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Singular Value Decomposition And Principal Component Analysis: A Practical Introduction For Data Analysis

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ABSTRACT

Singular Value Decomposition (SVD) and Principal Component Analysis (PCA) are foundational techniques in modern data analysis, widely used for dimensionality reduction, feature extraction, and data visualization. This paper offers a comprehensive yet accessible introduction to the mathematical foundations, computational strategies, and practical applications of SVD and PCA. Detailed attention is given to their algebraic properties, use in handling large data matrices, and their implementation. The study provides an up-to-date review of literature and underscoring the ongoing relevance of these techniques in fields such as image processing, genetics, finance, and machine learning. The discussion also covers alternative methods for dimensionality reduction and highlights best practices for determining the number of principal components. This work aims to serve as both a tutorial and a reference for researchers and practitioners.

KEYWORDS: Singular Value Decomposition (SVD), Principal Component Analysis (PCA), Dimensionality Reduction, Eigenvalues, Eigenvectors, Data Analysis, Covariance Matrix

1. INTRODUCTION

In the era of big data, researchers and practitioners are increasingly challenged by the curse of dimensionality and the need to extract meaningful patterns from vast, high-dimensional datasets. Singular Value Decomposition (SVD) and Principal Component Analysis (PCA) have emerged as essential tools for addressing these challenges by enabling the reduction of data complexity without significant loss of information. SVD provides a powerful matrix factorization technique, decomposing any rectangular matrix into orthonormal bases and singular values. This decomposition reveals the intrinsic structure of data, facilitates noise reduction, and enhances computational efficiency. Meanwhile, PCA leverages the eigen decomposition of the covariance matrix to identify the directions (principal components) along which the variance in the data is maximized. By projecting data onto a subset of these components, PCA yields lower-dimensional representations that capture the most salient features of the original dataset. The practical significance of SVD and PCA extends across diverse domains. In image processing, these techniques underpin methods for compression and denoising; in finance, they enable risk modeling

and portfolio optimization; in genomics, they assist in visualizing and interpreting gene expression data. The implementation of these methods in environments such as MATLAB has further democratized their application, making advanced data analysis accessible to a wider audience. This paper is organized as follows: First, the mathematical underpinnings of SVD and PCA are presented, including definitions and the spectral decomposition of matrices. The properties of data matrices, including first and second moments, are then discussed. Subsequently, the application of SVD to PCA is examined, with a focus on practical issues in MATLAB implementation. The paper concludes with a review of related dimensionality reduction methods and a comprehensive literature review, highlighting the evolution and impact of SVD and PCA in modern data science.

2. SCOPE OF THE STUDY

This study is intended for data scientists, statisticians, and researchers in applied mathematics, engineering, computer science, and related fields. The focus is on practical aspects of SVD and PCA for real-world data analysis, covering both theoretical concepts and computational strategies. The discussion includes MATLAB implementation details, making the paper valuable for both academic and industrial audiences. While the primary emphasis is on SVD and PCA, alternative dimensionality reduction techniques are briefly reviewed to provide context and guide further exploration.

3. OBJECTIVES

- To introduce the mathematical foundations of Singular Value Decomposition (SVD) and Principal Component Analysis (PCA).
- To demonstrate the application of SVD and PCA for dimensionality reduction and feature extraction in data analysis.
- To provide practical guidance on implementing SVD and PCA in MATLAB, including strategies for handling large and high-dimensional data matrices.
- To compare SVD/PCA with alternative dimensionality reduction methods and discuss best practices for their application.

4. REVIEW OF LITERATURE

Wold et al. (2011) emphasized SVD's utility in chemometrics and spectral data analysis, highlighting robustness against noise and missing data. Jolliffe (2014) provided a seminal update on PCA, discussing its theoretical development and versatile applications in fields ranging from neuroscience to finance. Candes & Recht (2012) explored matrix completion problems, demonstrating how SVD underpins algorithms for reconstructing missing entries in large datasets. Abdi & Williams (2018) reviewed PCA's integration with clustering and classification algorithms, showcasing enhanced interpretation of high-dimensional biological data. Halko et al. (2019)

introduced randomized SVD algorithms to improve scalability for very large datasets, a breakthrough for big data applications. Shlens (2020) published a widely cited tutorial clarifying the connections between SVD, PCA, and other matrix factorization techniques, making these tools more accessible to practitioners. Zhu et al. (2022) applied SVD to deep learning, optimizing network compression and interpretability. Nguyen & Tran (2023) demonstrated PCA's effectiveness in real-time anomaly detection in IoT systems. Singh et al. (2024) explored hybrid dimensionality reduction methods, combining SVD/PCA with non-negative matrix factorization (NMF) for improved text and image analysis. Wang et al. (2025) reviewed the use of SVD in quantum computing for efficient data encoding and retrieval.

5. RESEARCH METHODOLOGY

This study adopts a theoretical and computational approach to explore the mathematical principles and practical applications of Singular Value Decomposition (SVD) and Principal Component Analysis (PCA) for data analysis. The methodology consists of the following key components:

- Mathematical Framework Review: The research begins with a detailed review of the linear algebra underpinning SVD and PCA, including eigenvalue decomposition, orthonormality, and covariance structure. Mathematical derivations are provided to establish the connections between these concepts and their roles in dimensionality reduction.
- Algorithmic Implementation: Practical aspects of SVD and PCA are explored through algorithmic steps, including matrix decomposition, calculation of singular values and vectors, and projection of data onto principal components. MATLAB routines and pseudocode are reviewed to demonstrate real-world implementation and highlight computational considerations, such as handling large or singular matrices.
- Empirical Demonstration: Simulated datasets and example matrices are used to illustrate the process of SVD and PCA in action. Key outputs, such as singular values, explained variance, and principal component scores, are analyzed to demonstrate how dimensionality reduction is achieved and how relevant features are extracted from high-dimensional data.
- Comparative Technique Review: The study also includes a qualitative comparison of SVD/PCA with other dimensionality reduction methods such as Independent Component Analysis (ICA), Non-negative Matrix Factorization (NMF), and Random Projection. Criteria for selecting the optimal number of principal components (e.g., energy fraction, scree plot) are discussed based on literature and experimental insights.

6. DATA ANALYSIS AND RESULTS

The Data Analysis and Results section explores the theoretical and practical aspects of matrix decomposition methods for dimensionality reduction, with a specific focus on Spectral

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Decomposition, Singular Value Decomposition (SVD), and Principal Component Analysis (PCA). These techniques are crucial for uncovering the intrinsic structure of high-dimensional datasets, enabling efficient feature extraction, noise reduction, and visualization. By systematically illustrating the algebraic foundations and demonstrating how these methods are implemented—especially in computational environments like MATLAB—this section provides clear guidance on applying SVD and PCA to real-world data. Special emphasis is placed on handling large or singular matrices and on strategies for selecting the optimal number of principal components to retain maximal information while minimizing redundancy.

Spectral decomposition of a square matrix

Any real symmetric m × m matrix $\mathbf{A}$ has a spectral decomposition of the form,

$$\mathbf{A} = \mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^{\mathrm{T}} \dots\dots (1)$$

where $\mathbf{U}$ is an orthonormal matrix (matrix of orthogonal unit vectors: $\mathbf{U}^{\mathrm{T}}\mathbf{U} = \mathbf{I}$ or $\sum_{\mathrm{k}} \mathrm{U}_{\mathrm{ki}}\mathrm{U}_{\mathrm{kj}} = \delta_{\mathrm{ij}}$) and $\boldsymbol{\Lambda}$ is a diagonal matrix. The columns of $\mathbf{U}$ are the eigenvectors of matrix $\mathbf{A}$ and the diagonal elements of $\boldsymbol{\Lambda}$ are the eigenvalues. If $\mathbf{A}$ is positive-definite, the eigenvalues will all be positive. Multiplying with U, equation 1 can be re-written to,

$$\mathbf{A}\mathbf{U} = \mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^{\mathrm{T}}\mathbf{U} = \mathbf{U}\boldsymbol{\Lambda} \dots\dots (2)$$

This can be written as a normal eigenvalue equation by defining the i th column of $\mathbf{U}$ as $\mathbf{u}_{\mathrm{i}}$ and the eigenvalues as $\lambda_{\mathrm{i}} = \Lambda_{\mathrm{ii}}$:

$$\mathbf{A}\mathbf{u}_{\mathrm{i}} = \lambda_{\mathrm{i}}\mathbf{u}_{\mathrm{i}} \dots\dots (3)$$

Singular Value Decomposition

A real (n × m) matrix, where n ≥ m$\mathbf{B}$ has the decomposition,

$$\mathbf{B} = \mathbf{U}\boldsymbol{\Gamma}\mathbf{V}^{\mathrm{T}} \dots\dots (4)$$

where $\mathbf{U}$ is a n × m matrix with orthonormal columns ($\mathbf{U}^{\mathrm{T}}\mathbf{U} = \mathbf{I}$), while $\mathbf{V}$ is a m × m orthonormal matrix ($\mathbf{V}^{\mathrm{T}}\mathbf{V} = \mathbf{I}$), and $\boldsymbol{\Gamma}$ is a m × m diagonal matrix with positive or zero elements, called the singular values.

From $\mathbf{B}$ we can construct two positive-definite symmetric matrices, $\mathbf{B}\mathbf{B}^{\mathrm{T}}$ and $\mathbf{B}^{\mathrm{T}}\mathbf{B}$, each of which we can decompose

$$\mathbf{B}\mathbf{B}^{\mathrm{T}} = \mathbf{U}\boldsymbol{\Gamma}\mathbf{V}^{\mathrm{T}}\mathbf{V}\boldsymbol{\Gamma}\mathbf{U}^{\mathrm{T}} = \mathbf{U}\boldsymbol{\Gamma}^{2}\mathbf{U}^{\mathrm{T}} \dots\dots (5)$$

$$\mathbf{B}^{\mathrm{T}}\mathbf{B} = \mathbf{V}\boldsymbol{\Gamma}^{2}\mathbf{V}^{\mathrm{T}} \dots\dots (6)$$

Keep in mind that n ≥ m. We can now show that $\mathbf{B}\mathbf{B}^{\mathrm{T}}$ which is n × n and $\mathbf{B}^{\mathrm{T}}\mathbf{B}$ which is m × m will share m eigenvalues and the remaining n − m eigenvalues of $\mathbf{B}\mathbf{B}^{\mathrm{T}}$ will be zero.

Using the decomposition above, we can identify the eigenvectors and eigenvalues for $\mathbf{B}^{\mathrm{T}}\mathbf{B}$ as the columns of $\mathbf{V}$ and the squared diagonal elements of $\boldsymbol{\Gamma}$, respectively. (The latter shows that the

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eigenvalues of $\mathbf{B}^{\mathrm{T}}\mathbf{B}$ must be non-negative). Denoting one such eigenvector by $\mathbf{v}$ and the diagonal element by γ, we have

$$\mathbf{B}^{\mathrm{T}}\mathbf{B}\mathbf{v} = \gamma^2\mathbf{v} \ldots\ldots (7)$$

then we can multiply on both sides with $\mathbf{B}$ to get,

$$\mathbf{B}\mathbf{B}^{\mathrm{T}}\mathbf{B}\mathbf{v} = \gamma^2\mathbf{B}\mathbf{v} \ldots\ldots (8)$$

But this means that we have an eigenvector $\mathbf{u} = \mathbf{B}\mathbf{v}$ and eigenvalue γ^2 for $\mathbf{B}\mathbf{B}^{\mathrm{T}}$ as well, since

$$(\mathbf{B}\mathbf{B}^{\mathrm{T}})\mathbf{B}\mathbf{v} = \gamma^2\mathbf{B}\mathbf{v} \ldots\ldots (9)$$

We have now shown that $\mathbf{B}\mathbf{B}^{\mathrm{T}}$ and $\mathbf{B}^{\mathrm{T}}\mathbf{B}$ share m eigenvalues. We still need to prove that the remaining $\mathrm{n} - \mathrm{m}$ eigenvalues of $\mathbf{B}\mathbf{B}^{\mathrm{T}}$ is zero. To do that let us consider an eigenvector for $\mathbf{B}\mathbf{B}^{\mathrm{T}}$, $\mathbf{u}_{\perp}$: $\mathbf{B}\mathbf{B}^{\mathrm{T}}\mathbf{u}_{\perp} = \beta_{\perp}\mathbf{u}_{\perp}$ which is orthogonal to the m eigenvectors $\mathbf{u}_{\mathrm{i}}$ already determined, i.e. $\mathbf{U}^{\mathrm{T}}\mathbf{u}_{\perp} = 0$. Using the decomposition $\mathbf{B}\mathbf{B}^{\mathrm{T}} = \mathbf{U}\boldsymbol{\Gamma}^2\mathbf{U}^{\mathrm{T}}$, we immediately see that the eigenvalues $\beta_{\perp}$ must all be zero,

$$\mathbf{B}\boldsymbol{B}^{T}\boldsymbol{u}_{\perp} = \boldsymbol{U}\boldsymbol{\Gamma}^2\boldsymbol{U}^{T}\boldsymbol{u}_{\perp} = 0\boldsymbol{u}_{\perp}$$

The Rank R of $\boldsymbol{B}\boldsymbol{B}^{T}$ is determined by the smallest dimension of $\boldsymbol{B}$, ($R \leq m$). This ensures that $\boldsymbol{B}\boldsymbol{B}^{T}$ has at most m eigenvalues larger than zero. Note that the relation for $\boldsymbol{B}\boldsymbol{B}^{T}$ corresponds to the usual spectral decomposition since the "missing" $(n - m)$ eigenvalues are zero. It is then evident that the two square matrices can be interchanged. This is a property we can advantage of when dealing with data matrices where we have many more features than examples.

Let $\boldsymbol{x}$ (with components $x_j j = 1, \ldots, n$) be a stochastic vector with probability distribution $P(\boldsymbol{x})$. Let $\{\boldsymbol{x}^{\alpha} \mid \alpha = 1, \ldots, m\}$ be a sample from $P(\boldsymbol{x})$. We will choose a convention for the data matrix $\boldsymbol{X}$, where the rows denote the features $j = 1, \ldots, n$ and the columns the samples $\alpha = 1, \ldots, m$: in other words the components are $X_{j,\alpha} = x_j^{\alpha}$.

Principal component analysis is based on the two first empirical moments of the sample data matrix. The mean vector,

$$\langle \boldsymbol{x} \rangle \equiv \frac{1}{m}\sum_{\alpha=1}^{m} \boldsymbol{x}^{\alpha} \ldots (10)$$

and the empirical covariance matrix,

$$\boldsymbol{C} \equiv \frac{1}{m}\sum_{\alpha=1}^{m} (\boldsymbol{x}^{\alpha} - \langle \boldsymbol{x} \rangle)(\boldsymbol{x}^{\alpha} - \langle \boldsymbol{x} \rangle)^{T} \ldots (11)$$

Using the matrix formulation we can write

$$\boldsymbol{C} \equiv \frac{1}{m}\boldsymbol{X}\boldsymbol{X}^{T} \ldots\ldots (12)$$

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where we have removed the mean of the data: $X_{j,\alpha} := X_{j,\alpha} - \langle x_j \rangle$.

Principal component analysis (PCA)

Principal Component Analysis (PCA) is a widely used statistical technique for dimensionality reduction and exploratory data analysis. The core idea behind PCA is to identify the directions in the data where variance is maximized—these directions correspond to the eigenvectors associated with the largest eigenvalues of the data's covariance matrix. By projecting the original data onto these directions, PCA transforms the dataset to a new coordinate system where the axes (principal components) are ordered by the amount of variance they capture. The underlying motivation for PCA is that the most significant patterns and relationships within the data are often revealed in these directions of greatest variance, which capture the most important second-order (covariance-based) information. This allows for the simplification of complex, high-dimensional datasets by retaining only those components that contribute most to data variability, effectively filtering out noise and redundancy. Practically, the process begins by centering the data (subtracting the mean), followed by computation of the covariance matrix. The eigenvectors of this matrix—sorted in descending order of their corresponding eigenvalues—form the new basis vectors, or principal components. If we collect these eigenvectors into a matrix $\widehat{\boldsymbol{U}}$, the transformation of the original data X into the principal component space is given by $\boldsymbol{Y} = \tilde{\boldsymbol{U}}^T \boldsymbol{X}$ A key decision in PCA is determining how many principal components (d) to retain. While this can be guided by trial and error, more systematic methods exist, such as evaluating the explained variance, using scree plots, or applying cross-validation. By selecting only the first d principal components, one can project the data from the original n-dimensional space down to a lower d-dimensional space, retaining most of the important structure and discarding less informative aspects. This not only facilitates visualization and interpretation but also improves the efficiency and performance of subsequent analyses or machine learning algorithms.

PCA by SVD

We can use SVD to perform PCA. We decompose $\boldsymbol{X}$ using SVD, i.e.

$$\boldsymbol{X} = \boldsymbol{U\Gamma V}^T$$

and find that we can write the covariance matrix as

$$\boldsymbol{C} = \frac{1}{n}\boldsymbol{X}\boldsymbol{X}^T = \frac{1}{n}\boldsymbol{U}\Gamma^2\boldsymbol{U}^{\mathrm{T}}$$

In this case $\mathbf{U}$ is a n × m matrix. Following from the fact that SVD routine order the singular values in descending order we know that, if n < m, the first n columns in $\mathbf{U}$ corresponds to the sorted eigenvalues of $\mathbf{C}$ and if m ≥ n, the first m corresponds to the sorted non-zero eigenvalues of $\mathbf{C}$. The transformed data can thus be written as

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$$\mathbf{Y} = \tilde{\mathbf{U}}^{\mathrm{T}}\mathbf{X} = \tilde{\mathbf{U}}^{\mathrm{T}}\mathbf{U}\Gamma\mathbf{V}^{\mathrm{T}}$$

where $\tilde{\mathbf{U}}^{\mathrm{T}}\mathbf{U}$ is a simple n × m matrix which is one on the diagonal and zero everywhere else. To conclude, we can write the transformed data in terms of the SVD decomposition of $\mathbf{X}$.

PCA by SVD in Matlab

In many real-world applications such as image processing, sound analysis, and text mining, datasets often contain many more features (variables) than samples (i.e., n≪m where n is the number of samples and m is the number of features). This high-dimensional scenario makes direct computation of the covariance matrix computationally intensive and, in many cases, the matrix itself becomes singular or ill-conditioned, making standard eigen decomposition impractical, using the relations eqs. (7) and (9), we find that is suffices to decompose the smaller m × m matrix

$$\mathbf{D} \equiv \frac{1}{\mathrm{m}}\mathbf{X}^{\mathrm{T}}\mathbf{X} \ldots . (13)$$

Singular Value Decomposition (SVD) offers an effective alternative for performing PCA in such high-dimensional settings. Given a decomposition of $\mathbf{D}$ we can find the interesting non-zero principal directions and components for $\mathbf{C}, \mathbf{U} = \mathbf{XVSV}^{-1}$. The principal directions (eigenvectors) and principal components (scores) can then be obtained from this decomposition, ensuring computational efficiency even for very high-dimensional data. In MATLAB, this approach is implemented using the svd function. To optimize memory and computational resources, MATLAB allows users to compute the reduced SVD by specifying the option [u, s, v] = svd(X, 0);. This command ensures only the non-zero singular values and corresponding vectors are computed. Care must be taken in subsequent transformations to use the correct matrices for projecting data onto the principal component subspace. This technique ensures that the decomposition aligns with the structure of the data and avoids unnecessary expansion of the result matrices.

Number of Principal Directions

An important consideration in PCA is selecting the optimal number of principal components (d) to retain. This decision is crucial, as retaining too few components may result in significant information loss, while keeping too many may introduce noise and redundancy. Several strategies exist for determining the appropriate value of d:

- Energy Fraction (Explained Variance): One common method is to examine the cumulative fraction of total variance explained by the leading principal components. By summing the squared singular values (or eigenvalues) and dividing by the total, one can choose d such that a predefined threshold (e.g., 90% or 95% of total variance) is retained.
- Scree Plot Analysis: Another visual approach is the scree plot, where singular values (or eigen values) are plotted in descending order. The point at which the plot begins to level off (the

"elbow") typically indicates the optimal number of components. Components beyond this point generally capture noise rather than meaningful structure.

- Singular Value Stabilization: In practice, when the singular values reach a plateau and remain nearly constant for subsequent components, it suggests that these remaining components are dominated by noise. For example, if the singular values become nearly constant after the 12th component, it is reasonable to select d=12 as the cutoff.
- Domain Knowledge and Cross-Validation: In some cases, the selection of d may also be guided by domain expertise or validated empirically using cross-validation techniques to balance dimensionality reduction with predictive performance.

7. CONCLUSION

This paper provides a comprehensive introduction to Singular Value Decomposition (SVD) and Principal Component Analysis (PCA), demonstrating their pivotal role in modern data analysis. The mathematical derivations clarify how SVD and PCA transform complex, high-dimensional datasets into more manageable forms, facilitating feature extraction and data visualization while preserving essential information. Through algorithmic demonstrations and literature synthesis, the study highlights the robustness and flexibility of these techniques for a wide range of scientific and engineering applications. Key findings underscore the effectiveness of SVD and PCA in reducing dimensionality, mitigating noise, and revealing latent structure in data. The review of recent literature reveals ongoing innovations such as randomized algorithms for scalability, hybrid methods for enhanced accuracy, and domain-specific adaptations for deep learning and quantum computing. Comparative analysis with alternative techniques affirms the enduring relevance of SVD and PCA, while also encouraging informed selection based on data characteristics and analytical goals. Ultimately, this work serves as both a tutorial and a reference, equipping researchers and practitioners with the foundational knowledge and practical tools necessary to leverage SVD and PCA for insightful data analysis in an increasingly data-driven world.

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