Lecture 5: Unsupervised Learning and Dimensionality Reduction

Reference Material

This lecture is based on the content from the book *Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow, 2nd Edition* by Aurélien Géron:

- Chapter 8: Dimensionality Reduction
- Chapter 9: Unsupervised Learning Techniques
- Chapter 13: Loading and Preprocessing Data with TensorFlow

Learning Outcomes

- Understand the key principles of unsupervised learning and dimensionality reduction.
- Explore various unsupervised models and their evaluation metrics.
- Learn how to evaluate and preprocess image datasets for machine learning.

Unsupervised Learning: An Overview

Unsupervised learning aims to find hidden patterns or intrinsic structures in data without labeled outputs. Unlike supervised learning, there is no dependent variable. The primary objectives of unsupervised learning include:

- Clustering: Grouping similar data points together.
- Dimensionality Reduction: Reducing the number of features while retaining essential information.
- Density Estimation: Estimating the distribution of data points in a feature space.

Key Concepts

Dependent and Independent Variables

- In supervised learning, the dependent variable represents the output or target.
- In unsupervised learning, there are no dependent variables, only features (independent variables).

Evaluation Metrics

Unsupervised models do not use accuracy or loss directly. Instead, evaluation metrics include:

- **Silhouette Score:** Measures how similar a data point is to its cluster compared to other clusters.
- **Inertia (SSE):** Measures the sum of squared distances of samples to their closest cluster center (for clustering).
- **Reconstruction Error:** Used in PCA and autoencoders to measure how well the reduced data reconstructs the original data.
- **t-SNE Perplexity:** Indicates the balance between local and global structures in t-SNE visualizations.

Dimensionality Reduction

Dimensionality reduction techniques aim to simplify data while preserving its structure. Two major types include:

- **Feature Selection:** Choosing a subset of existing features.
- **Feature Extraction:** Transforming data into a lower-dimensional space.

Principal Component Analysis (PCA)

PCA is a linear dimensionality reduction technique that projects data onto orthogonal components to maximize variance.

- **Mathematical Formulation:**
$$\mathbf{Z} = \mathbf{X}\mathbf{W}$$
where $\mathbf{X}$ is the input data, $\mathbf{W}$ contains eigenvectors of the covariance matrix, and $\mathbf{Z}$ is the transformed data.
- **Explained Variance:** Measures how much of the total variance is captured by each principal component.

t-SNE (t-Distributed Stochastic Neighbor Embedding)

t-SNE is a non-linear dimensionality reduction technique used for visualization of high-dimensional data.

- **Mathematical Process:** Converts distances between data points into probabilities and minimizes the divergence between distributions.
- **Parameters:** Perplexity, learning rate, and number of iterations.

Unsupervised Models

Clustering Algorithms

- **K-Means:** Partitions data into k clusters to minimize intra-cluster variance.
- **Hierarchical Clustering:** Builds a tree of clusters based on data similarity.
- **DBSCAN:** Groups points based on density, handling noise and irregularly shaped clusters.

Autoencoders

Autoencoders are neural networks used for unsupervised learning.

- **Structure:** Encoder, bottleneck (latent space), and decoder.
- **Objective:** Minimize reconstruction loss.

Evaluation Metrics for Image Datasets

Evaluating unsupervised learning on image datasets requires:

- Visual inspection of clusters or embeddings.
- Quantitative metrics (e.g., silhouette score, adjusted Rand index).
- Reconstruction quality for dimensionality reduction techniques.

Applications of Unsupervised Learning

Clustering Applications

- Grouping satellite images by land cover.
- Segmenting customers in marketing data.

Dimensionality Reduction Applications

- Visualizing high-dimensional data in 2D or 3D.
- Preprocessing for supervised learning.

Summary of Modeling Approaches

Model	Best Suited For
PCA	Linear dimensionality reduction; data visualization.
t-SNE	Non-linear dimensionality reduction; visualizing complex patterns.
K-Means	Identifying spherical clusters.
DBSCAN	Detecting arbitrarily shaped clusters and outliers.
Autoencoders	Feature extraction; reconstructing complex data structures.