# Optimizing the Ledoit-Wolf Estimator through High-Dimensional Regularization

Youhong Lee (joint with Alex Shkolnik)

Department of Statistics and Applied Probability, UC Santa Barbara

August 2, 2023

1/26

### Outline



A High-Dimensional Approach to Optimizing the Ledoit-Wolf Estimator



### Section 1

# The Ledoit-Wolf (LW) Estimator for Covariance Estimation

# The Sample Covariance Matrix

#### The Sample Covariance Matrix

For a  $p \times n$  data matrix Y, let the sample covariance matrix be

$$S = \frac{1}{n}YY^{\top}$$

where p is the feature dimension and n is the sample size.

- For our calculation purposes, we make the assumption that the population mean equals zero.
- The sample covariance matrix characterizes the linear relationships among the variables in terms of their variances and covariances.
- The sample covariance matrix is recognized as a consistent estimator for the population covariance matrix, denoted by Σ.

# Properties of ${\rm S}$ in High Dimensions

#### The Sample Covariance Matrix

For a  $p \times n$  data matrix Y, let the sample covariance matrix be

$$S = \frac{1}{n}YY^{\top}$$

where p is the feature dimension and n is the sample size.

- However, in high-dimensional settings where *p* greatly exceeds *n*, S displays certain unfavorable characteristics.
- As suggested by Ledoit & Wolf (2004), S lacks invertibility when p > n (this can be a critical issue as the inverse of S may be required for computing the minimum variance portfolio).
- The Marchenko–Pastur law indicates that the spectrum of S deviates considerably from its population counterpart.

5 / 26

# The Ledoit-Wolf (LW) Estimator

#### Ledoit & Wolf (2004)

The Ledoit-Wolf (LW) Estimator is given by

$$\hat{\Sigma} = \alpha S + (1 - \alpha)F$$

where S denotes the sample covariance matrix, F stands for a shrinkage target, and  $\alpha \in [0, 1]$  represents a shrinkage constant.

- Ledoit & Wolf (2004) proposes a James-Stein type shrinkage estimator for the covariance matrix.
- This estimator is constructed as a linear combination of the sample covariance matrix and a predetermined shrinkage target.
- This approach leads us to two important questions:
  - What would be the most appropriate shrinkage target?
  - What degree of shrinkage is optimal?

#### The Ledoit-Wolf (LW) Estimator Ledoit & Wolf (2004)

The Ledoit-Wolf (LW) Estimator is given by

$$\hat{\Sigma} = \alpha S + (1 - \alpha) F$$

where S denotes the sample covariance matrix, F stands for a shrinkage target, and  $\alpha \in [0,1]$  represents a shrinkage constant.

• A simply structured deterministic matrix can be used as a shrinkage target.

F = identity, a factor model, constant correlation, etc.

• The optimal shrinkage constant is selected to minimize an error rate.

$$\alpha^* \in \arg\min_{\alpha \in [0,1]} \operatorname{Risk}(\alpha)$$

# A Choice of the Optimal Shrinkage Constant

#### Ledoit & Wolf (2004)

The Ledoit-Wolf (LW) Estimator is given by

$$\hat{\Sigma} = \alpha S + (1 - \alpha)F$$

where S denotes the sample covariance matrix, F stands for a shrinkage target, and  $\alpha \in [0, 1]$  represents a shrinkage constant.

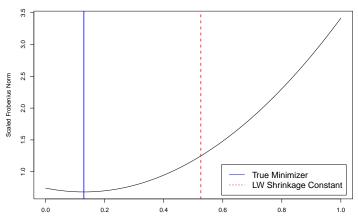
 More specifically, the optimal shrinkage constant is selected to asymptotically minimize the risk function of the Frobenius norm as loss.

$$\lim_{n \to \infty} \hat{\alpha}^* \in \arg\min_{\alpha \in [0,1]} \lim_{n \to \infty} \mathbb{E} \left[ \| \hat{\Sigma} - \Sigma \|^2 \right]$$

• In other words,  $\hat{\alpha}^*$  is a consistent estimator for the minimizer of the risk function.

## A Choice of the Optimal Shrinkage Constant

• However, empirical studies indicate that the optimal shrinkage constant may be overestimated in situations where the ratio n/p is relatively small.



Loss vs. Shrinkage Constant, n/p = 0.01

Shrinkage Constant

Youhong Lee (UCSB)

## **Refining the Optimal Shrinkage Constant Selection**

- We introduce a new analysis within the high-dimension, low-sample size (HL) regime.
- Our approach involves selecting an optimal shrinkage constant that minimizes its *p*-asymptotic loss as *p* → ∞.

$$\lim_{p \to \infty} \alpha^* \in \arg \min_{\alpha \in [0,1]} \lim_{p \to \infty} \operatorname{Error}(\alpha)$$

### Section 2

# A High-Dimensional Approach to Optimizing the Ledoit-Wolf Estimator

## A Loss Function with the Frobenius Norm

#### **Definition 1**

Our loss function is defined as the squared Frobenius norm between the true and estimated covariance matrices divided by p,

$$L(\alpha) = \frac{1}{\rho} \|\Delta(\alpha)\|^2 = \frac{1}{\rho} \operatorname{tr} \left(\Delta^2(\alpha)\right)$$

where  $\Delta = \Sigma - \hat{\Sigma}$  denotes the difference between the true and estimated covariance matrices with  $\hat{\Sigma} = \alpha S + (1 - \alpha)F$ .

# A Minimizer of the Loss Function

#### Lemma 1

A minimizer of the the loss function is given by

$$\alpha^* = \frac{\operatorname{tr}\left((\mathrm{F} - \mathrm{S})(\Sigma - \mathrm{S})\right)}{\operatorname{tr}\left((\mathrm{F} - \mathrm{S})^2\right)}$$

- The minimizer is unique almost surely.
- For a convex combination, the minimizer may be truncated to ensure  $\alpha \in [0, 1]$ .
- Note that the numerator can be expressed as

$$\mathrm{tr}\left((\mathrm{F}-\mathrm{S})(\Sigma-\mathrm{S})\right)=\mathrm{tr}(\mathrm{F}\Sigma)-\mathrm{tr}(\mathrm{S}\Sigma)-\mathrm{tr}\left(\mathrm{S}(\mathrm{F}-\mathrm{S})\right)$$

so we have two unobservable terms,  ${\rm tr}({\rm F}\Sigma)$  and  ${\rm tr}({\rm S}\Sigma).$ 

### The Market Model

• We adopt the assumption that that the population covariance matrix follows the market model

$$\boldsymbol{\Sigma} = \boldsymbol{p}\sigma^2\boldsymbol{u}\boldsymbol{u}^\top + \delta^2\mathbf{I}$$

where *u* is the leading eigenvector with its corresponding eigenvalue  $p\sigma^2 + \delta^2$  for some  $\sigma^2 > 0$  and  $\delta^2 > 0$  and I is the identity matrix.

• Correspondingly, we employ the single factor shrinkage target, represented as

$$\mathbf{F} = \boldsymbol{p}\boldsymbol{\sigma}_{\boldsymbol{F}}^2 \boldsymbol{q} \boldsymbol{q}^\top + \boldsymbol{\delta}_{\boldsymbol{F}}^2 \mathbf{I}$$

where q is an educated guess about the leading eigenvector and  $\sigma_F^2 > 0$  and  $\delta_F^2 > 0$  are constants.

## Lemmas for Unknown Quantities

• We derive random variables that are asymptotically equivalent to the two unknown quantities,  $tr(F\Sigma)$  and  $tr(S\Sigma)$ .

#### Lemma 2

For two sequences of random variables,  $a_p$  and  $b_p$ , denote  $a_p \sim b_p$  if  $\lim_{p\to\infty} \frac{a_p}{b_p} = 1$  almos surely. Then, under some assumptions, (a)  $\operatorname{tr}(S\Sigma) \sim p\sigma^2 s^2 \langle u, v \rangle^2$ 

where v is the leading eigenvector of S corresponding to the largest eigenvalue  $s^2$  with  $\Sigma = p\sigma^2 uu^{\top} + \delta^2 I$ .

(b)

$$\operatorname{tr}(\mathbf{F}\Sigma) \sim \sigma^2 \sigma_F^2 \langle u, q \rangle^2$$

with  $\mathbf{F} = p\sigma_F^2 q q^\top + \delta_F^2 \mathbf{I}$ .

## An Asymptotic Minimizer of the Loss Function

#### Theorem 1

Let  $\alpha' = \frac{p^2 \sigma^2 \sigma_F^2 \langle u, q \rangle^2 - p \sigma^2 s^2 \langle u, v \rangle^2 - tr(S(F-S))}{tr((F-S)^2)}$ . Then, under some assumptions,  $\alpha'$  asymptotically minimizes the loss function such that

$$\alpha' \sim \alpha^*$$

where  $\alpha^*$  is the true minimizer.

- We observe that  $\alpha'$  is composed of estimable quantities, specifically  $\sigma^2$ ,  $\langle u, q \rangle$ , and  $\langle u, v \rangle$ .
- Our analysis replicates the methods used in related literature, such as Jung et al. (2012), Goldberg et al. (2021), and Shkolnik (2022).

# **Consistent Estimators for Eigenvalues and Eigenvectors**

#### Lemma 3

Let  $\hat{\delta}^2 = \frac{(\operatorname{tr}(S) - s^2)m_p}{n - m_p}$  with  $m_p = 1 + n/p$  be an estimator of  $\delta^2$ , and let  $\hat{\sigma}^2 = s^2/p - \hat{\delta}^2/n$  be an estimator of  $\sigma^2$ . Then, under some assumptions,  $\hat{\sigma}^2 \sim \sigma^2$  and  $\hat{\delta}^2 \sim \delta^2$ . Moreover, if we define  $\psi \ge 0$  by  $\psi^2 = \hat{\delta}^2/s^2$ , then  $\psi \sim \langle u, v \rangle$  and  $\langle v, q \rangle/\psi \sim \langle u, q \rangle$ .

- Consequently, we derive *p*-consistent estimators for  $\sigma^2$ ,  $\langle u, q \rangle$ , and  $\langle u, v \rangle$ .
- These estimators contribute to the construction of a new shrinkage parameter,  $\hat{\alpha}'.$

17 / 26

## An Asymptotic Minimizer of the Loss Function

#### Theorem 2

Let  $\hat{\alpha}' = \frac{p^2 \hat{\sigma}^2 \sigma_F^2 \langle v, q \rangle^2 / \psi^2 - p \hat{\sigma}^2 s^2 \psi^2 - \operatorname{tr}(S(F-S))}{\operatorname{tr}((F-S)^2)}$  be an estimator of  $\alpha^*$ . Then, under some assumptions,  $\hat{\alpha}'$  asymptotically minimizes the loss function such that

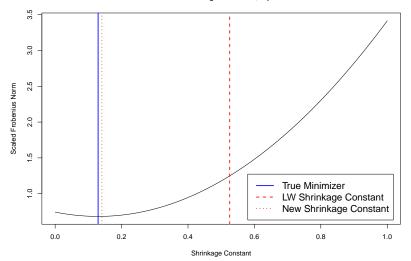
$$\hat{\alpha}' \sim \alpha^*$$

where  $\alpha^{\ast}$  is the true minimizer.

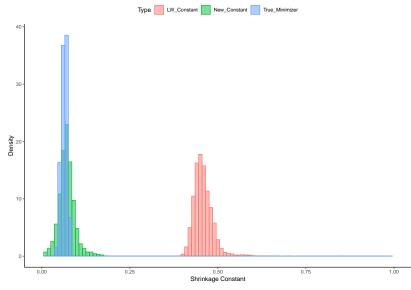
- We note that  $\hat{\alpha}'$  consists solely of sample quantities.
- Thus,  $\hat{\alpha}'$  offers a practical formula for determining the shrinkage constant, based on a *p*-asymptotic analysis.

## A Comparison of the Optimal Shrinkage Constants

Loss vs. Shrinkage Constant, n/p = 0.01

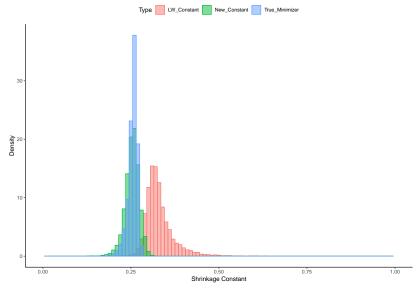


# Numerics: Distribution of Shrinkage Constants with n/p = 0.01

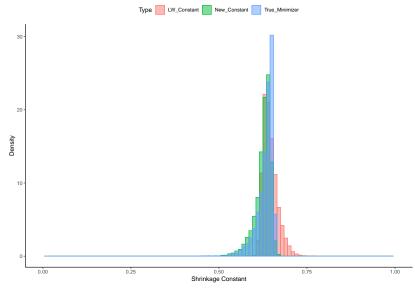


Youhong Lee (UCSB)

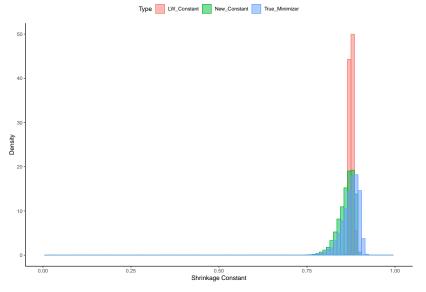
# Numerics: Distribution of Shrinkage Constants with n/p = 0.05



# Numerics: Distribution of Shrinkage Constants with n/p = 0.25



# Numerics: Distribution of Shrinkage Constants with n/p = 1



Youhong Lee (UCSB)

## Section 3

### **Summary**

## Summary

- The Ledoit-Wolf estimator is a widely adopted method for covariance estimation.
- We present a novel strategy for determining an optimal shrinkage constant using *p*-asymptotic analysis.
- Both theoretical and numerical results demonstrate that our new optimal constant delivers decreased error rates in situations where n/p is small.

# Thank You!