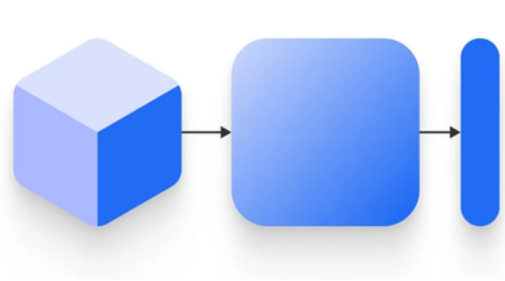
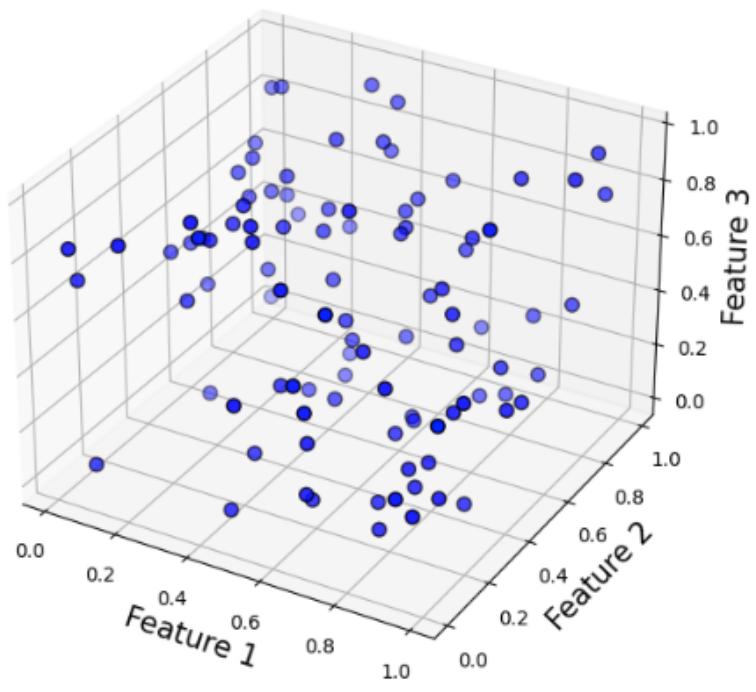
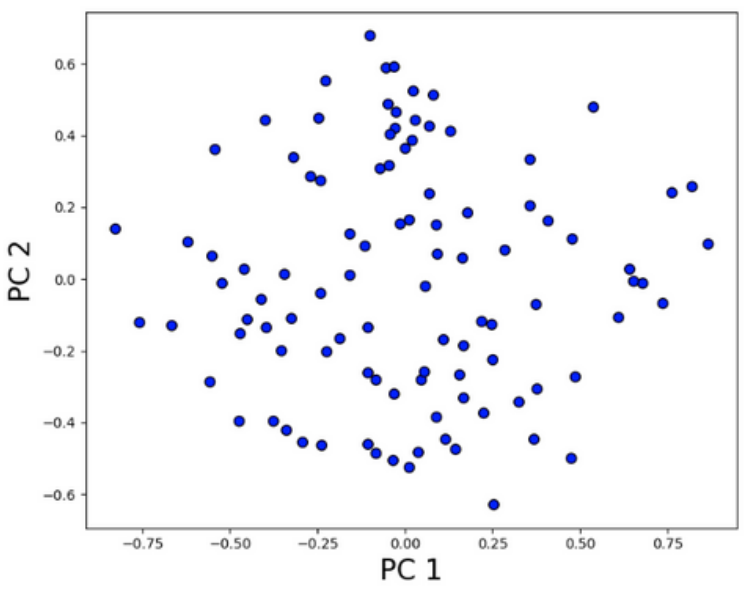
@shreyapatilu

Dimensionality Reduction Techniques



PCA, LDA, and KPCA Compared





Why do we need dimensionality reduction techniques?

- **Data simplification:** Reduces high-dimensional data to a more manageable form.
- **Sparsity reduction:** Creates a denser, more informative feature space.
- **Overfitting prevention:** Fewer features can lead to more generalizable models.
- **Improved visualization:** Allows high-dimensional data to be visualized in 2D or 3D.
- **Computational efficiency:** Reduces processing time and resource requirements.
- **Mitigates curse of dimensionality:** Addresses issues related to high-dimensional spaces.
- **Feature decorrelation:** Often produces less correlated features.
- **Noise reduction:** Can filter out less important variations in the data.
- **Enables advanced techniques:** Makes data more suitable for certain algorithms (e.g., kernel methods).

Potential drawbacks:

- New features may not have clear real-world meanings.
- Some methods can be intensive to compute.
- Some data characteristics may be lost in the process.

Three Fundamental Techniques

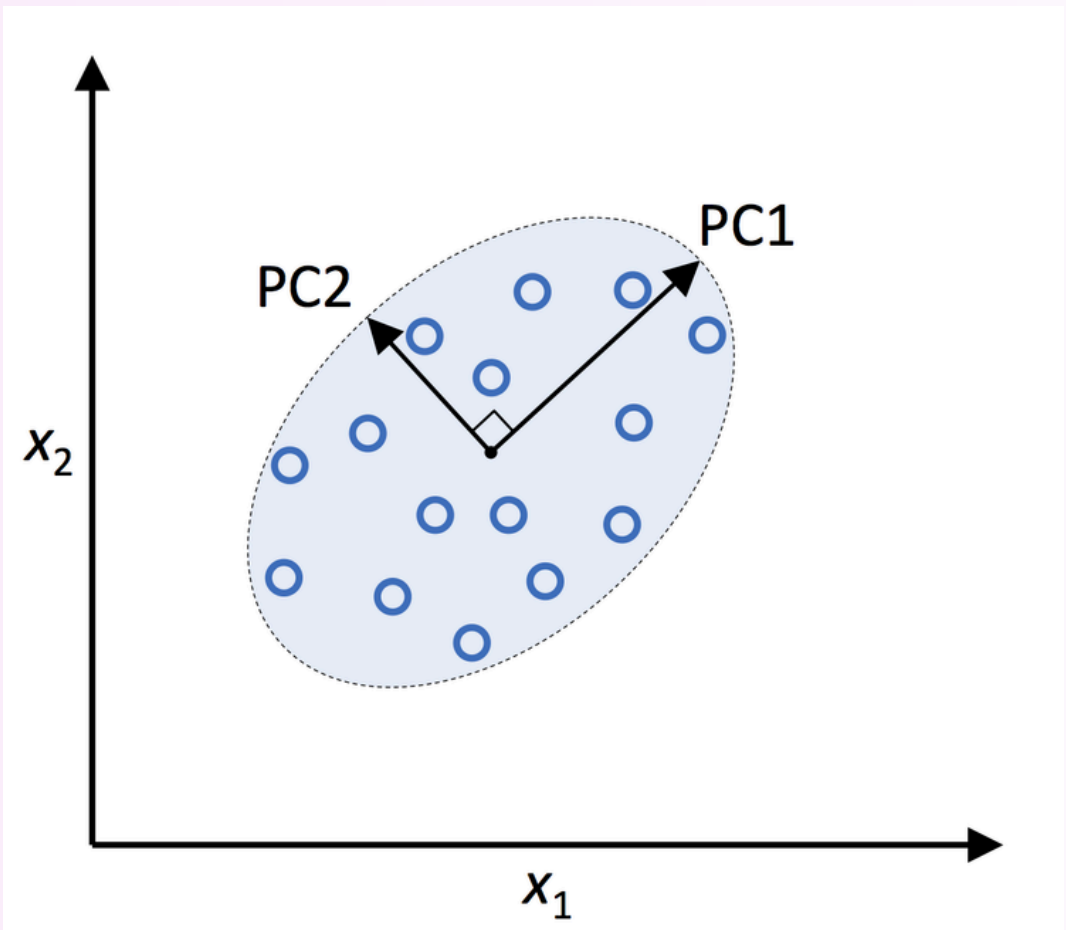
Feature	PCA	LDA	KPCA
Supervised/Unsupervised	Unsupervised	Supervised	Unsupervised
Linearity	Linear	Linear	Non-linear
Goal	Maximize variance	Maximize class separability	Maximize variance in higher-dimensional space
Class information	Not used	Used	Not used
Scalability	Moderate	Poor for high-dimensional data	Poor for large datasets
Interpretability	High	High	Low
Handles multicollinearity	Yes	Yes	Yes
Optimal for classification	No	Yes	No
Captures non-linear relationships	No	No	Yes
Requires parameter tuning	No	No	Yes (kernel selection)
Sensitive to feature scaling	Yes	Less sensitive	Depends on kernel

Principal Component Analysis (PCA):

PCA is an unsupervised dimensionality reduction technique used to transform high-dimensional data into a lower-dimensional space while preserving as much variance as possible.

Steps of PCA :

- Standardize the data
- Compute the covariance matrix
- Calculate eigenvectors and eigenvalues of the covariance matrix
- Sort eigenvectors by decreasing eigenvalues
- Choose top k eigenvectors as the new feature space
- Project the original data onto the new feature space



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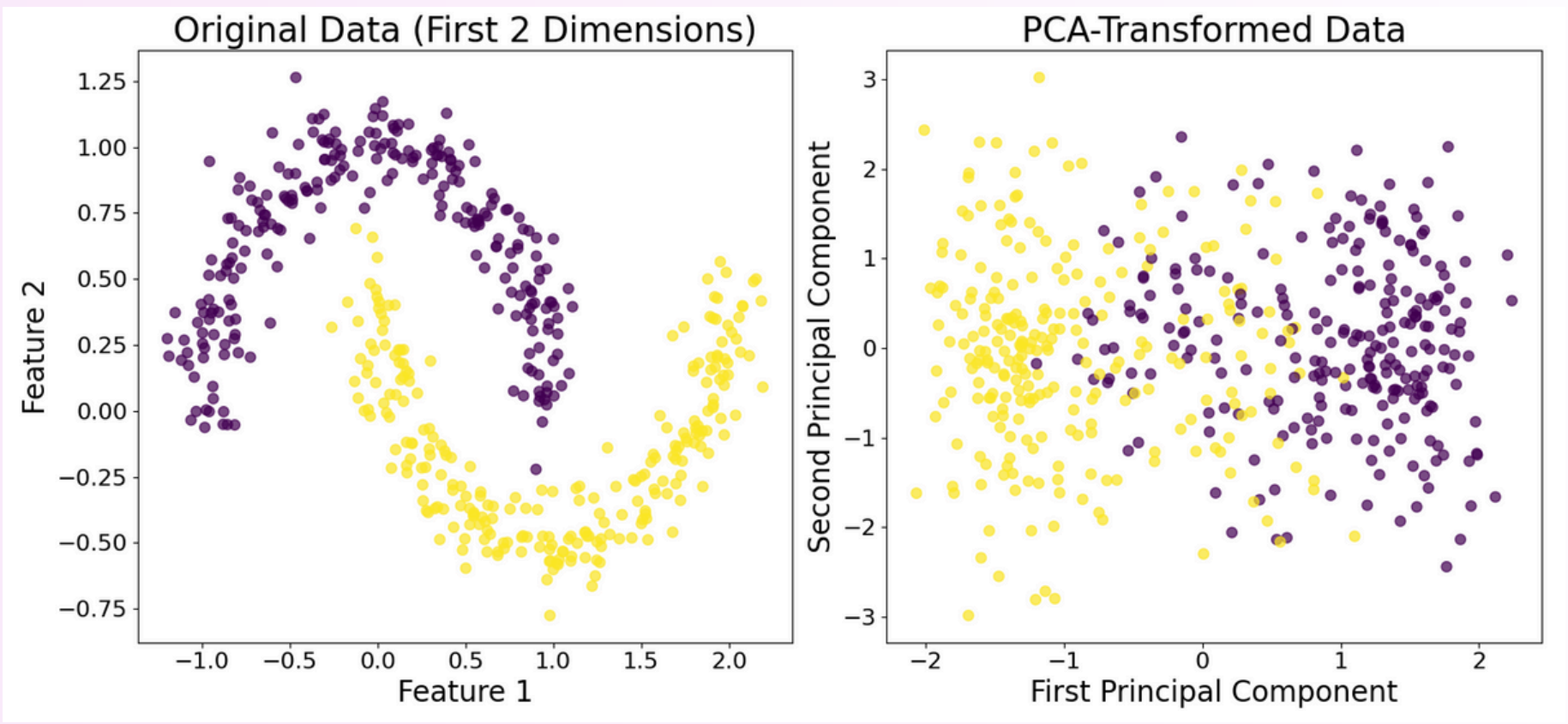
PCA finds orthogonal directions (principal components) in the feature space that capture the maximum variance in the data. It's particularly useful for visualization, noise reduction, and feature extraction.

```python
import numpy as np
import matplotlib.pyplot as plt
from sklearn.decomposition import PCA
from sklearn.datasets import make_moons
from sklearn.preprocessing import StandardScaler

# Generate complex dataset
def generate_data(n_samples=500):
    # Generate two interleaving moons
    X1, y1 = make_moons(n_samples=n_samples, noise=0.1)

    # Add some random noise dimensions
    noise_dims = np.random.randn(n_samples, 3) * 0.1
    X = np.hstack((X1, noise_dims))

    return X, y1

# Generate the data
X, y = generate_data(n_samples=500)

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

# Apply PCA
pca = PCA(n_components=2)
X_pca = pca.fit_transform(X_scaled)
```

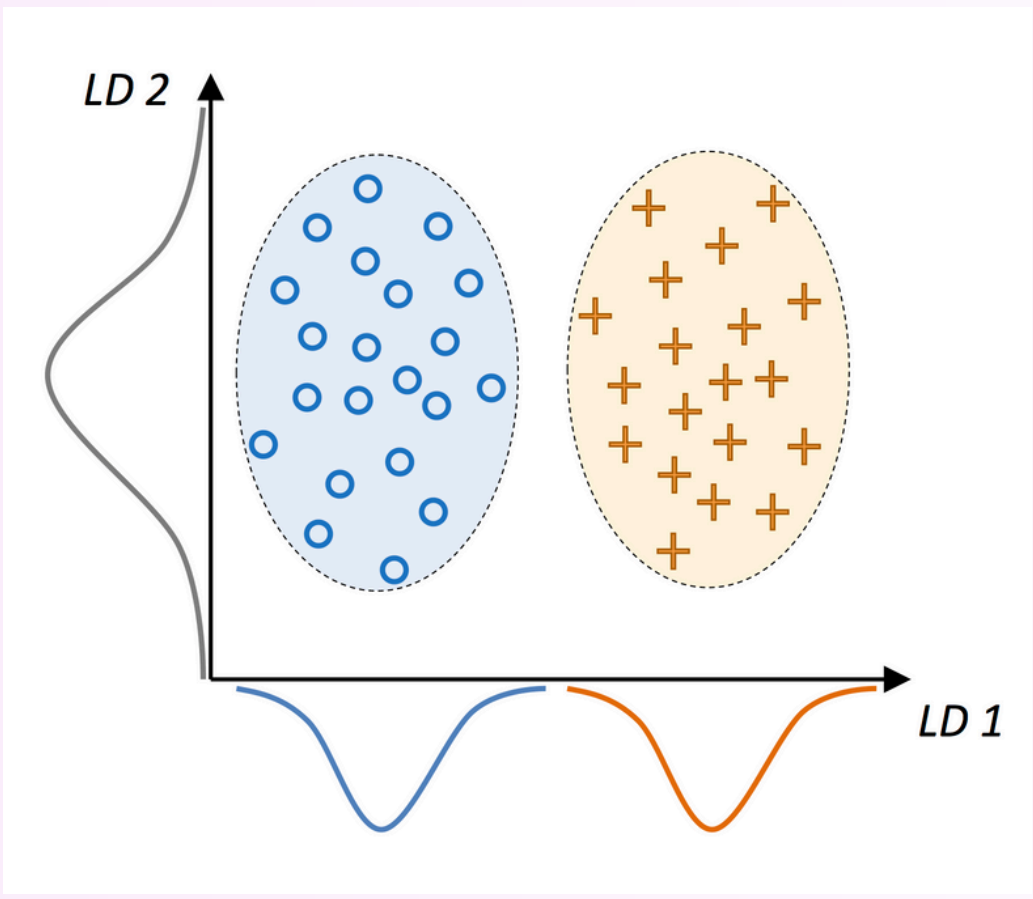


Linear Discriminant Analysis (LDA)

LDA is a supervised dimensionality reduction technique that aims to find a linear combination of features that best separates two or more classes.

Steps of LDA:

- Compute the mean vectors for each class
- Calculate the within-class and between-class scatter matrices
- Compute the eigenvectors and eigenvalues of the matrix product of the inverse within-class scatter matrix and the between-class scatter matrix
- Sort eigenvectors by decreasing eigenvalues
- Choose top k eigenvectors as the new feature space
- Project the original data onto the new feature space



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LDA maximizes the ratio of between-class variance to within-class variance, making it particularly useful for classification tasks.

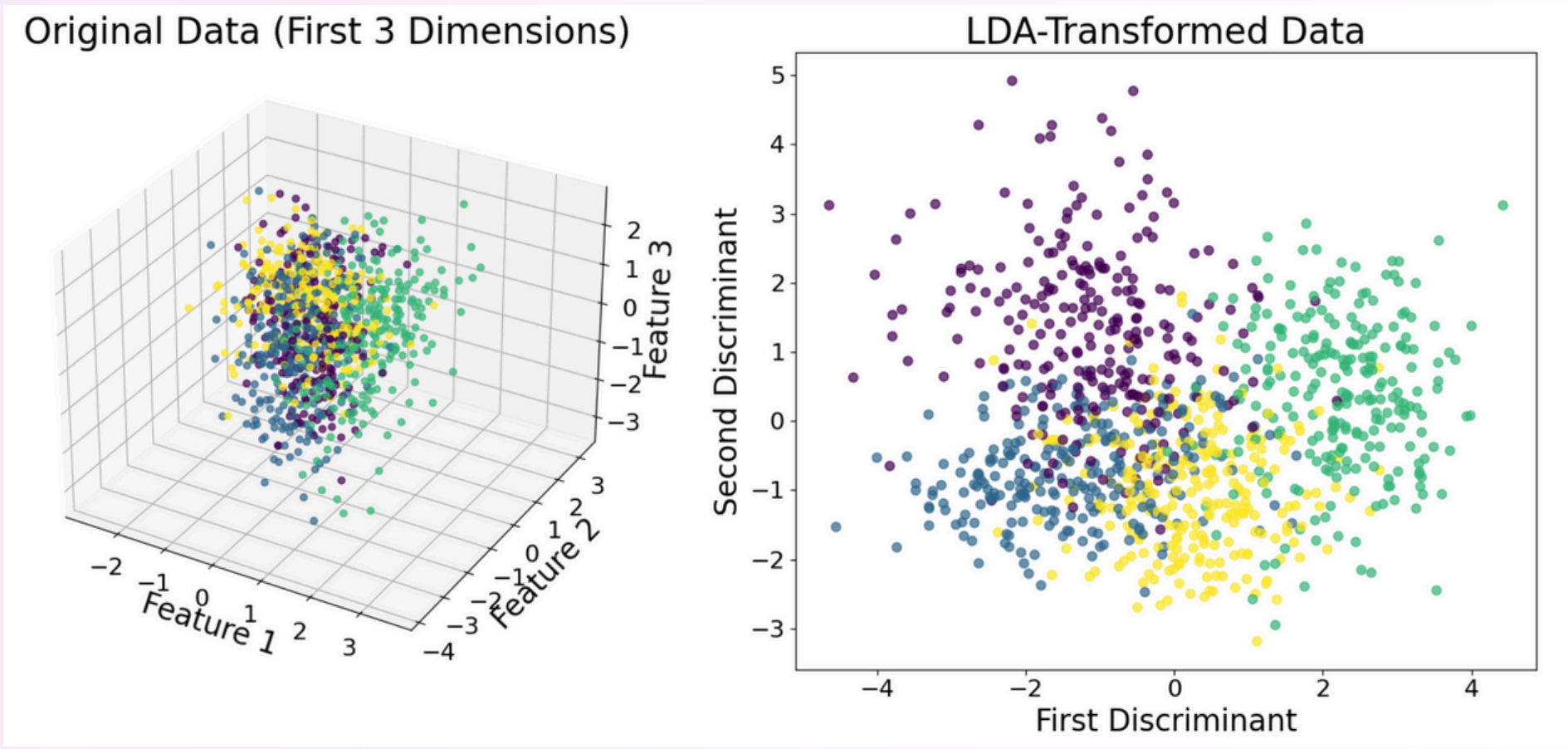
```
import numpy as np
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
from sklearn.discriminant_analysis import LinearDiscriminantAnalysis
from sklearn.datasets import make_classification
from sklearn.preprocessing import StandardScaler

# Generate complex dataset
def generate_complex_data_lda(n_samples=1000, n_features=20, n_classes=4):
    X, y = make_classification(n_samples=n_samples, n_features=n_features, n_classes=n_classes,
                               n_informative=10, n_redundant=5, n_repeated=3,
                               n_clusters_per_class=2, class_sep=1.5, random_state=42)
    return X, y

# Generate the complex data
X, y = generate_complex_data_lda(n_samples=1000)

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

# Apply LDA
lda = LinearDiscriminantAnalysis(n_components=2)
X_lda = lda.fit_transform(X_scaled, y)
```

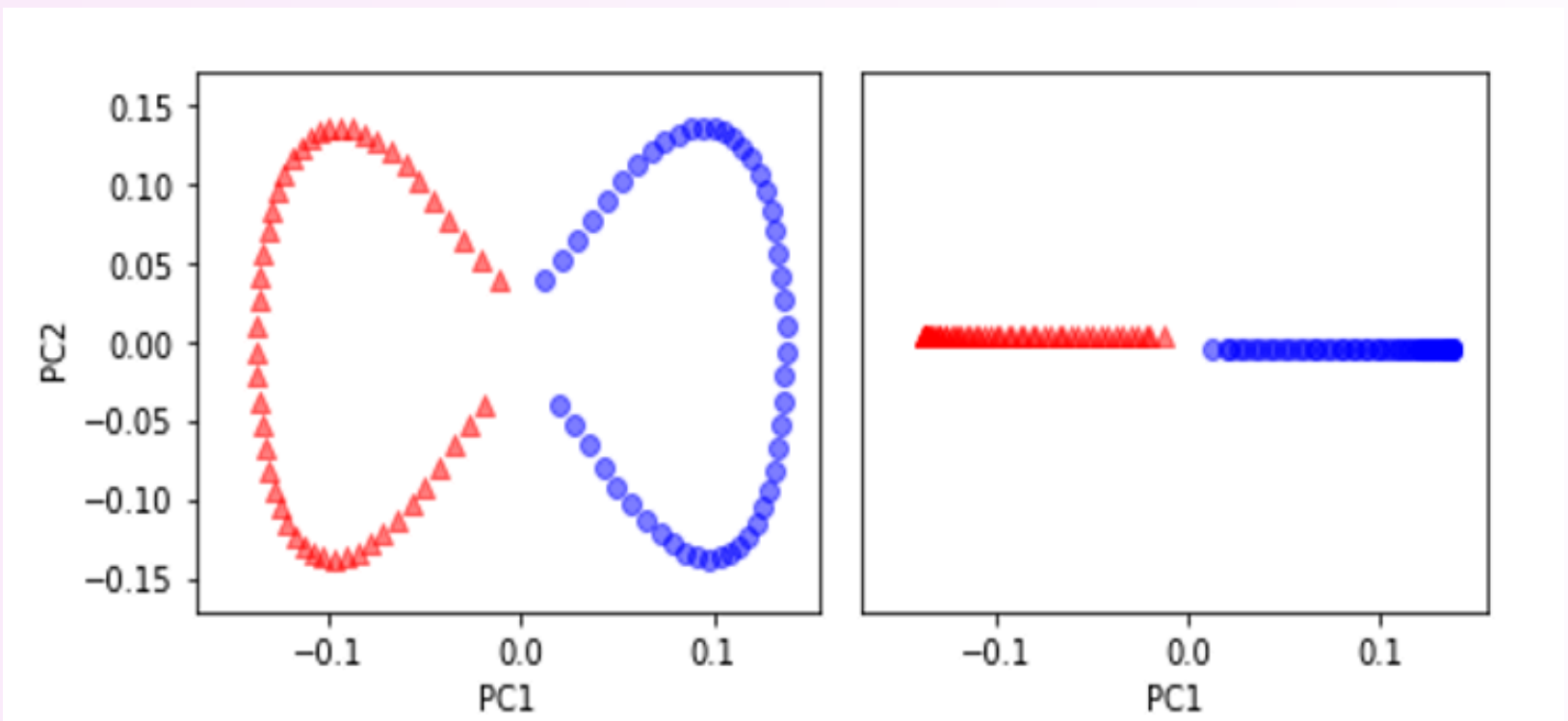


Kernel Principal Component Analysis (KPCA)

KPCA is a non-linear extension of PCA that uses kernel methods to perform dimensionality reduction in high-dimensional feature spaces.

Steps of KPCA:

- Choose a kernel function (e.g., Gaussian, polynomial)
- Compute the kernel matrix
- Center the kernel matrix
- Compute eigenvectors and eigenvalues of the centered kernel matrix Sort eigenvectors by decreasing eigenvalues
- Choose top k eigenvectors as the new feature space
- Project the original data onto the new feature space using the kernel trick



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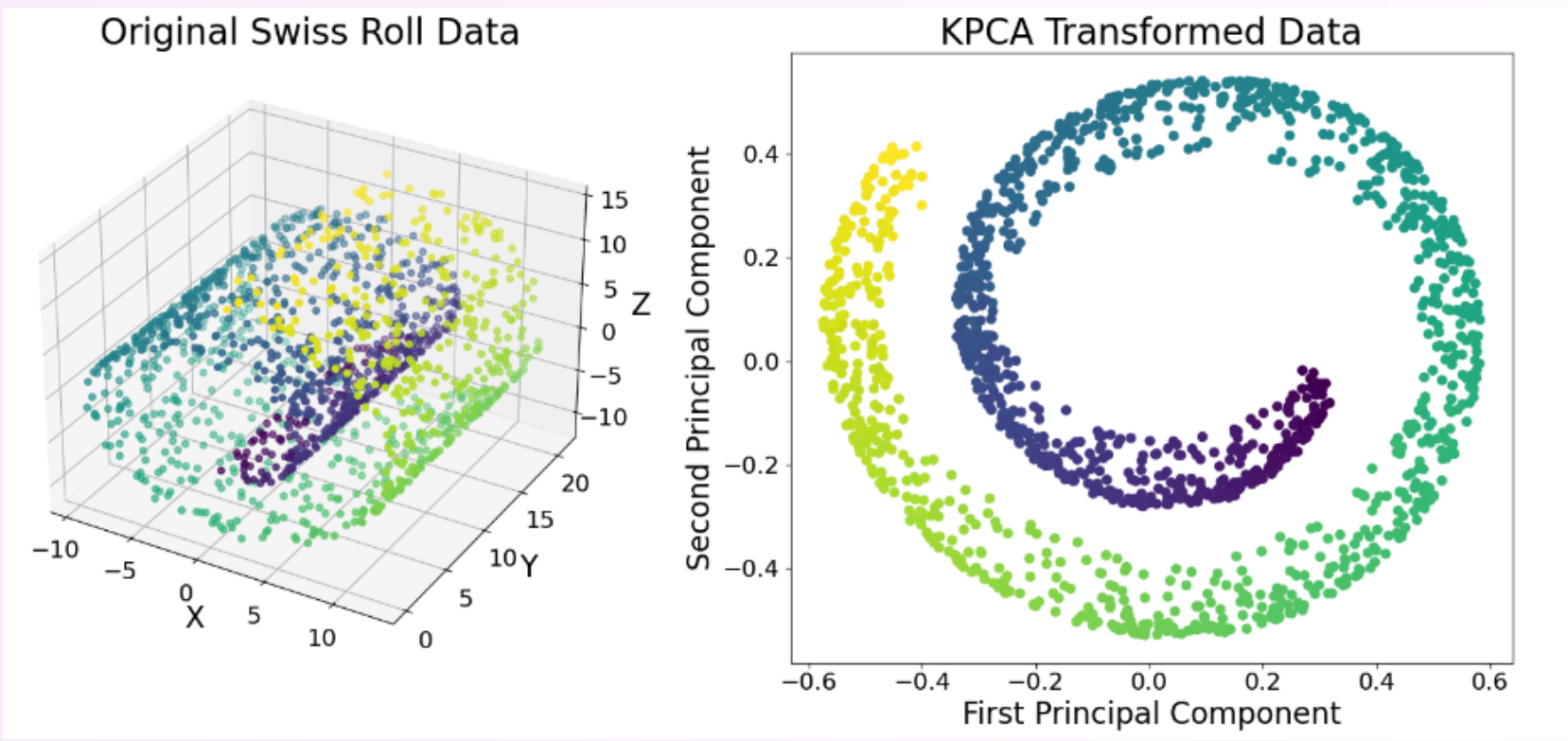
KPCA can capture non-linear relationships in the data, making it useful for datasets with complex structures that PCA might miss.

```python
import numpy as np
from sklearn.decomposition import KernelPCA
import matplotlib.pyplot as plt
from sklearn.datasets import make_swiss_roll
from mpl_toolkits.mplot3d import Axes3D

# Generate Swiss roll data
n_samples = 1500
noise = 0.05
X, color = make_swiss_roll(n_samples, noise=noise)

# Perform KPCA
kpca = KernelPCA(n_components=2, kernel='rbf', gamma=0.002)
X_kpca = kpca.fit_transform(X)
```



Resources

- Machine Learning with Python 3rd Edition, Chapter 5
- Hands-on Machine Learning with Scikit-Learn, Keras & TensorFlow, Chapter 8
- kernel-pca
- sklearn.decomposition.PCA
- GitHub Full Code