Data Mining: Term Paper

Topic: A Comparative Study of Dimensionality Reduction in High-Dimensional Data

1. Abstract

Dimensionality reduction is crucial for the study of high-dimensional data because it simplifies complex datasets, improves data visualization, and lowers computational requirements. Principal Component Analysis (PCA), T-Distributed Stochastic Neighbor Embedding (T-SNE), Linear Discriminant Analysis (LDA), and autoencoders are the four widely used dimensionality reduction techniques that are compared in this research. We assess each method's effectiveness in terms of computing efficiency, visual clarity, and knowledge retention using the MNIST dataset, which consists of handwritten digit images with over 750 features per sample. Our study illustrates the distinct benefits and drawbacks of each strategy, which helps us better understand the optimal machine learning application situations for each approach.

2. Table of Contents

e 3 e 4 -10
e 4 -10
-
e 10-17
e 18
e 18-19
•

3. Introduction

Traditional analysis techniques frequently find it difficult to keep up with the explosion of high-dimensional data in domains like computer vision, bioinformatics, and social network research. It becomes more difficult to store, process, and analyze data as it gets more complicated. The so-called "curse of dimensionality" postulates that the computational load and risk of overfitting in machine learning models increase with the number of features, which might make it challenging to identify significant patterns or insights in the data.

To overcome these obstacles, dimensionality reduction techniques are crucial. These techniques try to maintain a dataset's most important structures or patterns while reducing the number of characteristics in the dataset. Dimensionality reduction makes data easier to visualize by projecting it into a lower-dimensional space, which also increases computational efficiency and lowers the chance of overfitting. This makes it easier to find hidden linkages and patterns that might otherwise be overlooked.

Four widely used dimensionality reduction methods are compared in this paper: autoencoders, linear discriminant analysis (LDA), t-Distributed Stochastic Neighbor Embedding (t-SNE), and principal component analysis (PCA). Every approach has distinct advantages and works well with various kinds of data and analysis. While t-SNE is especially good at displaying high-dimensional data by maintaining local patterns, PCA, a linear approach, excels at retaining the most significant variance in the data. LDA maximizes separability across classes, which is very helpful in classification tasks. Conversely, autoencoders use neural networks to learn effective data representations and identify non-linear correlations.

For efficient analysis, researchers and practitioners need to use increasingly sophisticated tools as the amount and complexity of data continues to increase. By eliminating noise and superfluous features, dimensionality reduction not only simplifies data processing but also significantly improves machine learning model performance. Additionally, these methods offer insightful information about the fundamental structure of the data, which facilitates decision-making and raises forecast accuracy. This work attempts to advise the selection of the most relevant methodology based on dataset features and analysis objectives by comparing and comprehending the capabilities of techniques such as PCA, t-SNE, LDA, and autoencoders.

4. Related Work

"Dimensionality Reduction: A Comparative Review" by Postma and de Ridder

This review provides a comprehensive comparison of various dimensionality reduction techniques, discussing linear and non-linear methods. It explores approaches like Principal Component Analysis (PCA), Multidimensional Scaling (MDS), and non-linear methods such as t-SNE and Isomap, examining their strengths, weaknesses, and applications in handling high-dimensional data.

"Dimensionality Reduction and Classification through PCA and LDA " by Deshmukh Sachin

This paper offers an accessible introduction to PCA, breaking down its mathematical foundation and practical applications. It covers how PCA reduces dimensionality by transforming data to a lower-dimensional space while preserving maximum variance, making it useful in data visualization and noise reduction.

"Visualizing Data using t-SNE" by Laurens van der Maaten and Geoffrey Hinton

This paper introduces t-SNE, a non-linear technique particularly effective for visualizing high-dimensional data in two or three dimensions. It highlights t-SNE's ability to reveal clusters within complex data by preserving local structure, making it a popular tool in machine learning and data analysis.

"Evaluation of Dimensionality Reduction Techniques for Big Data" by Hemanth Kumar S. and Kumaravel A.

This paper provides an assessment of different dimensionality reduction techniques in the context of big data, specifically focusing on their scalability, accuracy, and suitability for high-dimensional datasets. It compares methods such as Principal Component Analysis (PCA), t-SNE, and autoencoders, discussing each technique's strengths and weaknesses when applied to large-scale data visualization and analysis. This comparative study helps in understanding which methods are best suited for retaining essential data structure in large datasets.

"Performance Evaluation of Dimensionality Reduction Techniques on High Dimensional Data" by Mandikal Vikram, Rakesh Pavan

This IEEE study assesses the effectiveness of dimensionality reduction techniques like PCA, t-SNE, and others when applied to high-dimensional data in big data contexts. The paper compares these methods based on scalability, accuracy, and suitability for retaining essential data structures, specifically in large datasets, making it valuable for understanding which methods are best for big data visualization and analysis.

5. Analysis of Dimensionality Reduction Techniques

5.1 Principal Component Analysis (PCA)

High-dimensional data can be transformed onto new, uncorrelated axes that capture the highest variance in the dataset using Principal Component Analysis (PCA), a conventional and popular linear dimensionality reduction technique. By determining the "principal components," or paths, along which the data varies the most, PCA reduces the number of features while keeping the most instructive elements of the original data. Data structures can be greatly simplified by this transformation, which minimizes information loss and facilitates visualization and analysis.

Mathematical Background

PCA reduces dimensionality while retaining as much information as feasible by projecting high-dimensional data onto a new set of axes that maximize variance. The following mathematical steps make up the process:

1. Centering the Data

Given a dataset X with n samples and p features, center the data by subtracting the mean of each feature:

$$X' = X - \mu$$
 where μ is the mean vector of X

Centering shifts the data to be centered around the origin, which is crucial for accurately computing the covariance matrix.

2. Covariance Matrix

The covariance matrix Σ of the centered data X' is calculated to understand the linear relationships between features. Each element in Σ represents the covariance between a pair of features:

$$\Sigma = (1 \div n - 1) X'T \times X$$

where:

- Σ (Sigma) is the covariance matrix.
- X' is the centered data matrix, meaning that each feature has been adjusted to have a mean of zero.
- X'T is the transpose of the centered data matrix X'.
- 'n' is the number of samples in the dataset.

3. Eigenvalues and Eigenvectors

To identify the principal components, we calculate the eigenvalues and eigenvectors of the covariance matrix Σ .

- Eigenvalues (λ): Represent the amount of variance explained by each principal component.
 Larger eigenvalues indicate components that capture more variance in the data.
- Eigenvectors (v): Define the direction of the principal components in the original feature space. Each eigenvector is associated with an eigenvalue, indicating its importance.

Mathematically, this can be expressed as:

$$\Sigma v = \lambda v$$

where λ is the eigenvalue and v is the corresponding eigenvector.

This equation indicates that multiplying an eigenvector v by Σ scales it by its eigenvalue λ , without changing its direction.

4. Selecting Principal Components

After calculating all eigenvalues and eigenvectors, we must sort the eigenvalues in descending order to identify the components that capture the most variance. Choose the top k eigenvectors corresponding to the largest k eigenvalues. These k eigenvectors form the principal components, defining a new subspace with reduced dimensionality.

5. Projection

To reduce the dimensionality of the original data, project it onto the new subspace defined by the selected principal components. Let W be the matrix containing the top k eigenvectors as columns. The projection of X' onto this new basis is given by:

$$Y = X' W$$

where Y is the transformed dataset in K-dimensional space.

This transformation preserves the essential variance in the data while reducing the number of dimensions, making it a powerful technique for data visualization.

Workflow

The following steps outline the workflow for PCA:

- 1. Input Data: Begin with the original high-dimensional dataset.
- 2. Data Centering: Center the data by subtracting the mean.

- 3. Covariance Matrix Calculation: Calculate the covariance matrix for the centered data.
- 4. Eigenvalue Decomposition: Perform eigenvalue decomposition to obtain eigenvalues and eigenvectors.
- 5. Component Selection: Sort and select the principal components based on eigenvalues.
- 6. Data Projection: Project the data onto the selected principal components for reduced dimensionality.

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

t-Distributed Stochastic Neighbor Embedding (t-SNE) is a non-linear dimensionality reduction technique particularly suited for visualizing high-dimensional data in two or three dimensions. Unlike linear methods such as PCA, t-SNE is designed to capture complex, non-linear relationships within data, making it highly effective for revealing clusters and substructures that traditional methods might miss. It is especially popular for exploring complex datasets, such as image or word embeddings, where clustering tendencies need to be emphasized.

Mathematical Background

T-SNE aims to preserve the local structure of data by keeping similar (neighboring) points close in a low-dimensional space.

- 1. High-Dimensional Similarity:
 - a. For each point pair in high-dimensional space, t-SNE calculates a similarity score using a Gaussian distribution. The similarity between two points, *pij*, is higher if the points are closer.
- 2. Low-Dimensional Similarity:
 - a. In the projected low-dimensional space, t-SNE calculates a new similarity score, qij, using a student's t-distribution. This distribution gives distant points low similarity, helping to spread out the points more naturally in the lower dimensions.

Workflow

The following steps outline the workflow for t-SNE:

- 1. Compute Pairwise Similarities in High Dimensions: Calculate pairwise probabilities in the original high-dimensional space based on Gaussian distributions.
- 2. Initialize Low-Dimensional Embedding: Initialize a random projection in a lower-dimensional space (often 2D or 3D).
- 3. Calculate Pairwise Similarities in Low Dimensions: Compute similarities in the low-dimensional embedding using a student's t-distribution.

- 4. Optimize with Gradient Descent: Iteratively adjust the positions in the low-dimensional space by minimizing the KL divergence between high-dimensional and low-dimensional similarity distributions.
- 5. Generate Final Low-Dimensional Map: Once convergence is achieved, the result is a low-dimensional representation of the data that captures its intrinsic clustering structure.

5.3 Linear Discriminant Analysis (LDA)

Linear Discriminant Analysis (LDA) is a supervised machine learning technique used for dimensionality reduction and classification. Unlike PCA, which focuses on maximizing the variance in the data, LDA maximizes the separability between different classes. It is useful when you have labeled data and want to reduce the number of features while maintaining the distinctiveness of each class. The goal is to project the data onto a lower-dimensional space in which the class separation is maximized.

Mathematical Background:

LDA works by optimizing the ratio of between-class variance to within-class variance. The main idea is to find a projection that maximizes class separability.

1. Within-Class Scatter Matrix S_w : Measures how much the data points within each class vary around their class mean.

$$S_w = \sum_{c=1}^{c} \sum_{x \in X_c} (x - \mu_c)(x - \mu_c)^T$$

2. Between-Class Scatter Matrix S_B : Measures how much the class means differ from the overall mean of the dataset.

$$S_B = \sum_{c=1}^{C} N_c (\mu_c - \mu)(\mu_c - \mu)^T$$

3. Maximizing the Class Separation: LDA finds the projection matrix *W* that maximizes the ratio:

maximize
$$\frac{\det(W^T S_B W)}{\det(W^T S_W W)}$$

This projection transforms the data into a new space where class separability is maximized.

Workflow

The following steps outline the workflow for LDA:

- 1. Compute Class Means
- 2. Compute Within-Class Scatter Matrix
- 3. Compute Between-Class Scatter Matrix
- 4. Solve for Eigenvalues and Eigenvectors
- 5. Select Top Eigenvectors
- 6. Project Data onto New Space

5.4 Autoencoders

Autoencoders are a type of artificial neural network used for unsupervised learning, particularly in dimensionality reduction. The goal of an autoencoder is to learn an efficient, compact representation (encoding) of input data by compressing it into a lower-dimensional space, then reconstructing the data back to its original form. This is achieved by training the network to minimize the reconstruction error between the input and the output. Autoencoders are useful for learning patterns in data, such as feature extraction, denoising, and reducing dimensionality.

Mathematical Background

1. Encoder

The encoder function f(x) maps the input data $x \in R^d$ to the lower-dimensional encoding $z \in R^k$. This is done through a transformation defined by weights W_1 and biases b_1 , typically using an activation function (e.g., ReLU):

$$z = f(x) = \sigma(W_1 x + b_1)$$

where:

$$W_1 \in R^{k \cdot d}$$

 $\sigma \in \text{is the activation function}$

2. Decoder

The decoder function g(z) reconstructs the original input $x' \in R^d$ from the encoding $z \in R^d$, using weights W_2 and biases b_2 :

$$x' = g(z) = \sigma(W_2 z + b_2)$$

where:

 $W_2 \in \mathbb{R}^{d \cdot k}$, is the weight matrix of decoder

$b_2 \in \mathbb{R}^d$ is the bias vector

3. Loss Function

The objective is to minimize the reconstruction error between the input and the reconstructed output x A common loss function used is Mean Squared Error (MSE).

4. Training

During training, the autoencoder network learns the weight matrices and bias vectors by minimizing the reconstruction error using optimization algorithms like Stochastic Gradient Descent (SGD) or Adam.

5. Dimensionality Reduction

Once trained, the encoder can be used to map high-dimensional input data to a lower-dimensional space z, which serves as the compressed representation of the original data.

Workflow

The following steps outline the workflow for Autoencoder:

- 1. Input Data: The raw data is fed into the encoder.
- 2. Encoder: The encoder processes the input and compresses it into a lower-dimensional representation (the bottleneck).
- 3. Bottleneck Layer: This layer holds the compressed version of the data, which is the most compact form that still retains key information.
- 4. Decoder: The decoder reconstructs the data from the compressed representation, aiming to produce an output as close as possible to the original input.

6. Application

6.1 Dataset Description

The MNIST dataset consists of gray-scale images of handwritten digits, ranging from 0 to 9. The dataset contains two main files: train.csv and test.csv.

- Image Dimensions: Each image is 28 pixels high and 28 pixels wide, resulting in a total of 784 pixels.
- Pixel Values: Each pixel has an integer value between 0 and 255, where 0 represents white and 255 represents black. These values correspond to the brightness or darkness of each pixel.

In the train.csv file:

- The first column, labeled "label", represents the digit (0-9) that corresponds to the handwritten image.
- The remaining 784 columns represent the pixel values for each image, named pixel0 through pixel783. Each pixel corresponds to the pixel at position x in the 28x28 image grid.

For simplicity, we have created 2 data frames X and y to store all the features and labels respectively.

Figure 1: Queries to understand the dataset

```
from sklearn.preprocessing import StandardScaler import pandas as pd import matplotlib.pyplot as plt from sklearn.decomposition import PCA

# Load MNIST dataset mnist = pd.read_csv("/content/train.csv")
#print(mnist.head())
#print(mnist.columns)

print("*"*100)
X = mnist.drop(columns=['label'])
y = mnist['label']

print(X.head(5))
print(y.head(5))
print("Shape of X :" , X.shape)
print("Shape of y :" ,y.shape)
```

Figure 2: Output screen after executing above queries

```
Fixels pixels pi
```

Observations:

- X is the feature matrix containing the pixel data for the images.
- 42000 represents the number of samples or images in the dataset.
- 784 is the number of features per sample, which corresponds to the total number of pixels in each 28x28 image (28 * 28 = 784).
- y is the target containing the labels for each image (0-9)
- 42000 indicates that there are 42,000 labels, one for each image in X.

6.2 Implementation of PCA

```
# Standardize the data
scaler = StandardScaler()
X_scaled = scaler.fit_transform(X)

# PCA (2D)
pca = PCA(n_components=2)
X_pca_2d = pca.fit_transform(X_scaled)

# PCA (3D)
pca = PCA(n_components=3)
X_pca_3d = pca.fit_transform(X_scaled)
```

We implemented PCA to reduce the dimensionality of the MNIST dataset and enable 2D and 3D visualization. We begin by identifying and removing constant features (those with zero variance) to eliminate redundant information. Next, we standardize the data so that each feature contributes equally, ensuring that PCA effectively captures the variance across features. Finally, we apply PCA to project the data into two and three dimensions, allowing us to visualize and explore underlying patterns and clusters while retaining the most significant variance in the dataset.

6.3 Implementation of T-SNE

```
# t-SNE (2D)
tsne_2d = TSNE(n_components=2, random_state=42, perplexity=30, n_iter=500)
X_tsne_2d = tsne_2d.fit_transform(X_scaled)

# t-SNE (3D)
tsne_3d = TSNE(n_components=3, random_state=42, perplexity=30, n_iter=600)
X_tsne_3d = tsne_3d.fit_transform(X_scaled)
```

In this code, we are applying t-Distributed Stochastic Neighbor Embedding (t-SNE) to reduce the original 784-dimensional MNIST dataset down to lower dimensions for visualization and analysis. Specifically, we perform two reductions: first to 2D (with n_components=2) and then 3D (with n_components=3).Parameters like perplexity (which controls the balance between local and global aspects) and n_iter (number of iterations) are tuned to optimize the visualization quality, with perplexity=30 helping manage the neighborhood size and n_iter ensuring convergence. By reducing from 784 dimensions to 2D and 3D, t-SNE allows us to visualize high-dimensional clusters and patterns that would otherwise be challenging to detect in the original dataset.

6.4 Implementation of LDA

```
# LDA (2D)
lda = LDA(n_components=2)
X_lda_2d = lda.fit_transform(X_scaled, y)

# LDA (3D)
lda = LDA(n_components=3)
X_lda_3d = lda.fit_transform(X_scaled, y)
```

In this code snippet, we perform dimensionality reduction using Linear Discriminant Analysis (LDA) to condense the original 784-dimensional input into both 3-dimensional and 2-dimensional spaces. The goal of LDA here is to project the data into a lower-dimensional space that maximizes the separability of the digit classes, guided by the labels provided in y.In the first step, LDA (2D), we project the data into two dimensions, creating a representation that is especially useful for visualization. Unlike PCA, which is unsupervised and aims to retain maximum variance without regard to class, LDA is a supervised method, focusing specifically on maximizing the distance between digit classes. By reducing from 784 dimensions to 2 or 3, we achieve a more interpretable dataset structure while retaining critical information in class. In the second step, LDA (3D), we specify three components, transforming the data into a 3D space that preserves class distinctions as much as possible, allowing us to explore how different digit classes are spread across three dimensions.

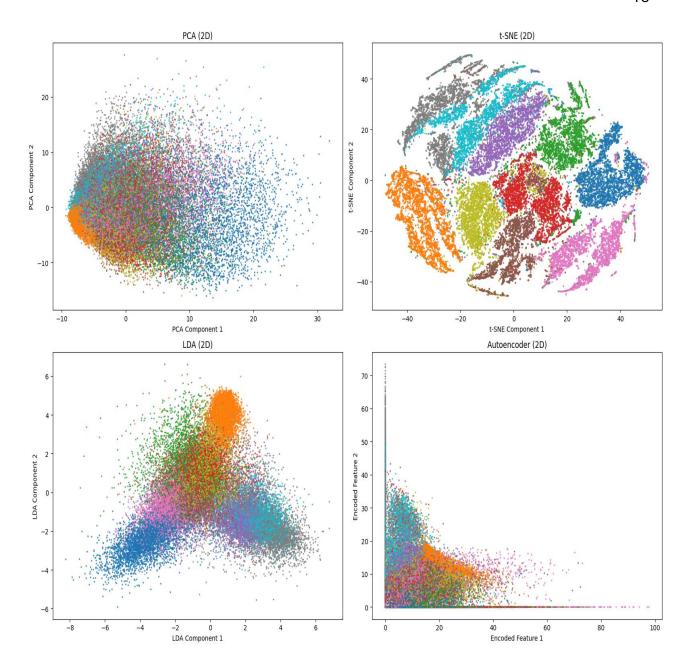
6.5 Implementation of Autoencoder

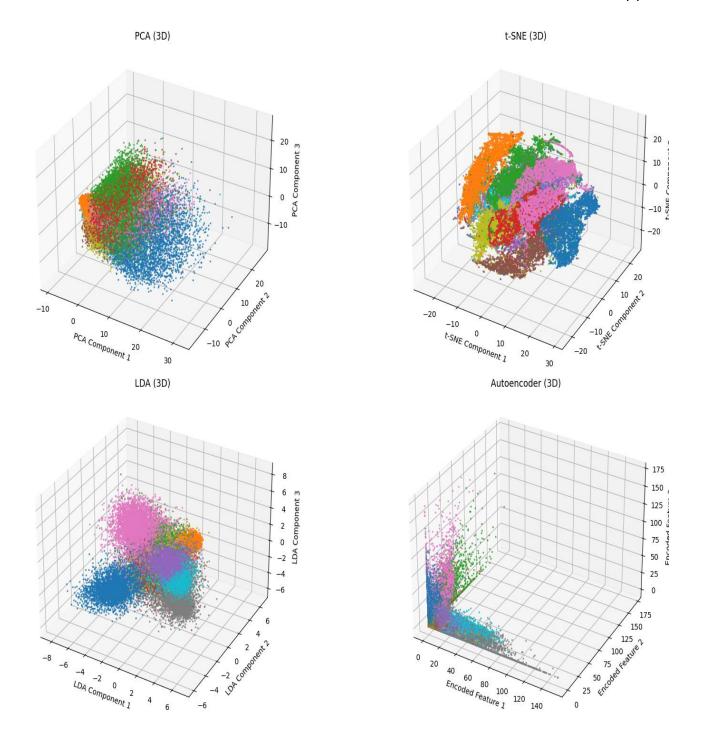
```
# Autoencoder (2D)
input_dim = X_scaled.shape[1] # Number of input features (784 for MNIST)
encoding_dim = 2 # Dimensionality for the encoding layer

input_layer = Input(shape=(input_dim,))
encoded = Dense(encoding_dim, activation='relu')(input_layer)
decoded = Dense(input_dim, activation='sigmoid')(encoded)
autoencoder = Model(input_layer, decoded)
encoder = Model(input_layer, encoded)
autoencoder.compile(optimizer='adam', loss='mse')
autoencoder.fit(X_scaled, X_scaled, epochs=50, batch_size=256, shuffle=True, validation_split=0.2)
X_autoencoder_2d = encoder.predict(X_scaled)
```

In this code, we implemented an autoencoder for dimensionality reduction using the MNIST dataset. The autoencoder consists of two parts: an encoder and a decoder. The encoder compresses the input data, reducing its dimensions to a specified size (2D or 3D in this case), while the decoder reconstructs the original data from the compressed form. We first trained the model with a 2-dimensional encoding (encoding_dim = 2) and then repeated the process with a 3-dimensional encoding (encoding_dim = 3). After training the autoencoder, we used the encoder to generate the reduced 2D and 3D representations of the original data.

6.6: Comparative Data Visualization of PCA, T-SNE, LDA and autoencoder in 2D





6.8 Comparision of accuracy after reducing 784 dimensions to 9 dimensions

We also tried reducing dimension to 9D to check which technique works better for MNIST Dataset.

We used all the above-mentioned techniques to train a logistic regression classifier and below is the analysis:

- LDA: Shows the highest accuracy of 88.24 %, as LDA is supervised and retains class-discriminative features.
- **PCA:** Performs similarly to the autoencoder of 78.30%, preserving variance in the data but not as class specific as LDA.
- **Autoencoder**: Performs reasonably well with 76.15% accuracy, as it preserves significant data structure in lower dimensions.
- T-SNE: It is computationally expensive to convert into lower dimensions using T-SNE. Due to the lack of memory, we decided to convert it into 2D which also took some time to process and achieved a very low classification accuracy of 42.5%, likely due to its unsuitability for high-dimensional reduction with a linear classifier since it is mainly a visualization tool.

6.9 Comparision of accuracy after reducing **784 dimensions to 9,50,100,200 dimensions** using PCA

```
PCA (50D) Classification Accuracy on Validation Data: 0.9011
PCA (9D) Classification Accuracy on Validation Data: 0.7830
Variance preserved with 50 components: 56.3588%
Variance preserved with 9 components: 26.8585%
PCA (100D) Classification Accuracy on Validation Data: 0.9146
Variance preserved with 100 components: 72.0968%
PCA (100D) Classification Accuracy on Validation Data: 0.9186
Variance preserved with 200 components: 87.9363%
```

We can observe that as the number of dimensions increases, variance is getting preserved more. Hence for 200D, variance preserved is 87.93%.

6.10: Comparision of accuracy after reducing **784 dimensions to 9,50,100,200 dimensions** using Autoencoder

```
Summary of Results (Accuracy and Reconstruction Errors):
                                  Train Reconstruction Error (MSE)
   Encoding Dimension Accuracy
0
                                                           0.721231
                       0.761905
1
                   50
                       0.900595
                                                           0.617557
2
                  100 0.916905
                                                           0.602225
3
                  200
                      0.925119
                                                           0.598040
  Validation Reconstruction Error (MSE)
0
                                 1.828591
1
                                 1.726254
2
                                 1.710927
3
                                 1.706581
```

We observed that as the encoding dimension increases from 9 to 200, the accuracy increases, and the reconstruction error on the training set decreases. This suggests that the autoencoder is learning better representations of the data with more encoding capacity.

The validation error reduces slightly with higher encoding dimensions but doesn't improve dramatically beyond 100. This suggests that increasing the encoding dimension further may lead to diminishing returns on generalization. If the validation error were to increase, that might indicate overfitting, where the model becomes too specialized to the training data.

7. Conclusion

In conclusion, this research demonstrates that the choice of dimensionality reduction method significantly affects classification accuracy. Supervised methods like LDA yield the highest accuracy by preserving class-discriminative features, while unsupervised methods like Autoencoders and PCA also show promising performance in capturing meaningful patterns in the data. T-SNE, being primarily a visualization tool, underperforms classification, highlighting the importance of aligning dimensionality reduction techniques with the objectives of the analysis.

For future research, the next steps could include:

- 1. Testing with Different Classifiers: Expanding the study to test these dimensionality reduction methods with a variety of classifiers (e.g., support vector machines, neural networks) could provide more insights into method compatibility with different models.
- Exploring Advanced Variants: Investigating advanced techniques like non-linear PCA, variational autoencoders, or discriminative t-SNE might reveal further gains in classification accuracy.
- 3. Applying to Different Datasets: Evaluating these methods on other high-dimensional datasets (e.g., medical imaging, genomics) would help generalize findings across various fields.
- 4. Parameter Tuning: Conducting hyperparameter optimization for each dimensionality reduction technique could uncover optimal configurations, enhancing performance.

8. References

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