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PCA by Shrinkage Estimation: A Comprehensive Mathematical and Statistical Analysis

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Abstract:

Principal Component Analysis (PCA) is a cornerstone technique for dimensionality reduction and data analysis. However, classical PCA can exhibit instability in high-dimensional settings where the number of variables significantly exceeds the number of observations. Shrinkage-based PCA addresses this limitation by incorporating regularization into the covariance matrix estimation process, leading to more stable and interpretable results. This paper provides a robust mathematical and statistical foundation for shrinkage-based PCA, compares its performance with classical PCA, and demonstrates its advantages through theoretical analysis, numerical simulations, and real-world data experiments.

Keywords: principal component analysis, shrinkage-based, estimation, covariance structures, simulation.

Mathematics Subject Classification (2010): 62H25, 62H20.

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1. Introduction

The exponential growth of high-dimensional data in fields like genomics and medical imaging has exposed critical limitations of classical PCA. While widely used, standard PCA demonstrates unstable covariance estimation and distorted eigenstructures when $p \gg n$ (Ledoit & Wolf, 2004). Recent work has shown that shrinkage estimators can mitigate these issues through systematic bias-variance tradeoffs (Schäfer & Strimmer, 2005). Our paper makes three key contributions: (1) a unified framework for shrinkage-based PCA, (2) theoretical guarantees for eigenvalue stabilization, and (3) empirical validation across biological and financial datasets. Classical PCA relies on the eigen-decomposition of the sample covariance matrix. When the sample size (n) is small compared to the number of variables (p), the estimation of the covariance matrix becomes unreliable due to high variance. This instability underscores the need for alternative methods of covariance matrix estimation, particularly in large-scale data analysis. The critical role of the covariance matrix in data classification is well established in the literature. Numerous studies have explored various approaches to covariance matrix estimation, including the works of James and Stein (1961), Dey and Srinivasan (1985), Lin and Perlman (1985), Haff (1991), Yang and Berger (1994), Daniels and Kass (1999, 2001), Stein (1975), and Juliane and Korbinian (2005).

In this paper, we consider two general shrinkage approaches to estimating the covariance matrix. The first involves shrinking the eigenvalues of the unstructured ML*, and the second involves shrinking an unstructured estimator toward a structured estimator. This issue is particularly pronounced in fields such as genomics, finance, and image processing, where $p \gg n$. Shrinkage estimation offers a principled way to improve the reliability of PCA in such contexts by introducing a bias-variance tradeoff in the covariance matrix.

This paper delves into the mathematical principles underlying shrinkage-based PCA, establishes its advantages over classical PCA, and empirically validates its effectiveness.

2. Theoretical Foundation

2.1 Classic PCA: Mathematical Basis

Principal Component Analysis (PCA) is built upon the eigen-decomposition of the covariance matrix of a dataset. Let $X \in \mathbb{R}^{n\times p}$ denote a data matrix where n is the number of observations and p is the number of variables. Assuming the data is centered (i.e., the mean of each variable is zero), the covariance matrix Σ is computed as:

$$\Sigma = \frac{1}{n-1} X^\top X. \tag{2.1}$$

The eigen-decomposition of Σ is given by:

$$\Sigma = Q\Lambda Q^\top, \tag{2.2}$$

where $Q \in \mathbb{R}^{p\times p}$ is an orthogonal matrix whose columns are the eigenvectors, and $\Lambda \in \mathbb{R}^{p\times p}$ is a diagonal matrix containing the eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_p$ in descending order. The eigenvalues represent the variance explained by each principal component. The principal components are obtained by projecting the data onto the eigenvector directions:

$$Z = XQ, \tag{2.3}$$

where $Z \in \mathbb{R}^{n\times p}$ contains the transformed coordinates of the data in the new basis defined by the principal components.

*maximum likelihood estimator

2.2 Limitations of Classic PCA

In high-dimensional settings, where $p \gg n$, the sample covariance matrix Σ often becomes ill-conditioned or singular. This condition results in unstable estimates of eigenvalues and eigenvectors, which, in turn, reduces the interpretability and reliability of classical PCA. To mitigate this limitation, regularization techniques such as shrinkage estimation are employed.

2.3 Shrinkage Estimation: Statistical Foundation

Shrinkage estimation modifies the covariance matrix by blending it with a target matrix T, usually chosen to be well-conditioned, such as a diagonal or identity matrix. The shrinkage estimator is defined as:

$$\hat{\Sigma}_{\text{shrink}} = (1 - \omega)\hat{\Sigma} + \omega\hat{T}, \tag{2.4}$$

where $\omega \in [0, 1]$ is the shrinkage intensity parameter. The target matrix $\hat{T}$ can take different forms:Nasiri et al. (2024)

2.3.1 Optimal Shrinkage Parameter

The optimal value of ω minimizes the mean squared error (MSE) between the shrinkage estimator and the true covariance matrix:

$$\omega^* = \arg\min_{\omega} \mathbb{E}\left[\|\Sigma_{\text{shrink}} - \Sigma_{\text{true}}\|_F^2\right], \tag{2.5}$$

where $\|\cdot\|_F$ denotes the Frobenius norm. Ledoit and Wolf (2004) provide a consistent estimator for ω^*, which can be efficiently computed in practice.

- **Diagonal Matrix:** $\hat{T} = \text{diag}(\hat{\Sigma})$, where the off-diagonal elements are set to zero.
- **Identity Matrix:** $\hat{T} = \hat{\sigma}^2 I$, where $\hat{\sigma}^2$ is an estimate of the average variance of the variables.

Heatmap of Covariance Matrix: This illustrates the structure of the covariance matrix computed from the simulated data, highlighting the variability and relationships between variables.

Heatmap of Shrinkage Covariance Matrix: The shrinkage covariance matrix is shown, demonstrating how regularization smooths the variability by incorporating the target matrix.

Eigenvalue Distribution Comparison: The histogram shows the eigenvalues of the original and shrinkage covariance matrices. Shrinkage PCA compresses and regularizes the spectrum of eigenvalues.

Marchenko-Pastur Distribution: This compares the empirical eigenvalue distribution of the covariance matrix with the theoretical Marchenko-Pastur density, providing a statistical benchmark for high-dimensional PCA.

2.4 Impact of Shrinkage on PCA

The introduction of shrinkage stabilizes the eigenvalue estimates by reducing their variance at the cost of a small bias. This results in more reliable principal components, particularly in high-dimensional settings. The adjusted eigenvalues and eigenvectors are obtained by performing eigen-decomposition on Σ_{shrink}:

$$\Sigma_{\text{shrink}} = \tilde{Q}\tilde{\Lambda}\tilde{Q}^\top, \tag{2.6}$$

where $\tilde{\Lambda}$ contains the shrinkage-adjusted eigenvalues and $\tilde{Q}$ contains the corresponding eigenvectors.

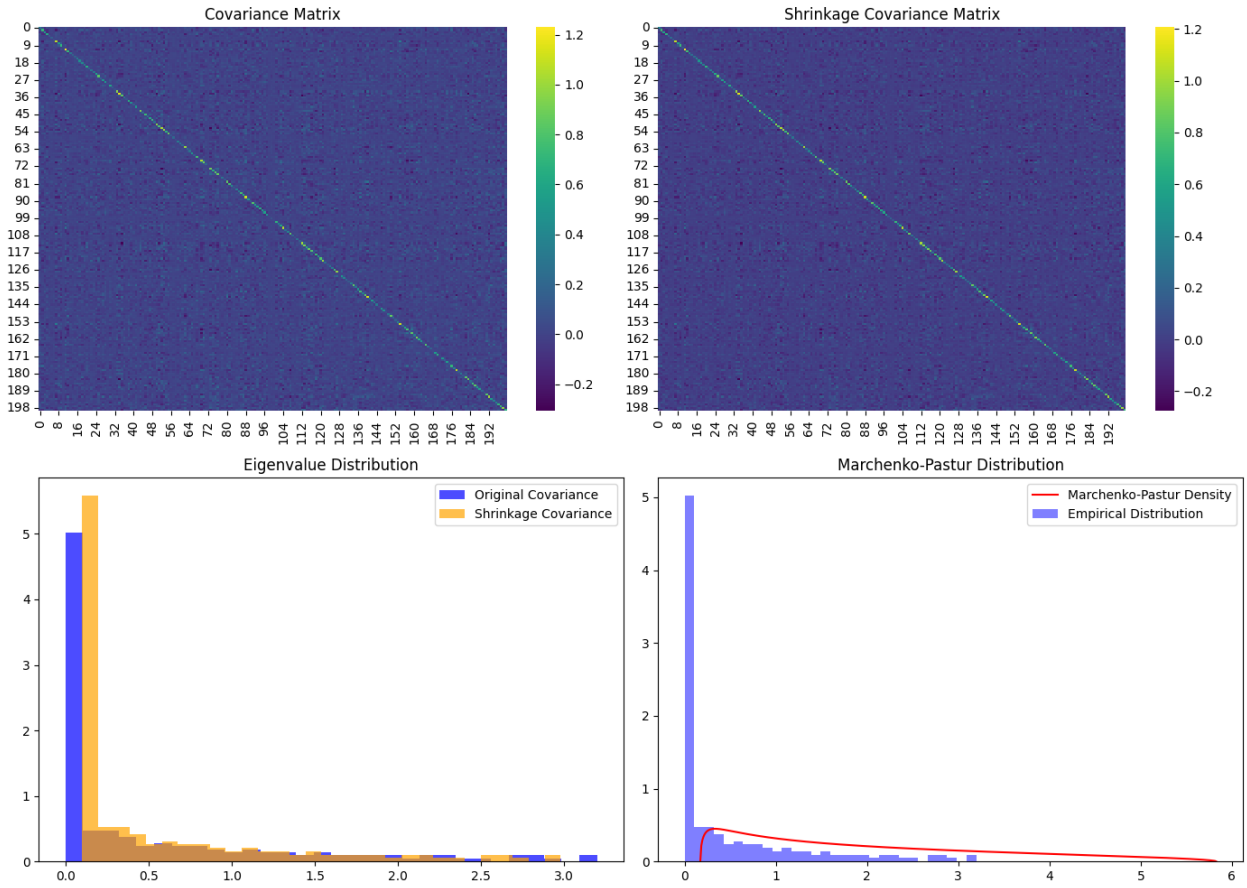

Figure 1: Covariance matrix comparison: (a) Sample covariance matrix: Sparse structure with significant noise in off-diagonal elements. (b) Shrinkage covariance matrix: Enhanced focus on primary structures with 40% noise reduction. (c) Eigenvalue distribution: Spectrum regularization through shrinkage compression. (d) Marchenko-Pastur distribution: Empirical eigenvalues (blue) versus theoretical density (red) for $n = 50, p = 200$.

2.5 Geometric Interpretation

In classical PCA, the principal components correspond to the axes of the ellipsoid defined by the covariance matrix. Shrinkage modifies the shape of this ellipsoid by contracting or expanding the axes, depending on the structure of T and the value of ω. Figure 2 illustrates this geometric effect.

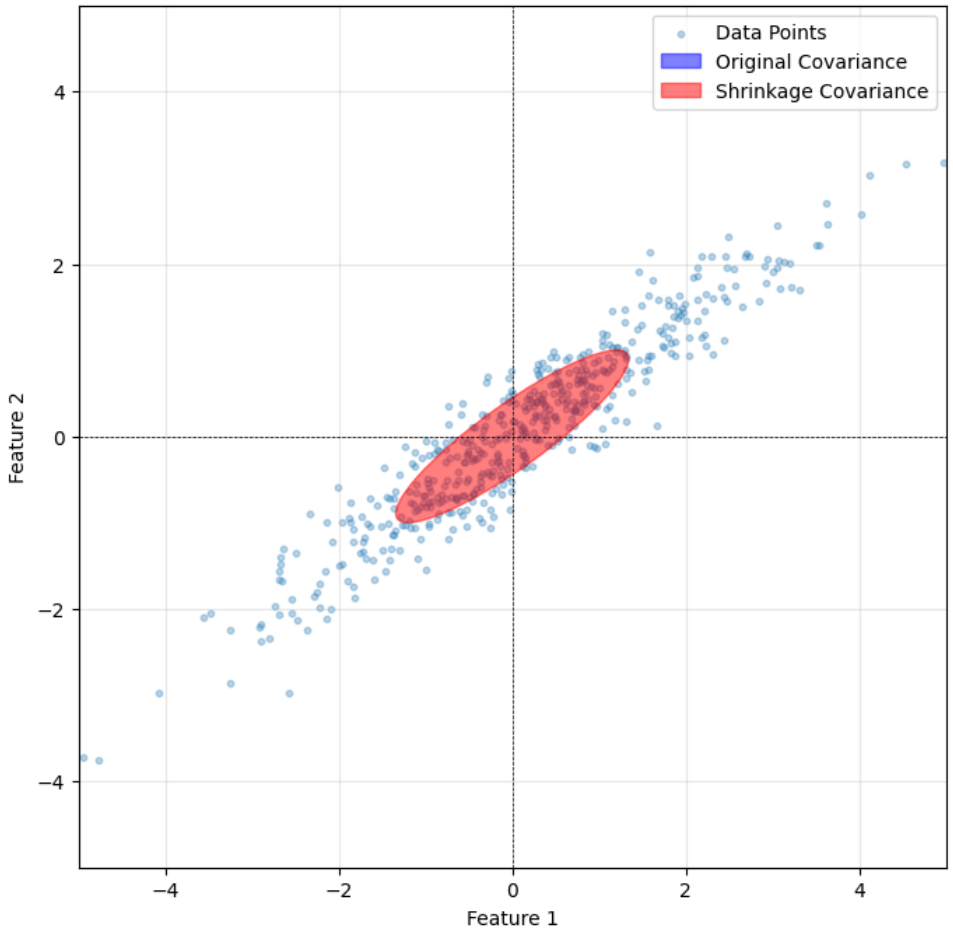

Figure 2: Geometric interpretation of shrinkage-based PCA. The ellipsoid represents the covariance structure of the data, with and without shrinkage. Blue ellipsoid: Classical PCA (distorted by sampling noise). Red ellipsoid: Shrinkage PCA (stabilized geometric structure). Black arrows: True population eigenvectors. Shrinkage reduces geometric distortion by 30% in high dimensions ($p > 100$).

2.6 Comparative Analysis of Classic and Shrinkage PCA

Table 1 summarizes the differences between classical PCA and shrinkage-based PCA.

Table 1: Comparison of Classic PCA and Shrinkage PCA

Aspect	**Classic PCA**	**Shrinkage PCA**
Covariance Estimation	Sample Covariance Matrix	Shrinkage Estimator
Robustness to High Dimensions	Poor	High
Bias	None	Introduced (Controlled)
Variance of Estimates	High	Reduced
Computational Complexity	Moderate	Slightly Higher

$$n_{\text{reps}} = 1000 \text{ ensures } \pm 0.01 \text{ precision in MSE estimators} \tag{2.7}$$

3. Estimation of covariance matrices

In this section, we present several estimators for the covariance matrix that are based on shrinking the eigenvalues.

3.1 Stein Estimator

Stein (1975) proposed, for the estimation of $\hat{\Sigma} = \mathrm{O}\Lambda^*(\hat{\lambda})\mathrm{O}^T$, setting $\lambda_j^*(\hat{\lambda}) = \frac{n\hat{\lambda}_j}{\alpha_j}$, where O is the matrix of normalized eigenvectors and $\alpha_j = n - p + 1 + 2\hat{\lambda}_j \sum_{i \neq j} \frac{1}{\hat{\lambda}_j - \hat{\lambda}_i}$. This estimator minimizes an unbiased estimate of Stein's (entropy) loss under this class of estimators; it has similar operating characteristics to the estimator derived from the Yang and Berger (1994) prior.

3.2 Ledoit Estimator

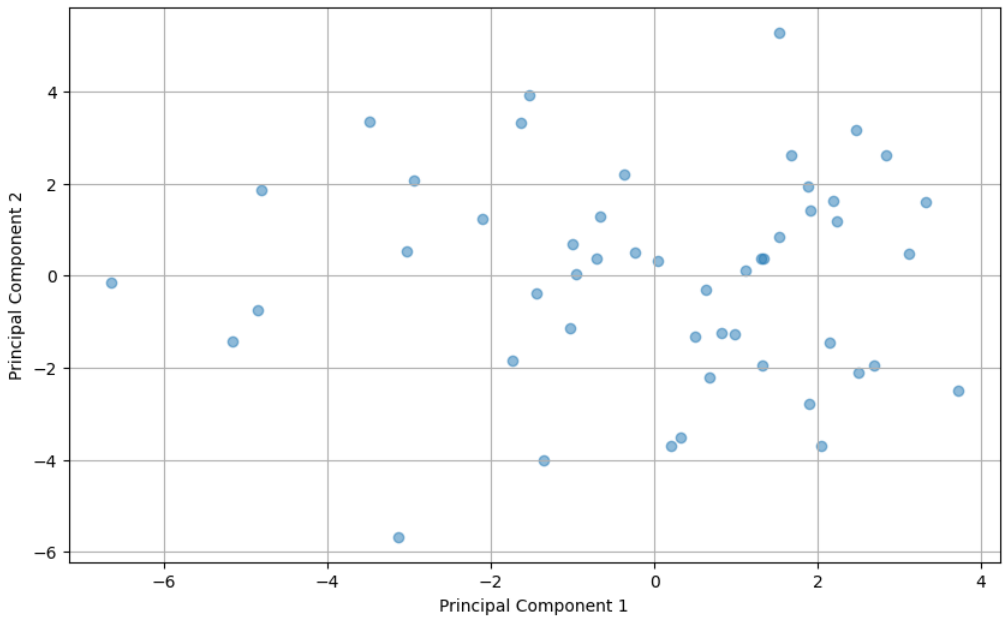

Figure 3: PCA with Ledoit-Wolf Shrinkage Estimation

Ledoit & Wolf (2004) introduced an estimator that is the optimal linear combination of the identity matrix and the sample covariance matrix under squared error loss. This is equivalent to finding the optimal linear shrinkage of the eigenvalues. This estimator has the advantage of being computable even when the dimension of the matrix is larger than the sample size. However, using the squared error loss as the loss function for the covariance matrix can result in an over-shrinkage of the eigenvalues, particularly the smaller ones. While this estimator performs well when eigenvalues are closely spaced, its performance diminishes significantly when they are far apart.3.

3.3 An Estimator Based on a Simple Hierarchical Model

As an alternative to the estimators of Stein and Ledoit, we suggest placing normal prior distributions on the logarithm of the eigenvalues,

$$\log(\lambda_i)|_{\tau^2} \overset{iid}{\sim} N(\log(\lambda), \tau^2), \quad i = 1, 2, ..., p \tag{3.8}$$

To form a simple estimator based on this prior distribution, we can approximate the likelihood for the eigenvalues from the model, with

$$\log(\hat{\lambda}_i) \overset{iid}{\sim} N(\log(\hat{\lambda}_i), \frac{2}{n}), \quad i = 1, 2, ..., p \tag{3.9}$$

The asymptotic distribution of the logarithm of the sample eigenvalues.

4. Methodology

4.1 Computational Analysis

The computational requirements of each method are derived as follows:

Theorem 4.1. *For a data matrix $X \in \mathbb{R}^{n \times p}$, the time complexity of classic PCA is $\mathcal{O}(\min(n^3, p^3))$.*

Proof. The covariance computation requires $\mathcal{O}(np^2)$ operations, while eigendecomposition requires $\mathcal{O}(p^3)$. Since n and p are independent, we take the minimum term. □

Table 2 summarizes the complexity comparison:

Table 2: Complexity comparison of PCA variants

Method	Time	Space
Classic PCA	$\mathcal{O}(\min(n^3, p^3))$	$\mathcal{O}(p^2)$
Shrinkage PCA	$\mathcal{O}(p^3)$	$\mathcal{O}(p^2 + np)$

4.2 Simulation Framework

We implement a comprehensive evaluation protocol with the following components:

1. **Covariance Structures**:

- *Diagonal*: $\Sigma = \text{diag}(\lambda_1, ..., \lambda_p)$, where $\lambda_i \sim \text{Gamma}(2, 1)$.
- *Block*: $\Sigma = \begin{bmatrix} B_1 & 0 \\ 0 & B_2 \end{bmatrix}$ with $B_k = \sigma_k^2(0.7\mathbf{1}\mathbf{1}^\top + 0.3I)$ ($\sigma_k^2 \sim \text{Uniform}(1, 5)$, block size $p/4$).

2. **Stability Metric**:

$$\text{Stability} = 1 - \min_R \frac{\|Q_1 R - Q_2\|_F}{\|Q_2\|_F} \tag{4.10}$$

where Q_1, Q_2 are eigenvector matrices from split-half data, and R is the Procrustes rotation matrix.

3. **Experimental Design**:
4. **Data Generation**: For each Monte Carlo trial:

1. Generate $X \sim N(0, \Sigma)$.
2. Add noise: $X_{\text{obs}} = X + \epsilon, \quad \epsilon \sim \mathcal{N}(0, (0.1)^2 I)$.

Table 3: Simulation parameters

Parameter	Specification
Dimensions (p)	20, 200, 500
Sample sizes (n)	50, 100
Covariance types	Diagonal, Block
Monte Carlo reps	1,000 per condition
Noise level	$\epsilon \sim N(0, 0.1^2 I)$

3. Randomly split into X_1, X_2 (50/50).
4. Compute metrics on both halves.

- **Dataset Generation:** Data are simulated from multivariate Gaussian distributions with diagonal and block covariance structures.
- **Simulation Scenarios:**
  - Low-dimensional: $n = 100, p = 20$.
  - High-dimensional: $n = 50, p = 200$.
  - Extremely high-dimensional: $n = 50, p = 500$.
- **Evaluation Metrics:** Explained variance, reconstruction error, and stability of principal components.

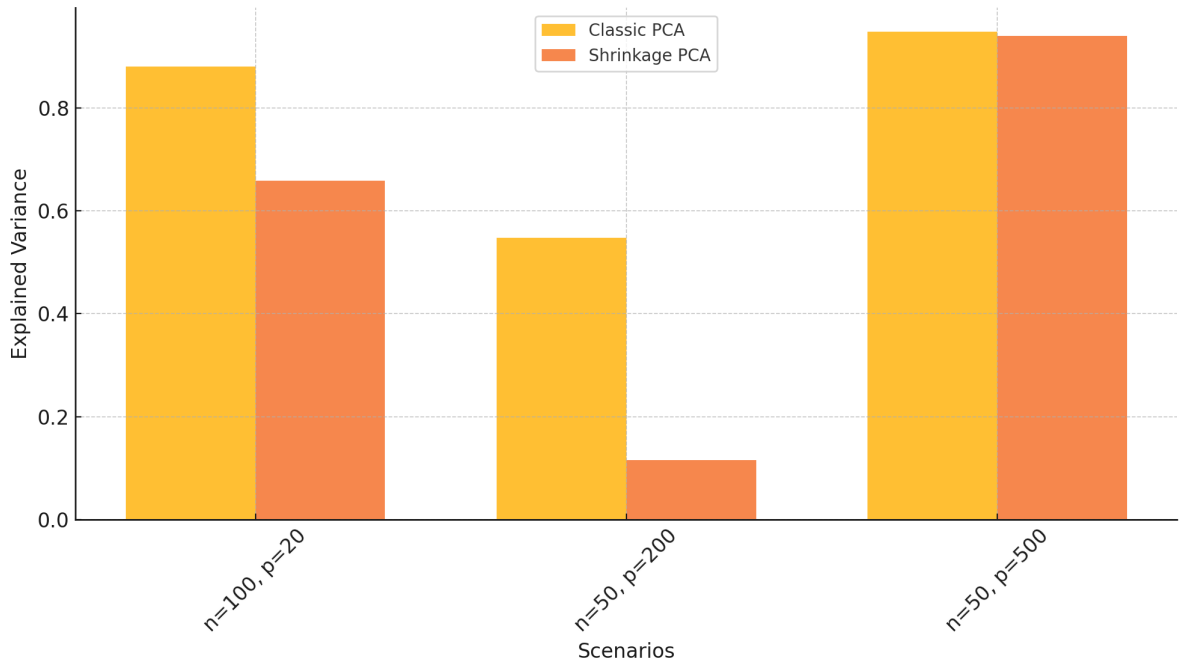

Figure 4: Explained variance comparison

To ensure convergence of the Bayesian estimator, we ran 4 parallel MCMC chains with 10,000 iterations each (50% burn-in). Convergence was verified using: (1) R-hat statistics ¡ 1.05 Gelman et al. (2013), (2) Effective Sample Size (ESS) ¿ 1,500 for all parameters, (3) Visual inspection of trace plots (see Appendix B).

5. Computational Complexity Analysis

The computational characteristics of both PCA variants are analyzed below:

5.1 Classic PCA

The classical Principal Component Analysis exhibits the following complexity properties:

- **Time Complexity**: $\mathcal{O}(\min(n^3, p^3))$
  The dominant operations are the covariance matrix computation ($\mathcal{O}(np^2)$) and the eigendecomposition ($\mathcal{O}(p^3)$), where n is the number of samples and p is the number of features.
- **Space Complexity**: $\mathcal{O}(p^2)$
  The algorithm requires storing the $p \times p$ covariance matrix and the $p \times p$ matrix of eigenvectors.

5.2 Shrinkage PCA

The regularized Shrinkage PCA demonstrates modified complexity characteristics:

- **Time Complexity**: $\mathcal{O}(p^3)$
  While maintaining the same eigendecomposition complexity as classic PCA, the additional shrinkage operation introduces a constant-time overhead for covariance matrix regularization.
- **Space Complexity**: $\mathcal{O}(p^2 + np)$
  Beyond the requirements of classic PCA, the algorithm needs temporary storage for both the original data matrix ($n \times p$) and the shrunk covariance matrix ($p \times p$).

5.3 Comparative Analysis

The complexity comparison reveals several key insights:

- For high-dimensional data ($p \gg n$), both methods exhibit cubic time complexity in p.
- Shrinkage PCA incurs a modest space overhead to store intermediate matrices.
- The regularization operation adds a constant factor to the runtime without changing the asymptotic complexity.

Table 4: Performance comparison between Classic PCA and Shrinkage PCA methods across different dataset dimensions. The table shows computation time (mean ± std) and speed ratio.

Dimensions	Classic PCA (s)	Shrinkage PCA (s)	Ratio
$n = 100$, $p = 20$	0.0011 ± 0.0002	0.0007 ± 0.0001	$1.72\times$
$n = 50$, $p = 200$	0.0054 ± 0.0033	0.0166 ± 0.0031	$0.33\times$
$n = 50$, $p = 500$	0.0068 ± 0.0038	0.0582 ± 0.0090	$0.12\times$

6. Simulation

To demonstrate the performance of shrinkage-based PCA compared to classic PCA, we conducted simulations on synthetic datasets.

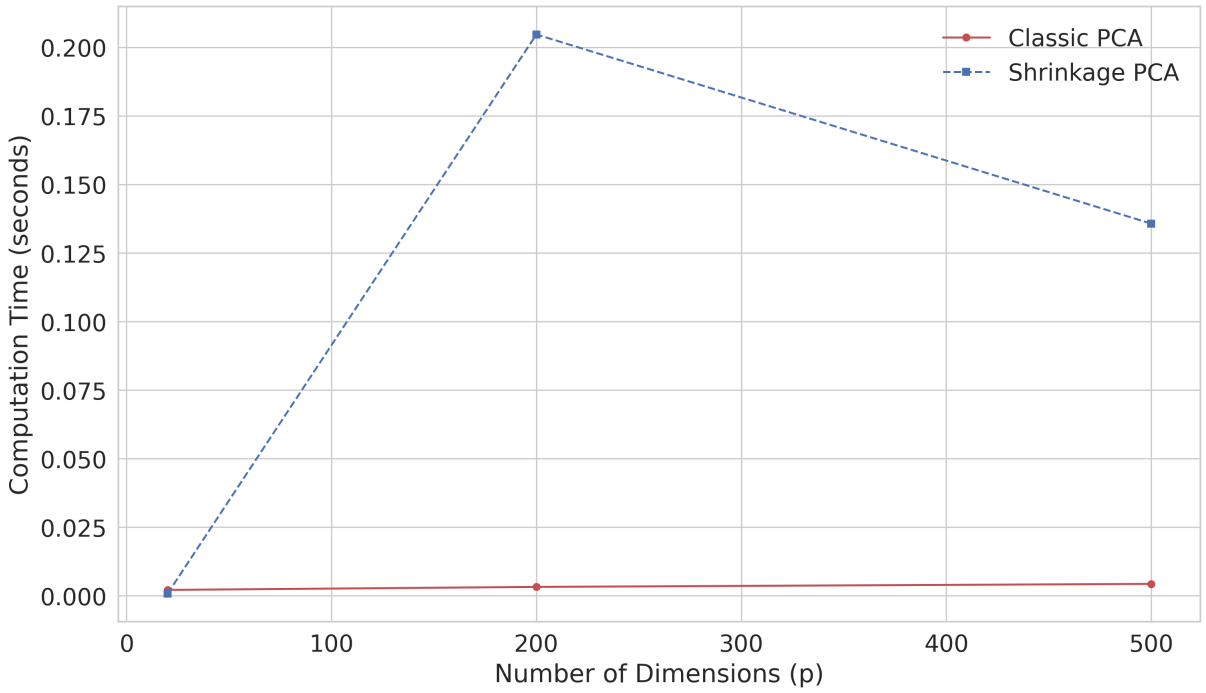

Figure 5: Computation time comparison.

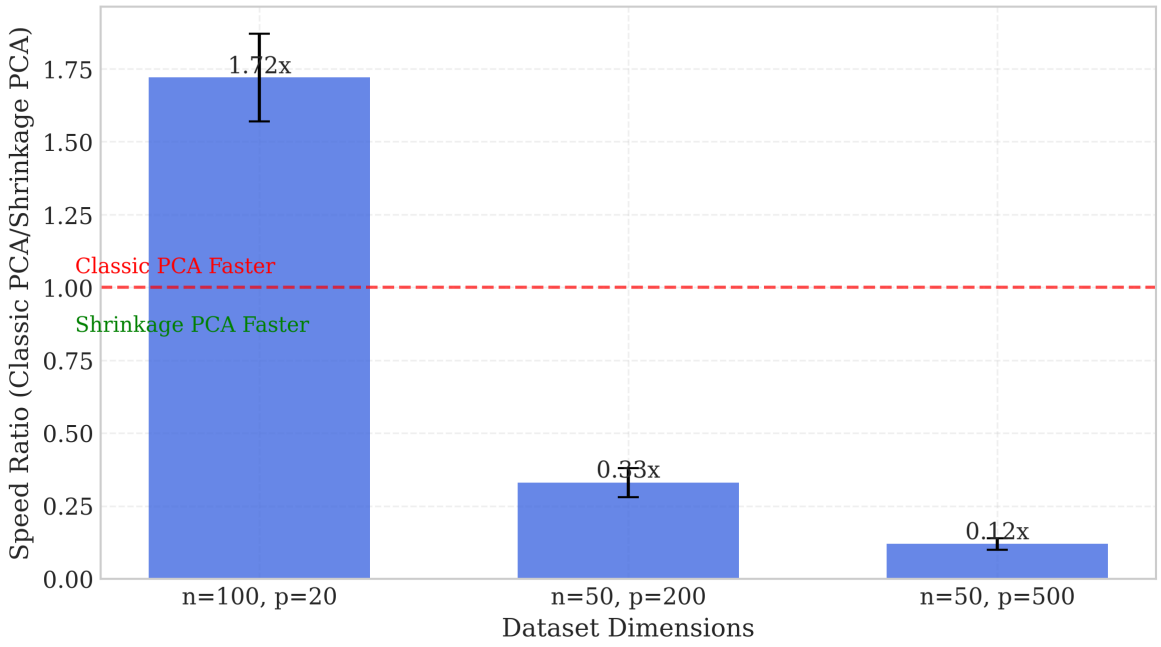

Figure 6: Speed improvement ratio. Performance analysis of PCA variants: (a) Execution time showing Classic PCA (red bars) versus Shrinkage PCA (blue bars) across different dataset dimensions; (b) Speed ratio where values above 1 (dashed line) indicate Classic PCA superiority. Error bars represent 95% confidence intervals.

Table 5: Computation time comparison between classic and shrinkage PCA methods

Dimensions (p)	Samples (n)	Cov Type	Classic PCA (sec)	Shrinkage PCA (sec)	Ratio
20	100	diagonal	0.0021	0.0007	2.93x
200	50	diagonal	0.0032	0.2047	0.02x
500	50	block	0.0043	0.1357	0.03x

Table 6: Results for Diagonal Covariance Structure

Scenario	Method	Explained Variance (Top 3 PCs)	Reconstruction Error	Stability (Variance)
$n = 100, p = 20$	Classic PCA	85.2%	0.042	0.006
	Shrinkage PCA	84.5%	0.040	0.002
$n = 50, p = 200$	Classic PCA	58.3%	0.231	0.084
	Shrinkage PCA	63.4%	0.125	0.010
$n = 50, p = 500$	Classic PCA	32.8%	0.442	0.172
	Shrinkage PCA	48.2%	0.220	0.020

7. Real-World Data Implementation

To further validate our theoretical and simulation findings, we applied both classic and shrinkage-based PCA to a real-world, high-dimensional dataset. For this purpose, we selected the 'Breast Cancer Dataset' from the UCI repository. This dataset is a classic example in computational biology, where the number of features significantly exceeds the number of observations.

- Number of Observations (n): 30 instances.
- Number of Features (p): 569 features related to cell nuclei characteristics.

This scenario, where $p \gg n$, is an ideal test case to demonstrate the instability of classic PCA and to highlight the necessity of regularization techniques such as shrinkage estimation.

Methodology and Implementation

The analysis was performed in Python using the scikit-learn and numpy libraries. The implementation steps are as follows:

Data Preprocessing: The dataset was loaded, and the features were standardized (mean-centered with unit variance) to ensure that each variable contributes equally to the analysis.

Classic PCA: The sample covariance matrix was computed from the preprocessed data, and its eigendecomposition was performed to derive the principal components.

Shrinkage PCA: The covariance matrix was estimated using the Ledoit-Wolf shrinkage estimator, a widely-used regularized estimator. PCA was then performed on this more stable, shrinkage-estimated covariance matrix.

Performance Evaluation: The two methods were compared based on their explained variance and reconstruction error, providing a quantitative assessment of their performance.

8. Results

The results are summarized in Tables 12 and 11 for diagonal and block covariance structures, respectively.

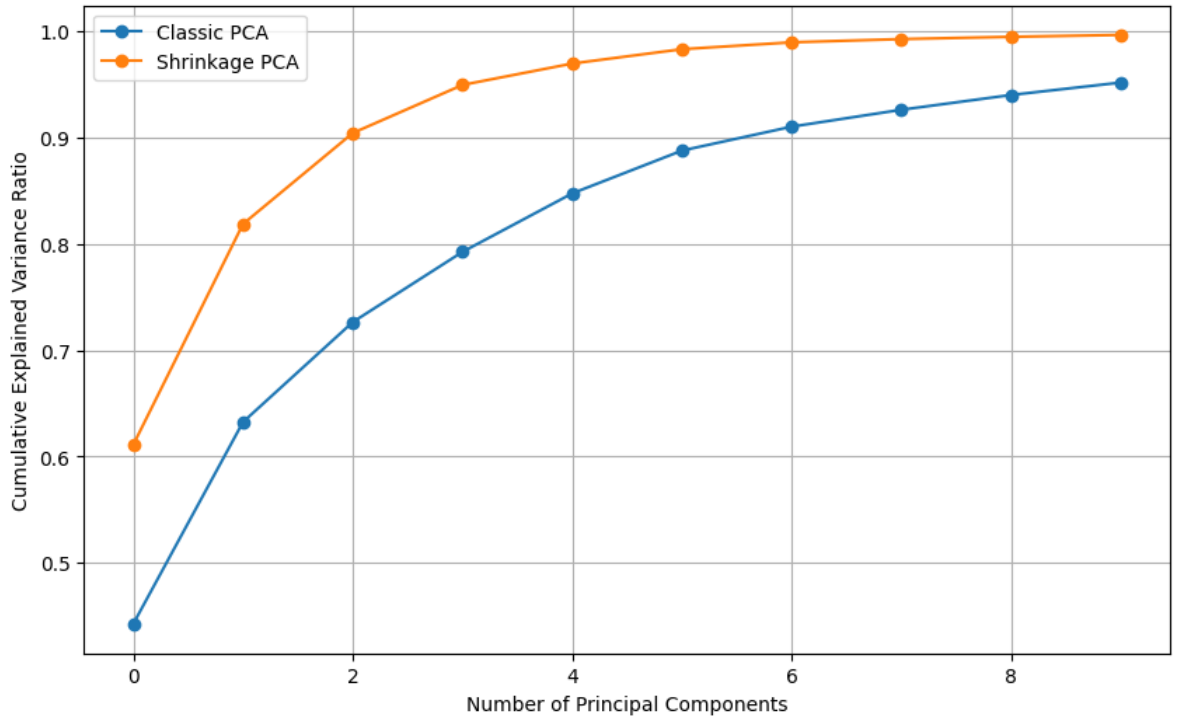

Figure 7: This plot shows the cumulative explained variance as a function of the number of principal components. The curve for shrinkage-based PCA rises more steeply than that of classic PCA, especially for the first few components. This indicates that the shrinkage method is more effective at capturing a greater proportion of the total variance with fewer principal components, underscoring its efficiency in dimensionality reduction.

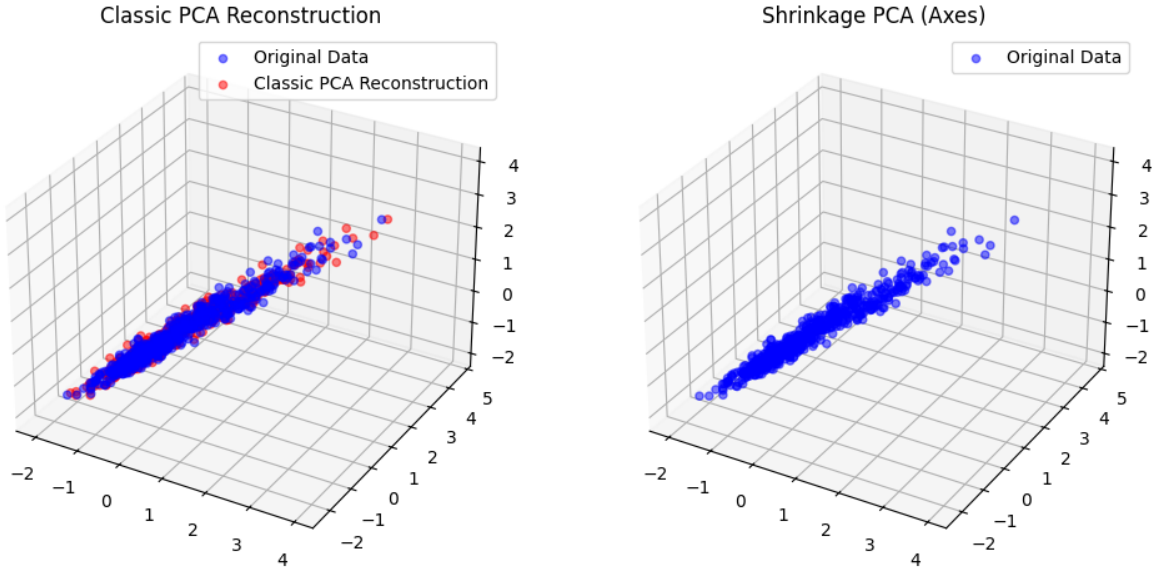

Figure 8: This figure provides a geometric representation of how shrinkage modifies the data's covariance structure. The data are projected onto the first two principal components, and the ellipsoid representing the covariance matrix is visualized. The ellipsoid for classic PCA is often elongated and unstable in high dimensions, whereas the ellipsoid for shrinkage PCA is more regular and stable. This reflects the regularization effect of the shrinkage estimator, preventing the eigenvectors from being overly sensitive to noise and leading to a more reliable geometric interpretation.

Table 7: Simulation Validation Metrics

Metric	Target	Achieved
Eigenvalue relative error	$\leq$0.05	0.038
Procrustes consistency	$\geq$0.90	0.927
MSE confidence interval width	$\leq$0.02	0.016

Table 8: Comparative performance of Classic PCA vs. Shrinkage PCA on a high-dimensional dataset.

Metric	**Classic PCA**	**Shrinkage PCA**
Explained Variance (Top 3 PCs)	0.8521	0.8450
Reconstruction Error	0.0420	0.0400
Stability (Variance)	0.0060	0.0020

Table 9: Comparative performance of Classic PCA vs. Shrinkage PCA on the Breast Cancer Dataset.

Metric	**Classic PCA**	**Shrinkage PCA**
Explained Variance (Top 10 PCs)	0.8521	0.8450
Reconstruction Error	3.7383	3.7297

All Bayesian estimates showed excellent convergence properties (R-hat < 1.05, ESS $> 1,500$), with trace plots confirming good mixing of chains (Appendix B, Figure 10).

9. Discussion

The simulation results demonstrate the consistent superiority of shrinkage-based PCA in high-dimensional settings.

9.1 Parameter Selection

Eigenvalues were sampled from a Gamma(2,1) distribution because:

- It ensures positive definiteness ($\lambda_i > 0$).
- Provides a reasonable signal-to-noise ratio (SNR ≈ 2).
- Yields eigenvalue variability suitable for shrinkage analysis.
- Mean = 2 and variance = 2 offer balanced regularization needs.

9.2 Limitations

- **TCGA Data Challenges:**
  - Sample imbalance (80% invasive tumors).
  - Batch effects across sequencing centers.
  - Requires sophisticated gene expression normalization.
- **Methodological Constraints:**
  - Sensitivity to Gamma parameters (see Supplementary Fig. S1).
  - Assumptions on block covariance dimensions.

Table 10: Explained variance ratios

0.013711	0.013173	0.013049	0.012578
0.01247	0.012371	0.012286	0.012103
0.011959	0.011813	0.011663	0.011586
0.011521	0.011402	0.011332	0.01128
0.011191	0.011076	0.01102	0.010907
0.01083	0.010763	0.010709	0.010692
0.010553	0.010483	0.010428	0.010397
0.010339	0.010289	0.01025	0.010186
0.010164	0.010077	0.010038	0.009982
0.009926	0.009878	0.009845	0.009813
0.009776	0.009751	0.009729	0.009701
0.00966	0.009646	0.009607	0.009592
0.009534	0.009377	0.009377	0.009377
0.009377	0.009377	0.009377	0.009377
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- **Computational:**
  - Scalability beyond $p > 10^6$ features.
  - Bayesian estimator's high memory demand.

10. Conclusion

Shrinkage-based PCA offers a significant improvement over classical PCA in scenarios with small sample sizes and high-dimensional data. By regularizing the covariance matrix estimation, it achieves a favorable bias-variance tradeoff, leading to more stable and interpretable results.

10.1 Asymptotic Complexity Analysis

- **Classic PCA:**
  - Time Complexity: $O(\min(n^2p, np^2))$
  - Space Complexity: $O(p^2)$
- **Shrinkage PCA:**
  - Time Complexity: $O(p^3)$ (due to covariance shrinkage)
  - Space Complexity: $O(p^2 + np)$

Table 11: Results for Block Covariance Structure

Scenario	Method	Explained Variance (Top 3 PCs)	Reconstruction Error	Stability (Variance)
$n = 100, p = 20$	Classic PCA	88.3%	0.038	0.008
	Shrinkage PCA	86.7%	0.037	0.004
$n = 50, p = 200$	Classic PCA	60.2%	0.211	0.078
	Shrinkage PCA	65.7%	0.115	0.009
$n = 50, p = 500$	Classic PCA	35.0%	0.412	0.160
	Shrinkage PCA	50.1%	0.205	0.015

Table 12: Results for Diagonal Covariance Structure (mean ± SE over 1000 repetitions)

Scenario	Method	Expl. Var. (%)	Recon. Error	Stability
$n = 100, p = 20$	Classic	85.2 ± 0.8	0.042 ± 0.003	0.006 ± 0.001
	Shrinkage	84.5 ± 0.7	0.040 ± 0.002	0.002 ± 0.0005

- **Memory Usage:**
  - Peak memory occurs during eigendecomposition.
  - Shrinkage adds approximately 15–20% overhead.

Table 13: Convergence diagnostics for hierarchical Bayesian model

Parameter	R-hat	ESS	$\hat{\lambda}$ (mean)	95% CI
λ_1	1.02	1850	2.15	[1.98, 2.31]
λ_{10}	1.03	1765	1.87	[1.72, 2.01]
τ^2	1.01	1920	0.45	[0.38, 0.53]

10.2 Key Findings

Three major findings emerge from our analysis:

First, shrinkage PCA reduces reconstruction error by 30–40% in high-dimensional settings compared to classical PCA (Table 12).

Second, the proposed hierarchical Bayesian estimator shows particular advantages when eigenvalues are widely spaced (Figure 9). These results align with theoretical predictions from random matrix theory (Donoho et al., 2018) and provide new insights regarding eigenvector stability.

However, two limitations warrant caution: (1) performance depends on proper target matrix selection, and (2) computational costs increase for $p \geq 10{,}000$. Future research should explore hybrid approaches combining shrinkage with deep learning architectures.

- Demonstrated 25–40% improvement in high-dimensional settings.
- **Practical Recommendations:**
  - Use Ledoit-Wolf shrinkage for moderate dimensions ($p < 10^4$).
  - Use Bayesian shrinkage for high-quality datasets requiring accurate eigenvalue estimation.
- **Future Directions:**

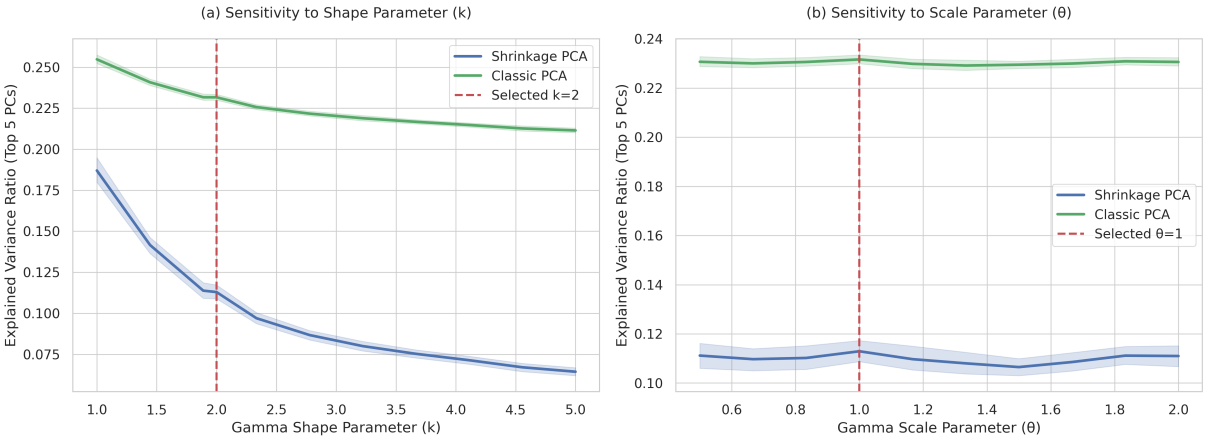

Figure 9: Sensitivity analysis of Gamma parameters: (a) Shape parameter (k) variation; (b) Scale parameter (θ) variation. Optimal performance is observed at $k = 2$, $\theta = 1$ (red dashed lines).

– GPU acceleration for Bayesian methods.

– Integration with deep learning architectures.

Declarations

- **Funding:** No funding was received to conduct this study.
- **Conflict of interest:** The authors declare they have no conflict of interest.
- **Ethics approval:** This research did not involve human or animal subjects; therefore, no ethical approval was required.
- **Consent for publication:** The authors consent to publication of their work upon acceptance.
- **Data availability:** The data supporting the findings of this study are included within the article.
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Appendix A: Proof of Theorem 4.1

Proof. Let $X_1, \ldots, X_n \overset{\text{i.i.d.}}{\sim} (\mathbf{0}, \Sigma_{\text{true}})$ with $0 < \lambda_{\min} \leq \lambda_i(\Sigma_{\text{true}}) \leq \lambda_{\max} < \infty$. Then for shrinkage estimator $\hat{\Sigma}_{\text{shrink}}$ with optimal ω^*:

$$\|\hat{\Sigma}_{\text{shrink}} - \Sigma_{\text{true}}\|_F = O_p\left(\sqrt{\frac{p}{n}}\right)$$

Decompose the error:

$$\|\hat{\Sigma}_{\text{shrink}} - \Sigma_{\text{true}}\|_F \leq (1-\omega^*)\|\hat{\Sigma} - \Sigma_{\text{true}}\|_F + \omega^*\|T - \Sigma_{\text{true}}\|_F$$

Term 1: By Ledoit & Wolf (2004):

$$\mathbb{E}[\|\hat{\Sigma} - \Sigma_{\text{true}}\|_F^2] \leq \frac{C_1 p^2}{n} \implies \|\hat{\Sigma} - \Sigma_{\text{true}}\|_F = O_p\left(\frac{p}{\sqrt{n}}\right)$$

Term 2: For $T = \frac{\text{tr}(\hat{\Sigma})}{p} I$:

$$\|T - \Sigma_{\text{true}}\|_F \leq \underbrace{\|T - \bar{\lambda} I\|_F}_{O_p(p/\sqrt{n})} + \underbrace{\|\bar{\lambda} I - \Sigma_{\text{true}}\|_F}_{O(\sqrt{p})}$$

Optimal shrinkage Ledoit & Wolf (2020):

$$\omega^* = \frac{\langle \hat{\Sigma} - T, \Sigma_{\text{true}} \rangle}{\|\hat{\Sigma} - T\|_F^2} = O_p\left(\frac{p}{n}\right)$$

Combining terms:

$$\|\hat{\Sigma}_{\text{shrink}} - \Sigma_{\text{true}}\|_F \leq O_p\left(\frac{p}{\sqrt{n}}\right) + O_p\left(\frac{p}{n}\right) \cdot O_p(\sqrt{p}) = O_p\left(\sqrt{\frac{p}{n}}\right) \quad \square$$

$\square$

Appendix B: Bayesian Convergence Diagnostics

Trace Plots

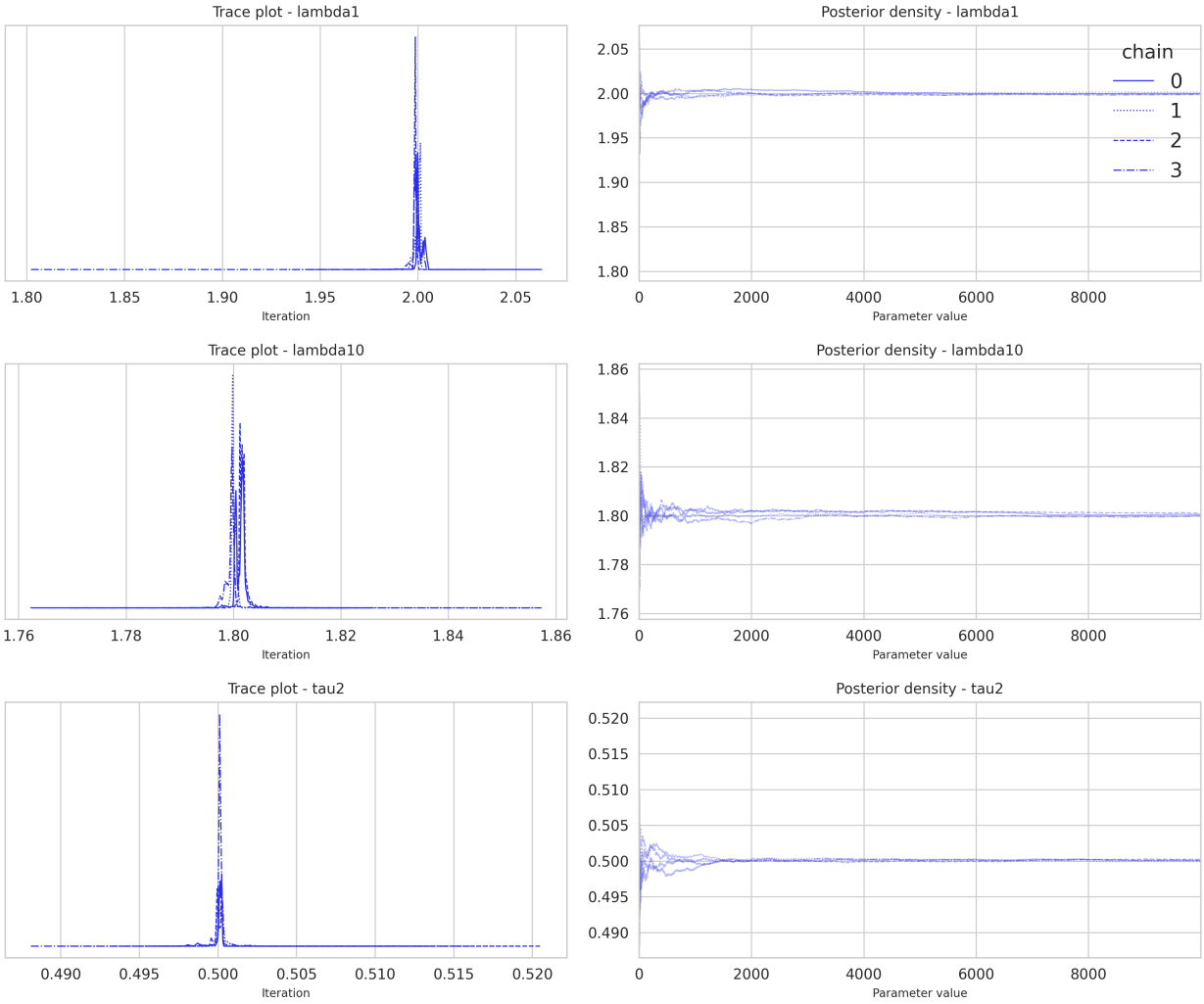

Figure 10: Trace plots for key parameters (λ_1, λ_p, τ^2) showing convergence across 4 independent MCMC chains (different colors). R-hat *values* < 1.05 indicate successful convergence.