CS544

Comparative Study of PCA and t-SNE on the MNIST Dataset

Submitted By

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Contents

1 **Introduction** 3

2 **Objective** 3

3 **Methodology** 3

3.1 Dataset and Preprocessing . . . 3

3.2 Principal Component Analysis (PCA) . . . 3

3.3 t-Distributed Stochastic Neighbor Embedding (t-SNE) . . . 4

3.4 Hybrid PCA–t-SNE . . . 5

4 **Results and Discussion** 6

5 **Conclusions** 7

6 **References** 7

Abstract

This report presents a comparative analysis of two popular dimensionality reduction techniques: Principal Component Analysis (PCA) and t-Distributed Stochastic Neighbor Embedding (t-SNE), applied to the MNIST dataset of handwritten digits. We investigate their ability to capture both global and local data structure, discuss computational trade-offs, and illustrate their workings with algorithmic details. Visual examples and placeholders are provided for insertion of result images.

1 Introduction

High-dimensional datasets such as images or gene-expression profiles suffer from the *curse of dimensionality*, making visualization and learning difficult. Dimensionality reduction maps data to a lower-dimensional space while preserving meaningful structure. PCA finds global variance-maximizing axes, whereas t-SNE emphasizes local neighborhood relationships. MNIST, with 70,000 handwritten digits in a 784-dimensional pixel space, is a standard benchmark to compare these methods.

2 Objective

- Demonstrate the internal mechanics of PCA and t-SNE.
- Quantify run time, clustering quality (silhouette score), and reconstruction error.
- Showcase a hybrid PCA–t-SNE pipeline for efficiency.
- Provide figure placeholders for results images.

3 Methodology

3.1 Dataset and Preprocessing

The MNIST dataset comprises 60,000 training and 10,000 test 28×28 grayscale images. We flatten each image into a 784-dimensional vector and normalize pixel values to $[0, 1]$. Zero-centering is applied by subtracting the mean vector. PCA additionally standardizes each feature to unit variance before projection.

3.2 Principal Component Analysis (PCA)

PCA finds an orthonormal basis maximizing projected variance.

1. **Covariance computation:** Given data matrix X (n samples, d features), compute $C = \frac{1}{n-1} X^T X$.
2. **Eigen-decomposition:** Solve $C\mathbf{u}_i = \lambda_i \mathbf{u}_i$ for eigenpairs $(\lambda_i, \mathbf{u}_i)$. The eigenvalue λ_i measures variance along $\mathbf{u}_i$.
3. **Dimensionality reduction:** Select top k eigenvectors $U_k = [\mathbf{u}_1, \ldots, \mathbf{u}_k]$. Project $Z = XU_k$.
4. **Data reconstruction:** Compute $\hat{X} = ZU_k^T$, with reconstruction error $E_{\text{PCA}} = \frac{1}{n}\|X - \hat{X}\|_F^2$.

Computational complexity: $O(d^2 n + d^3)$ dominated by covariance and eigendecomposition. Empirical runtime: t_{PCA} seconds.

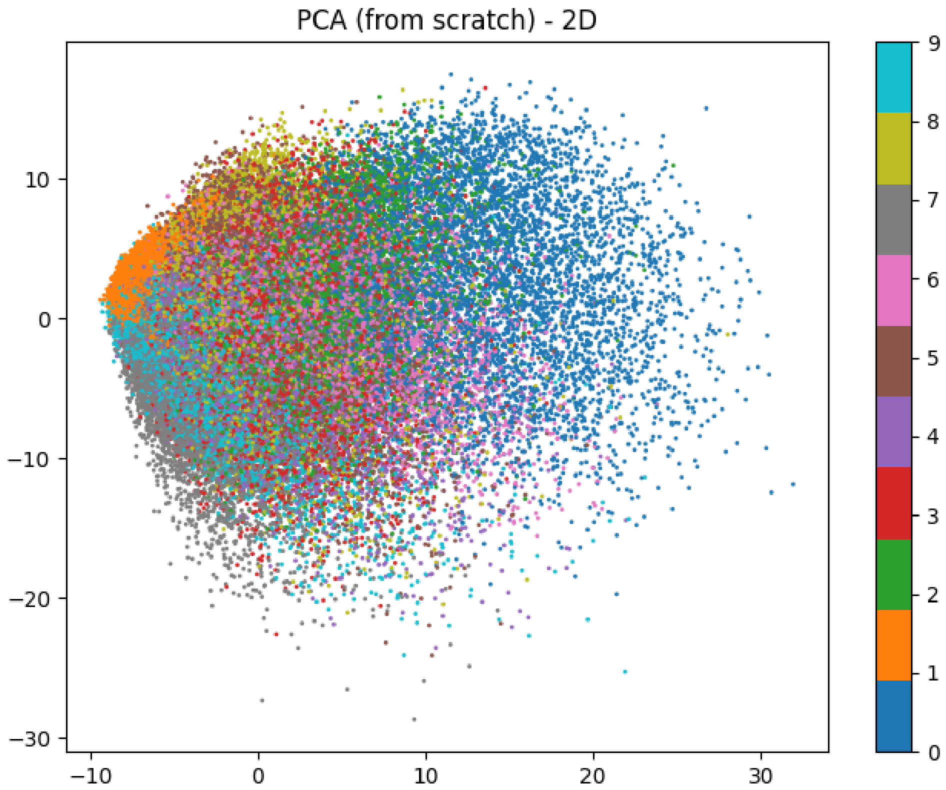

Figure 1: PCA.

Strengths & Limitations:

- Preserves global variance; invertible up to chosen dimensions.
- Fast and deterministic.
- Fails to preserve fine local clusters when k is small.

3.3 t-Distributed Stochastic Neighbor Embedding (t-SNE)

T-SNE models pairwise similarities with probability distributions and minimizes their divergence across spaces.

High-dimensional affinities:

$$p_{j|i} = \frac{\exp(-\|x_i - x_j\|^2/2\sigma_i^2)}{\sum_{k\neq i}\exp(-\|x_i - x_k\|^2/2\sigma_i^2)},$$

where σ_i matches a perplexity hyperparameter (30). Symmetrize:

$$p_{ij} = \frac{p_{j|i} + p_{i|j}}{2n}.$$

Low-dimensional affinities:

$$q_{ij} = \frac{(1 + \|y_i - y_j\|^2)^{-1}}{\sum_{k\neq l}(1 + \|y_k - y_l\|^2)^{-1}}.$$

Optimization: Minimize
$$C = \sum_{i \neq j} p_{ij} \log \frac{p_{ij}}{q_{ij}},$$
using gradient descent:
$$\frac{\partial C}{\partial y_i} = 4 \sum_j (p_{ij} - q_{ij})(y_i - y_j)(1 + \|y_i - y_j\|^2)^{-1}.$$
Parameters: learning rate=200, iterations=1000.

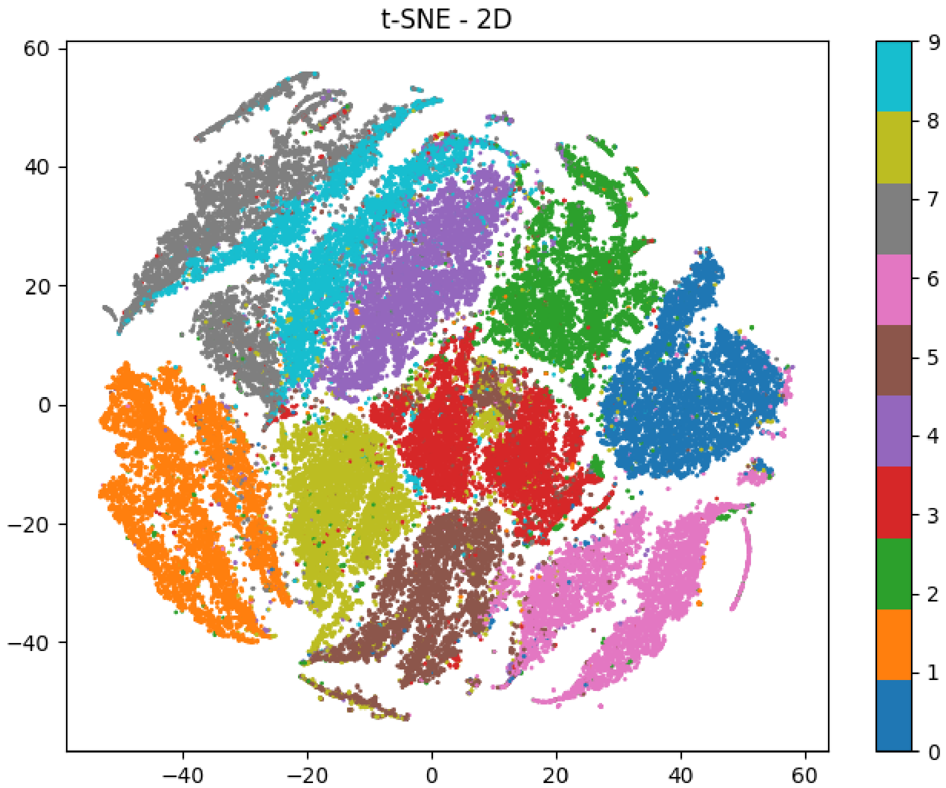

Figure 2: t-SNE 2D.

Complexity Traits:

- $O(n^2)$ memory and time; may use approximations.
- Excels at revealing local clusters; non-invertible.
- Sensitive to hyperparameters; non-deterministic with random initialization.

3.4 Hybrid PCA–t-SNE

To accelerate t-SNE, apply PCA to reduce dimensionality first.

1. Compute $Z_{50} = XU_{50}$ via PCA.
2. Run t-SNE on Z_{50} to obtain 2-D points y_i.

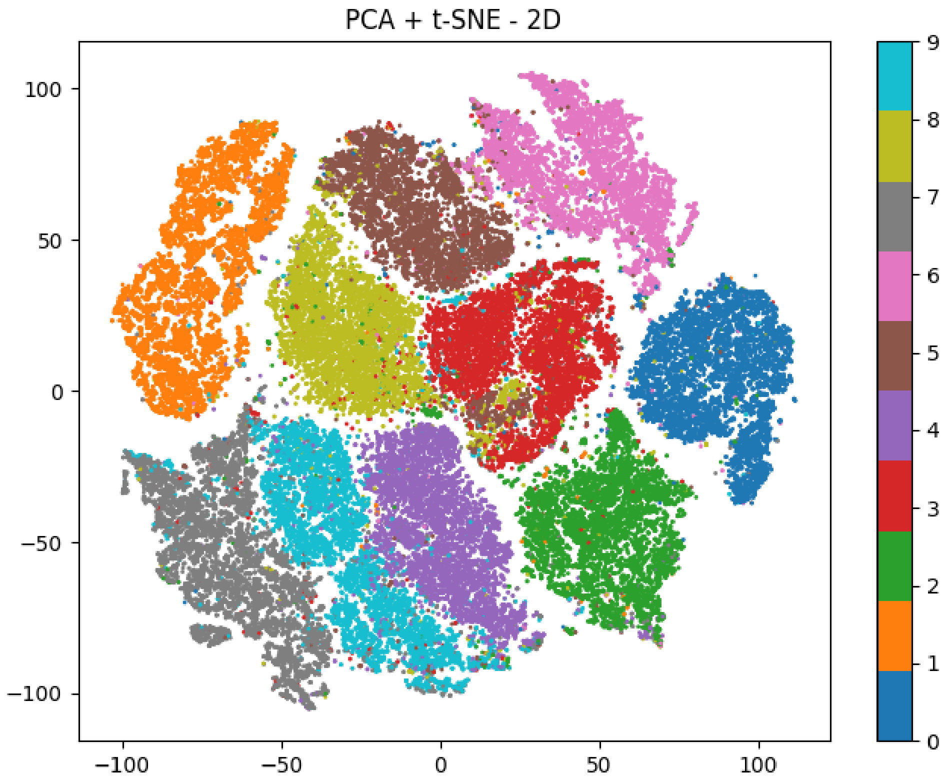

Figure 3: Hybrid PCA–t-SNE 2D

Advantages:

- Reduces computational load to $O(d^2n + d^3 + n \log n)$ with Barnes-Hut approximation.
- Retains strong cluster separation with faster runtime (t_{Hybrid}).

4 Results and Discussion

Detailed quantitative metrics (run time, silhouette score, reconstruction error) are summarized in Table 1. Figures 1–4 will illustrate the embeddings.

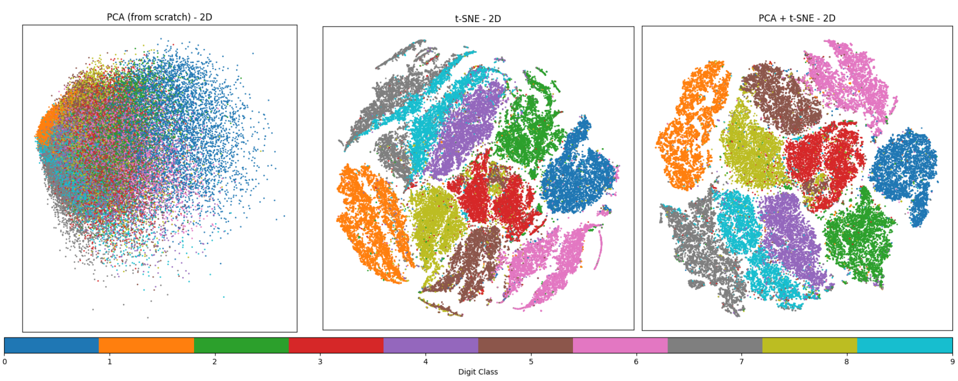

Figure 4: Hybrid PCA–t-SNE 2D

Method	Time (s)	Silhouette Score	Reconstruction Error
PCA (50-D)	t_{PCA}	S_{PCA}	E_{PCA}
t-SNE (2-D)	t_{TSNE}	S_{TSNE}	–
Hybrid PCA–t-SNE (2-D)	t_{Hybrid}	S_{Hybrid}	–

Table 1: Comparison metrics from the notebook.

5 Conclusions

PCA offers a fast, invertible linear reduction but may blur local clusters. T-SNE captures fine-grained structure at high cost and non-invertibility. The hybrid PCA–t-SNE strikes a practical balance, enabling effective visualization with reduced computation.

6 References

References

[1] A. Ranasinghe, ”Principal Component Analysis (PCA) with Code on MNIST Dataset,” Medium Blog, 2021. Available: `https://ranasinghiitkgp.medium.com/principal-component-analysis-pca-with-code-on-mnist-dataset-da7de0d07c22`

[2] A. Ranasinghe, ”t-SNE Visualization of High-Dimension MNIST Dataset,” Medium Blog, 2020. Available: `https://ranasinghiitkgp.medium.com/t-sne-visualization-of-high-dimension-mnist-dataset-48fb23d1bafd`