0}{\hat{\theta}_{p,n}(k_{p,n}) - \theta_0} \overset{p}{\to} 1.
\]

Letting \( Z_{1,n} := (n(1 - p_n))^{\gamma}(\hat{\theta}_{p,n}(k_{p,n}) - \theta_0) \) and \( Z_{2,n} := n^{\gamma}(\hat{\theta}_{n}(k_{n}) - \theta_0) \), and assuming that the sufficient condition in Equation (11) of the main text holds, we find that \( Z_{1,n}/Z_{2,n} \overset{d}{\to} 1 \) by the Continuous Mapping Theorem. Then, notice that

\[
\frac{Z_{1,n}}{Z_{2,n}} = \frac{(1 - p_n)^{\gamma}(\hat{\theta}_{p,n}(k_{p,n}) - \theta_0)}{\hat{\theta}_{n}(k_{n}) - \theta_0},
\]

which yields the desired sufficient condition when \( p_n \to 0 \). In the case of single-split validation, \( Z_{2,n} \overset{d}{=} Z_{1,n}/(1 - p_n) \), and so \( Z_{2,n} \overset{d}{\to} Z \) implies that \( (Z_{1,n}, Z_{2,n}) \overset{d}{\to} (Z,Z) \).

**Remark 1.** We assume throughout this work that \( \mathbb{E}_{\mathbb{P}_0}[X] = 0 \) without loss of generality. In practice, however, the mean vector is generally unknown. Consider the uniformly bounded random vector \( \hat{Y} \) such that \( X = Y - \mathbb{E}_{\mathbb{P}_0}[Y] \). We might therefore consider using the demeaned random vector \( \tilde{Y} = Y - \hat{Y} \) instead, where \( \hat{Y}^{(j)} = 1/n \sum Y_i^{(j)} \). Employing \( \tilde{Y} \) in place of \( X \) in Lemma 1, and denoting \( \tilde{Z}_k := L(\tilde{Y}; \hat{\Psi}_k(P_{n,B_n}^0)) - L(\tilde{Y}; \psi_0) \), we find that \( \mathbb{E}_{\mathbb{P}_0}[\tilde{Z}_k|P_{n,B_n}^0, B_n] = \sum (\psi_0^{(j)} - \hat{\Psi}_k^{(j)}(P_{n,B_n}^0))(n - 2)\psi_0^{(j)} / n - \hat{\Psi}_k^{(j)}(P_{n,B_n}^0)) \). It then follows that, as \( n \to \infty \), \( \mathbb{E}_{\mathbb{P}_0}[\tilde{Z}_k|P_{n,B_n}^0, B_n] = \mathbb{E}_{\mathbb{P}_0}[Z_k|P_{n,B_n}^0, B_n] \). The asymptotic results of Theorem 1 and Corollary 1 are therefore achievable when \( \mathbb{E}_{\mathbb{P}_0}[Y] \) is unknown. The same cannot be said for the finite sample result of Theorem 1: \( \mathbb{E}_{\mathbb{P}_0}[\tilde{Z}_k|P_{n,B_n}^0, B_n] \) is not strictly nonegative. For large enough values of \( n \), however, we do expect these finite bounds to be approximately correct.

## 2 Additional Figures and Tables
### Table 1: Families of candidate estimators used by cvCovEst in the simulation study (74 distinct estimators in total)

| Estimator                                         | Hyperparameters                                              |
|---------------------------------------------------|--------------------------------------------------------------|
| Sample covariance matrix                          | Not applicable                                               |
| Hard thresholding (Bickel and Levina, 2008a)      | Thresholds = \{0.1, 0.2, \ldots, 1.0\}                      |
| SCAD thresholding (Fan and Li, 2001; Rothman et al., 2009) | Thresholds = \{0.1, 0.2, \ldots, 1.0\}                      |
| Adaptive LASSO (Rothman et al., 2009)             | Thresholds = \{0.1, 0.2, \ldots, 0.5\}; exponential weights = \{0.1, 0.2, \ldots, 0.5\} |
| Banding (Bickel and Levina, 2008b)                | Bands = \{1, 2, \ldots, 5\}                                 |
| Tapering (Cai et al., 2010)                       | Bands = \{2, 4, \ldots, 10\}                               |
| Linear shrinkage (Ledoit and Wolf, 2004)          | Not applicable                                               |
| Dense linear shrinkage (Schäfer and Strimmer, 2005) | Not applicable                                               |
| Nonlinear shrinkage (Ledoit and Wolf, 2018)       | Not applicable                                               |
| POET (Fan et al., 2013) using hard thresholding   | Latent factors = \{1, 2, \ldots, 5\}; thresholds = \{0.1, 0.2, 0.3\} |

### Table 2: Families of candidate estimators used in single-cell transcriptomic data analyses

| Estimator                                         | Hyperparameters                                              |
|---------------------------------------------------|--------------------------------------------------------------|
| Sample covariance matrix                          | NA                                                           |
| Hard thresholding                                 | Thresholds = \{0.05, 0.10, \ldots, 0.30\}                   |
| SCAD thresholding                                 | Thresholds = \{0.05, 0.10, \ldots, 0.50\}                   |
| Adaptive LASSO                                    | Thresholds = \{0.1, 0.2, \ldots, 0.5\}; exponential weights = \{0.1, 0.2, \ldots, 0.5\} |
| Linear shrinkage                                  | NA                                                           |
| Dense linear shrinkage                            | NA                                                           |
| POET using hard thresholding                      | Latent factors = \{5, 6, \ldots, 10\}; thresholds = \{0.05, 0.10, \ldots, 0.3\} |

Table 1: Families of candidate estimators used by cvCovEst in the simulation study (74 distinct estimators in total)

Table 2: Families of candidate estimators used in single-cell transcriptomic data analyses
Figure 1: Comparison of the cross-validated ($\hat{k}_{p,n}$) and cross-validated oracle ($\tilde{k}_{p,n}$) selections’ cross-validated conditional risk differences. The proposed cross-validated selection procedure achieves asymptotic equivalence in most settings for relatively small sample sizes and numbers of features.
Figure 2: Zeisel dataset: Diagnostic plots and tables generated using the cvCovEst R package. The components in (A) can be interpreted in the same manner as the previous figure, with the exception of the top-left panel. In this table, a five number summary of the cross-validated Frobenius risk is given for each class of estimators considered across all possible combinations of hyperparameters, if any. It is clear from the tables in (A) that the cvCovEst selection is essentially equivalent in terms of cross-validated risk to the sample covariance matrix. The plots in (B) further highlight that the 20 leading eigenvalue of the cvCovEst estimate and the sample covariance matrix are indistinguishable.

| Estimator               | Mean   | 2.5%   | 25%    | 75%    | 97.5%  | 99.75  |
|-------------------------|--------|--------|--------|--------|--------|--------|
| LinearShrinkLWEst       | 2801.794 | 2801.794 | 2801.794 | 2801.794 | 2801.794 | 2801.794 |
| denoiserShrinkLWEst     | 2805.000 | 2805.000 | 2805.000 | 2805.000 | 2805.000 | 2805.000 |
| sampleCovEst            | 2825.010 | 2825.010 | 2825.010 | 2825.010 | 2825.010 | 2825.010 |
| jpeeEst                 | 2832.400 | 2798.900 | 2798.900 | 2798.900 | 2798.900 | 2798.900 |
| FixedShrinkLWEst        | 2794.080 | 2698.100 | 2698.100 | 2698.100 | 2698.100 | 2698.100 |
| leaveEst                | 3225.400 | 6777.400 | 6030.640 | 6287.960 | 7310.310 | 3823.410 |
| adaptiveLW_shrinkEst    | 6442.850 | 2931.790 | 2931.790 | 2931.790 | 2931.790 | 2931.790 |

Best Hyperparameter Values by Class

| Estimator            | Hyperparameters | CV-Risk |
|----------------------|-----------------|---------|
| LinearShrinkLWEst    | lambda = NA     | 2801.794 |
| denoiserShrinkLWEst  | lambda = NA     | 2805.000 |
| sampleCovEst         | hyperparameters | 2825.010 |
| jpeeEst              | lambda = 10     | 2832.400 |
| FixedShrinkLWEst     | lambda = 0.05   | 2794.080 |
| leaveEst             | gamma = 0.05    | 3225.400 |
| shrinkEst            | lambda = 0.5    | 6442.850 |
| adaptiveLW_shrinkEst | lambda = 0.5    | 6442.850 |
3 Extended Simulation Results

We compared the estimates generated by our method against those of the individual candidate procedures using the simulated data sets. This was accomplished by computing the Frobenius norm of each estimate against the corresponding true covariance matrix. The mean norms over all simulations were then computed for each covariance matrix estimation procedure, again stratified by $n$, $J/n$, and the covariance matrix model (Figure 3). Our CV scheme was used to select hyperparameters of these competing approaches where necessary. As stated previously, our CV approach is generally equivalent to these estimators’ hyperparameter selection procedures. The hyperparameters considered are provided in Table 3. Where appropriate, the competing methods’ hyperparameters are more varied than those used by cvCovEst, reflecting more aggressive estimation procedures that one might employ when only using a single family of estimators.

We repeated this benchmarking experiment using the spectral norm to assess the accuracy of our estimation procedure with respect to the leading eigenvalue of the covariance matrix. Recall that the spectral norm of a square matrix is defined as its largest absolute eigenvalue. Though our theoretical results do not relate to this norm, outcomes similar to those in Figure 3 are expected given the relationship between these two norms for reasons previously described.

The results, presented in Figures 3 and 4, demonstrate that our estimator selection procedure performs at least as well as the best alternative estimation strategy. This suggests that procedures dedicated to or relying upon the accurate estimation of leading eigenvalues and eigenvectors, like principal component analysis and latent variable estimation, might benefit from the integration of our cross-validated covariance matrix estimation framework.
Figure 3: Comparison of competing, bespoke covariance matrix estimation procedures to our cross-validated selection approach in terms of the Monte Carlo mean Frobenius norm under a variety of data-generating processes. Note that the scales of the y-axis are tailored to the covariance matrix model.
Figure 4: Comparison of competing, bespoke covariance matrix estimation procedures to our cross-validated selection approach in terms of the Monte Carlo mean spectral norm under a variety of data-generating processes. Note that the scales of the y-axis are tailored to the covariance matrix model.
4 Candidate Covariance Matrix Estimators

Using the proposed cross-validated selection procedure effectively requires a large and diverse set of candidate covariance matrix estimators. In this spirit, we provide in the sequel a brief overview of select covariance matrix estimators that have proven to be effective in a variety of settings. Note, however, that the proposed selection framework need not be limited to those described here. Thorough reviews of estimators have been provided by Pourahmadi (2013), Fan et al. (2016), and Ledoit and Wolf (2020), to name only a few.

4.1 Thresholding Estimators

An often natural, simplifying assumption about the true covariance matrix’s structure is that it is sparse, that is, a non-negligible portion of its off-diagonal elements have a value near zero or equal to zero. This assumption is not altogether unreasonable: Given a system of numerous variables, it seems unlikely in many settings that a majority of these variables would depend on one another. The class of generalized thresholding estimators (Bickel and Levina, 2008a; Rothman et al., 2009; Cai and Liu, 2011) is one collection of covariance matrix estimators based upon this structural assumption. Given the sample covariance matrix $S_n$, the generalized thresholding estimator is defined as

$$\hat{\Psi}_{gt}(P_n; t) := \{ t \left( S_n^{(jl)} \right) : j, l = 1, \ldots, J \},$$

where $t(\cdot)$ is a thresholding function that often requires one or more hyperparameters dictating the amount of regularization. The hard, soft, smoothly clipped absolute deviation (SCAD) (Fan and Li, 2001), and adaptive LASSO (Rothman et al., 2009) functions are among the collection of suitable thresholding operators. As an example, the hard-thresholding function is defined as $t_u(S_n^{(jl)}) \equiv S_n^{(jl)} I(S_n^{(jl)} > u)$ for some threshold $u > 0$. Cai and Liu (2011) also demonstrated that element-specific thresholding functions might be useful when the features’ variances are highly variable. The hyperparameters for any specific thresholding function are often selected via CV. Regardless of the choice of $t(\cdot)$, these estimators preserve the symmetry of the sample covariance matrix and are invariant under permutations of the features’ order.
Bickel and Levina (2008a) and Rothman et al. (2009) have shown that these estimators are consistent under the spectral norm (which is defined as a square matrix’s largest absolute eigenvalue), assuming that \( \log J/n \to 0 \), that the observations’ marginal distributions satisfy a tail condition, and that the true covariance matrix is a member of the class of matrices satisfying a particular notion of “approximate sparsity.” Cai and Liu (2011) have derived similar results for their entry-specific thresholding estimator over an even broader parameter space of sparse covariance matrices.

### 4.2 Banding and Tapering Estimators

A family of estimators related to thresholding estimators are banding and tapering estimators (Bickel and Levina, 2008b; Cai et al., 2010). Like thresholding estimators, these estimators rely on the assumption that the true covariance matrix is sparse. However, the structural assumption of these estimators on \( \varphi_0 \) is much more rigid than that of thresholding estimators. Specifically, such estimators assume that the true covariance matrix is a **band matrix**, that is, a sparse matrix whose non-zero entries are concentrated about the diagonal. These estimators therefore require a natural ordering of the observations’ features, operating under the assumption that “distant” variables are uncorrelated. Such structure is often encountered in longitudinal and time-series data.

Given the sample covariance matrix \( S_n \), the banding estimator of Bickel and Levina (2008b) is defined as

\[
\hat{\Psi}_{\text{band}}(P_n; b) := \left\{ S_{n}(jl) \mathbb{I}(|j - l| \leq b) : j, l = 1, \ldots, J \right\},
\]

where \( b \) is a hyperparameter that determines the number of bands to retain from the sample covariance matrix and is chosen via a CV procedure. For the class of “bandable” covariance matrices, i.e., the set of well-conditioned matrices whose elements not in the central bands of the matrix decay rapidly, this banding estimator has been shown to be uniformly consistent in the spectral norm so long as \( \log(J)/n \to 0 \).

The tapering estimator of Cai et al. (2010) is the smooth generalization of the banding estimator, gradually shrinking the off-diagonal bands of the sample covariance matrix towards zero. It is defined as

\[
\hat{\Psi}_{\text{tap}}(P_n; b) := W_b \circ S_n,
\]

for some weight matrix \( W_b \). Here, “\( \circ \)” denotes the Hadamard (element-wise) matrix product. Clearly, letting \( W_b^{(jl)} = \mathbb{I}(|j - l| \leq b) \) for some positive integer \( b \) results in the banding estimator. A popular weighting scheme derived by Cai et al. (2010) is

\[
W_b^{(jl)} := \begin{cases} 
1, & \text{when } |j - l| \leq \frac{b}{2} \\
2 - \frac{|j - l|}{b}, & \text{when } \frac{b}{2} < |j - l| \leq b \\
0, & \text{otherwise}
\end{cases}
\]

which we use in our simulation study presented in Section 4 of the main text. Cai et al. (2010) also derived the optimal rates of convergence for this estimator under the Frobenius and spectral norms, considering a class of bandable covariance matrices that is more general than that considered by Bickel and Levina (2008b): The smallest eigenvalue of the covariance matrices in this class can take on a value of zero. However, this estimator does not improve upon the bounds set by the banding estimator.
4.3 Shrinkage Estimators

We next consider the linear and non-linear shrinkage estimators inspired by Stein’s work on empirical Bayesian methods. These estimators are rotation-equivariant, shrinking the eigenvalues of the sample covariance matrix towards a set of target values, whilst leaving its eigenvectors untouched. In doing so, the resultant estimators are better-conditioned than the sample covariance matrix in a manner guaranteeing that the resultant covariance matrix estimator be non-singular. Further, these estimators do not rely on sparsity assumptions about the true covariance matrix, setting them apart from those previously discussed.

One of the first shrinkage estimators, the linear shrinkage estimator of the sample covariance matrix, was proposed by Ledoit and Wolf (2004). This estimator is defined as the convex combination of the sample covariance matrix and the identity matrix. Hence, it represents a compromise between $S_n$, an unbiased but highly variable estimator of $\psi_0$ in high dimensions, and $I_{J \times J}$, a woefully biased but fixed estimator. Ledoit and Wolf (2004) found that, under mild conditions, the asymptotically optimal shrinkage intensity with respect to the scaled (by $J$) Frobenius norm can be estimated consistently in high dimensions. This estimator is defined as

$$\hat{\Psi}_{ls}(P_n) := \frac{b_n^2}{d_n^2} m_n I + \frac{a_n^2}{d_n^2} S_n,$$

for $m_n = \text{tr}(S_n)/J$, $d_n^2 = \|S_n - m_n I\|_{F,1/J}^2$, $b_n^2 = n^{-2} \sum_i \|X_i X_i^\top - S_n\|_{F,1/J}^2$, $b_n^2 = \min(\bar{b}_n^2, \bar{d}_n^2)$, and $a_n^2 = d_n^2 - b_n^2$.

Bespoke shrinkage targets may be used in place of the identity. For example, one might consider a dense matrix target whose diagonal elements are the average of the sample covariance matrix’s diagonal elements and whose off-diagonal elements are equal to the average of all the sample covariance matrix’s off-diagonal elements. For the sake of brevity, discussion of such estimators is omitted, but examples are provided by, among others, Ledoit and Wolf (2003) and Schäfer and Strimmer (2005), particularly for use in financial economics and statistical genomics applications, respectively.

When assumptions about the true covariance matrix’s structure are unfounded, it can become impossible to select an appropriate linear shrinkage target. Instead, one might consider generalizing these estimators to shrink the eigenvalues of the sample covariance matrix in a non-linear fashion. That is, an estimator that shrinks the sample covariance matrix’s eigenvalues not by a common shrinkage factor (as with linear shrinkage estimators) but with shrinkage factors tailored to each sample eigenvalue. As with the aforementioned linear shrinkage estimators, such non-linear shrinkage estimators produce positive-definite estimates so long as the shrunken sample eigenvalues are positive and rotation-equivariant. These estimators belong to a class initially introduced by Stein (1986) and have since seen a resurgence in the work of Ledoit and Wolf (2012, 2015). More recently, Ledoit and Wolf (2018) derived an analytical non-linear shrinkage estimator that is asymptotically optimal in high dimensions and more computationally efficient than their previously formulated estimators.

4.4 Estimators Based on Factor Models

Covariance matrix estimators based on factor models form another broad family of estimators that do not assume sparsity of the true covariance matrix. Often encountered in econometrics and finance, these estimators utilize the operating assumption that the dataset’s observations are functions of a few common, often latent, factors. The factor model can be described as follows:

$$X = \mu + \beta F + \epsilon,$$  \hspace{1cm} (3)
where \( X_{J \times 1} \) represents a random observation, \( \mu_{J \times 1} \) a mean vector, \( \beta_{J \times L} \) a matrix of factor coefficients, \( F_{L \times 1} \) a random vector of \( L \) common factors, and \( \epsilon_{J \times 1} \) a random error vector. Assuming that \( F \) and \( \epsilon \) are uncorrelated, the covariance matrix of \( X \) is given by

\[
\psi = \beta \text{Cov}(F) \beta^\top + \psi_\epsilon,
\]

(4)

where \( \psi_\epsilon \) is the covariance matrix of the random error.

For a review on estimating the covariance matrix in the presence of observable factors, see Fan et al. (2016). We now briefly discuss the estimation of \( \psi \) when the factors are unobservable. Notice that when \( \psi_\epsilon \) is not assumed to be diagonal, the decomposition of \( \psi \) in Equation (4) is not identifiable for fixed \( n \) and \( J \), since the random vector \( X \) is the only observed component of the model. By letting \( J \to \infty \), and assuming that the eigenvalues of \( \psi_\epsilon \) are uniformly bounded or grow at a slow rate relative to \( J \) and that the eigenvalues of \( (1/J) \beta^\top \beta \) are uniformly bounded away from zero and infinity, it can be shown that \( \beta \text{Cov}(F) \beta^\top \) is asymptotically identifiable (Cai et al., 2010). It follows from these assumptions that the signal in the factors increases as the number of features increases, while the noise contributed by the error term remains constant. The eigenvalues associated with \( \beta \text{Cov}(F) \beta^\top \) therefore become easy to differentiate from those of \( \psi_\epsilon \).

Now, even with \( \beta \text{Cov}(F) \beta^\top \) being asymptotically identifiable, \( \beta \) and \( F \) cannot be distinguished. As a solution, the following constraint is imposed on \( F \): \( \text{Cov}(F) = I_{L \times L} \). It then follows that

\[
\psi = \beta \beta^\top + \psi_\epsilon.
\]

Under the additional assumption that the columns of \( \beta \) be orthogonal, Fan et al. (2013) found that the leading \( L \) eigenvalues of \( \psi \) are spiked, meaning that they are bounded below by some constant (Johnstone, 2001), and grow at rate \( O(J) \) as the dimension of \( \psi \) increases. The remaining \( J - L \) eigenvalues are then either bounded above or grow slowly. This implies that the latent factors and their loadings can be approximated via the eigenvalues and eigenvectors of \( \psi \).

Fan et al. (2013) therefore proposed the Principal Orthogonal compleEment Thresholding (POET) estimator of \( \psi \), which was motivated by the spectral decomposition of the sample covariance matrix

\[
S_n = \sum_{j=1}^{J} \lambda_j V_{j \cdot} V_{j \cdot}^\top \\
\approx \sum_{j=1}^{L} \beta_{\cdot j} \beta_{\cdot j}^\top + \sum_{j=L+1}^{J} \lambda_j V_{j \cdot} V_{j \cdot}^\top,
\]

where \( \lambda_j \) and \( V_{j \cdot} \) are the \( j \)th eigenvalues and eigenvectors of \( S_n \), respectively, and \( \beta_{\cdot j} \) is the \( j \)th column of \( \beta \). For ease of notation, we denote the second term by \( S_\epsilon \) and refer to this matrix as the principal orthogonal complement. The estimator for \( L \) latent variables is then defined as

\[
\hat{\Psi}_{\text{POET}}(P_n; L, s) := \sum_{j=1}^{L} \lambda_j V_{j \cdot} V_{j \cdot}^\top + T_{\epsilon,s},
\]

where \( T_{\epsilon,s} \) is the generalized thresholding matrix of \( S_\epsilon \)

\[
T_{\epsilon,s}^{(jl)} := \begin{cases} 
S_\epsilon^{(jj)}, & \text{when } j = l \\
s(S_\epsilon^{(jl)}), & \text{otherwise}
\end{cases}
\]
for some generalized thresholding function $s$.

Although this estimator is computationally efficient, the assumptions encoding the factor based model under which it is derived are such that the latent features’ eigenvalues grow in $J$. This results in a poor convergence rate under the spectral norm (Fan et al., 2016).

References

Bickel, P. J. and Levina, E. (2008a), “Covariance Regularization by Thresholding,” *Annals of Statistics*, 36, 2577–2604, URL http://www.jstor.org/stable/25464728.
— (2008b), “Regularized Estimation of Large Covariance Matrices,” *Annals of Statistics*, 36, 199–227, URL http://www.jstor.org/stable/25464621.

Cai, T. and Liu, W. (2011), “Adaptive Thresholding for Sparse Covariance Matrix Estimation,” *Journal of the American Statistical Association*, 106, 672–684, URL https://doi.org/10.1198/jasa.2011.tm10560.

Cai, T. T., Zhang, C.-H., and Zhou, H. H. (2010), “Optimal rates of convergence for covariance matrix estimation,” *Annals of Statistics*, 38, 2118–2144.

Dudoit, S. and van der Laan, M. J. (2005), “Asymptotics of cross-validated risk estimation in estimator selection and performance assessment,” *Statistical Methodology*, 2, 131–154.

Fan, J. and Li, R. (2001), “Variable Selection via Nonconcave Penalized Likelihood and its Oracle Properties,” *Journal of the American Statistical Association*, 96, 1348–1360.

Fan, J., Liao, Y., and Liu, H. (2016), “An overview of the estimation of large covariance and precision matrices,” *The Econometrics Journal*, 19, C1–C32, URL https://onlinelibrary.wiley.com/doi/abs/10.1111/ectj.12061.

Fan, J., Liao, Y., and Mincheva, M. (2013), “Large covariance estimation by thresholding principal orthogonal complements,” *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 75, 603–680.

Johnstone, I. M. (2001), “On the distribution of the largest eigenvalue in principal components analysis,” *Annals of Statistics*, 295–327.

Ledoit, O. and Wolf, M. (2003), “Improved estimation of the covariance matrix of stock returns with an application to portfolio selection,” *Journal of Empirical Finance*, 10, 603 – 621.
— (2004), “A well-conditioned estimator for large-dimensional covariance matrices,” *Journal of Multivariate Analysis*, 88, 365 – 411.
— (2012), “Nonlinear shrinkage estimation of large-dimensional covariance matrices,” *Annals of Statistics*, 40, 1024–1060.
— (2015), “Spectrum estimation: A unified framework for covariance matrix estimation and PCA in large dimensions,” *Journal of Multivariate Analysis*, 139, 360 – 384.
— (2018), “Analytical nonlinear shrinkage of large-dimensional covariates,” ECON – Working Papers 264, Department of Economics - University of Zurich, URL https://EconPapers.repec.org/RePEc:zur:econwp:264.
— (2020), “The Power of (Non)-Linear Shrinking: A Review and Guide to Covariance Matrix Estimation,” *Journal of Financial Econometrics*.

Pourahmadi, M. (2013), *High-dimensional covariance estimation*, Wiley series in probability and statistics, Wiley.

Rothman, A. J., Levina, E., and Zhu, J. (2009), “Generalized Thresholding of Large Covariance Matrices,” *Journal of the American Statistical Association*, 104, 177–186, URL https://doi.org/10.1198/jasa.2009.0101.

Schäfer, J. and Strimmer, K. (2005), “A Shrinkage Approach to Large-Scale Covariance Matrix Estimation and Implications for Functional Genomics,” *Statistical Applications in Genetics and Molecular Biology*, 4.

Stein, C. (1986), “Lectures on the theory of estimation of many parameters,” *Journal of Soviet Mathematics*, 34, 1373–1403, URL https://doi.org/10.1007/BF01085007.