INT104 ARTIFICIAL INTELLIGENCE

LECTURE 3- DIMENSIONALITY REDUCTION

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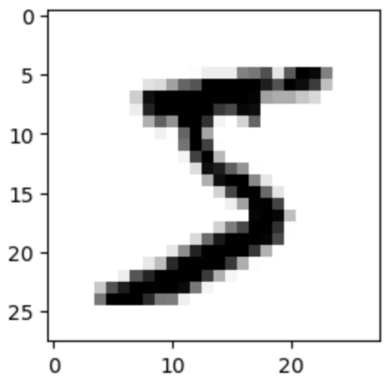
CONTENT

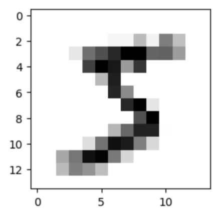
- Why need Dimensionality Reduction
- Principal Component Analysis (PCA)
- Locally Linear Embedding (LLE)
- Other Dimensionality Reduction Techniques

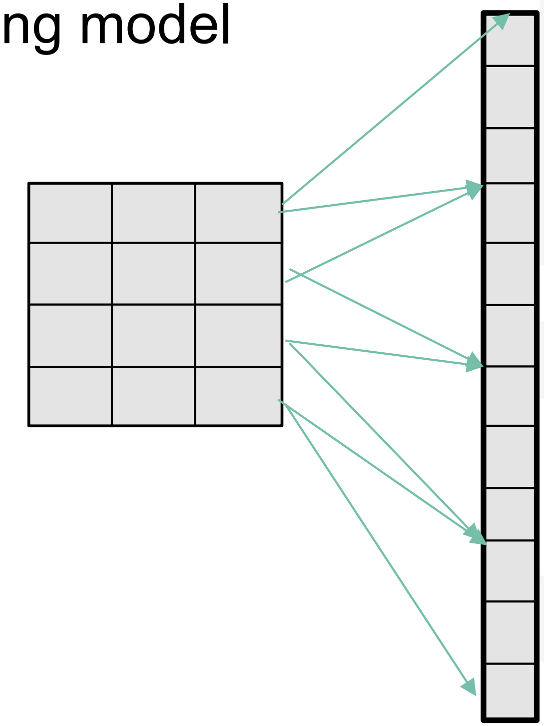
Dimensionality Reduction

Data with high dimensions:

- High computational complexity
- May contain many irrelevant or redundant features
- Difficulty in visualization
- With high risk of getting an overfitting model



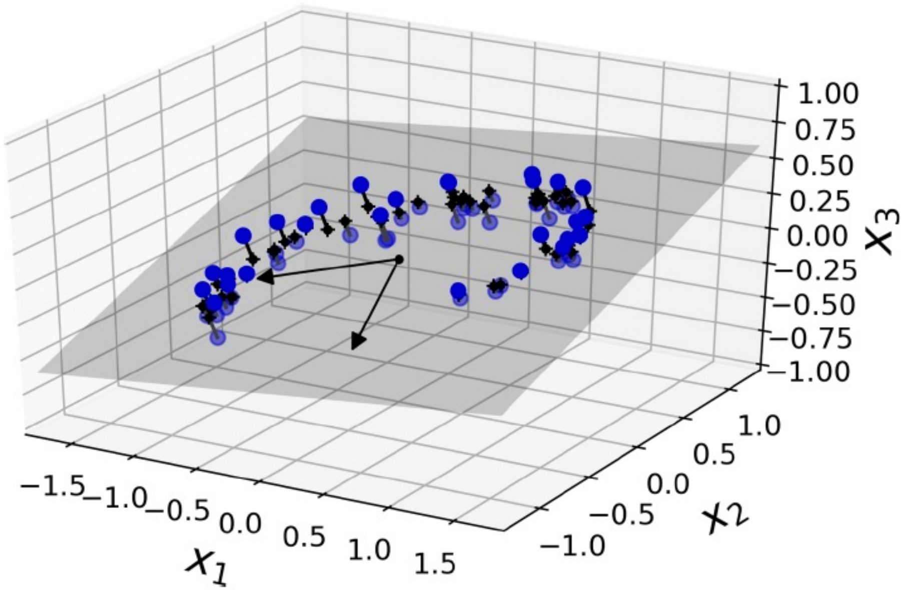


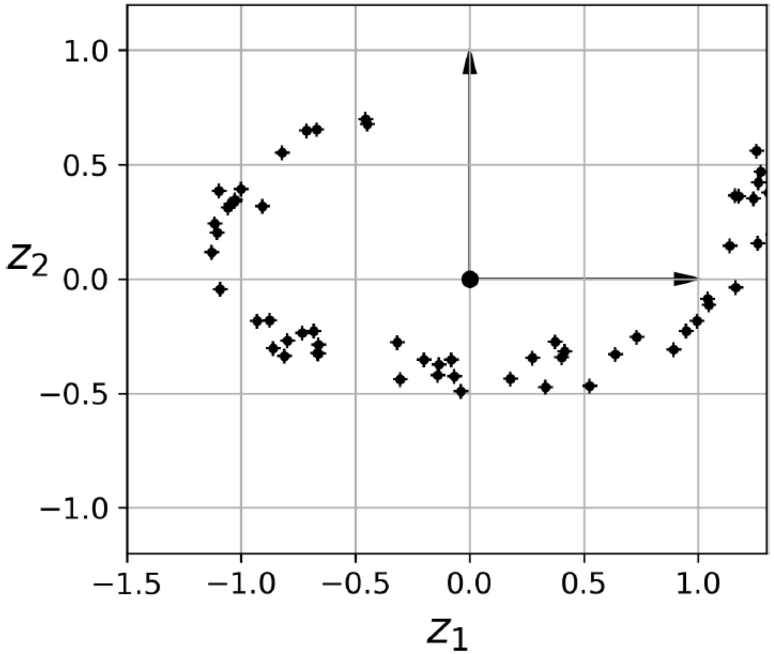


Approaches for Dimensionality Reduction

Projection:

- Data is not spread out uniformly across all dimensions. (All the data lies within (or close to) a much lower-dimensional subspace of the high-dimensional space.





Principal Component Analysis (PCA)

Preserving the Variance:

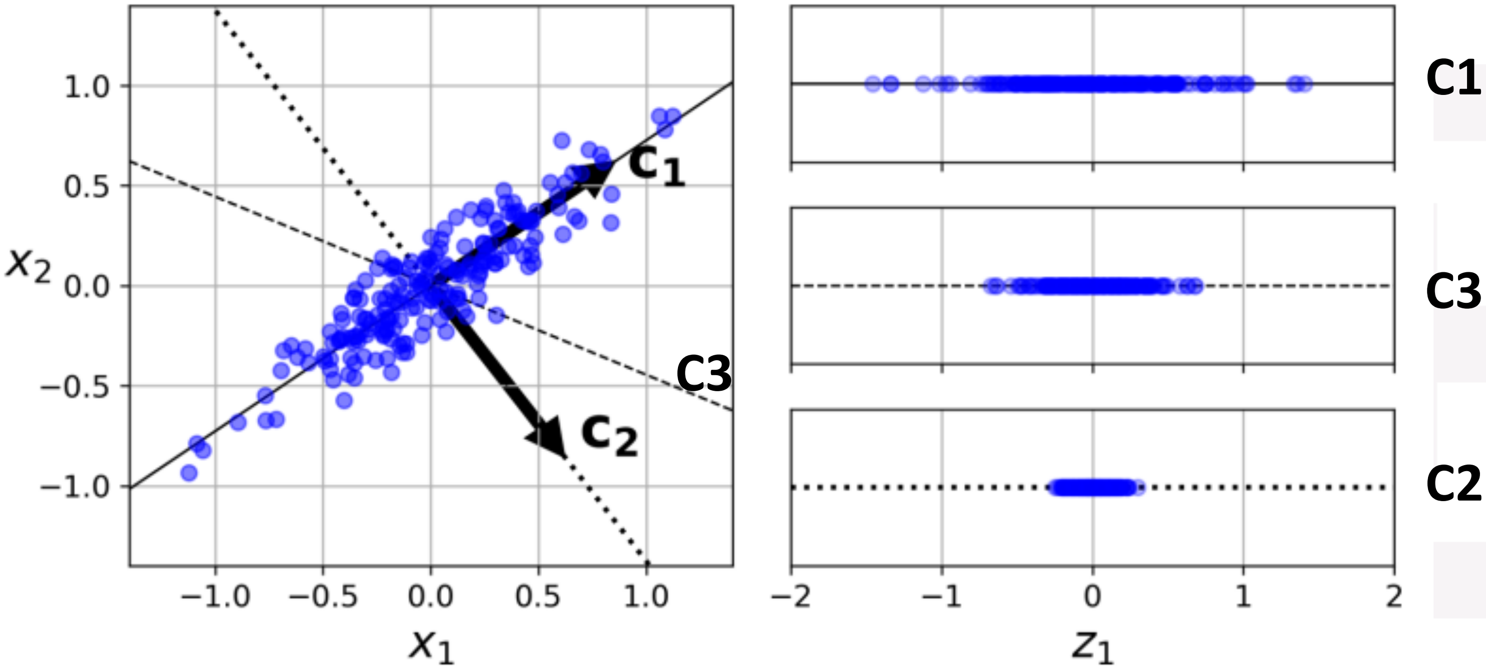


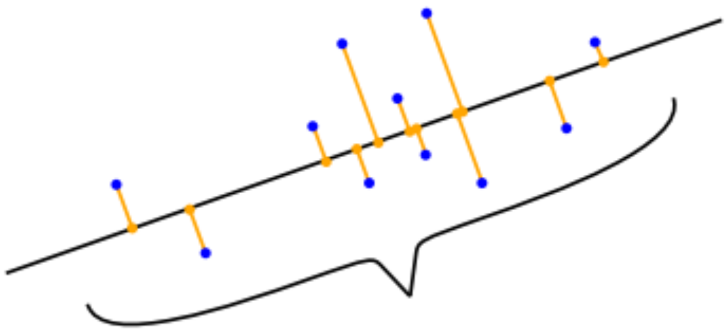
Figure 8-7. Selecting the subspace to project on

PCA identifies the axis that accounts for the largest amount of variance in the training set.

Principal Component Analysis (PCA)

-Variance on C1

$$V_1 = \frac{1}{M}\sum_{i=1}^{M}(\boldsymbol{c}_1^\intercal \boldsymbol{x}^{(i)})^2 = \frac{1}{M}\sum_{i=1}^{M}\boldsymbol{c}_1^\intercal \boldsymbol{x}^{(i)}\boldsymbol{x}^{(i)\intercal}\boldsymbol{c}_1 = \boldsymbol{c}_1^\intercal(\frac{1}{M}\sum_{i=1}^{M}\boldsymbol{x}^{(i)}\boldsymbol{x}^{(i)\intercal})\boldsymbol{c}_1$$
$$= \boldsymbol{c}_1^\intercal S \boldsymbol{c}_1$$



-Data covariance matrix

$$S = \frac{1}{M}\sum_{i=1}^{M}\boldsymbol{x}^{(i)}\boldsymbol{x}^{(i)\intercal}$$

- S is an N*N matrix, N is the number of features, M is the total number of data points.

Principal Component Analysis (PCA)

-Constrained optimization problem

$$\max_{\boldsymbol{c}_1} \boldsymbol{c}_1^{\intercal} S \boldsymbol{c}_1$$

subject to $||\boldsymbol{c}_1||^2 = 1$

-Lagrange equation $\mathcal{L}(\boldsymbol{c}_1, \lambda_1) = \boldsymbol{c}_1^{\intercal} S \boldsymbol{c}_1 + \lambda_1 (1 - \boldsymbol{c}_1^{\intercal} \boldsymbol{c}_1)$

-Solve this constrained optimization problem

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{c}_1} = 2S\boldsymbol{c}_1 - 2\lambda_1 \boldsymbol{c}_1 \qquad \frac{\partial \mathcal{L}}{\partial \lambda_1} = 1 - \boldsymbol{c}_1^{\intercal} \boldsymbol{c}_1$$

- Setting these partial derivatives to 0 gives us the relations:

$S\boldsymbol{c}_1 = \lambda_1 \boldsymbol{c}_1$ and $\boldsymbol{c}_1^{\intercal} \boldsymbol{c}_1 = 1$

- Variance on C1

$$V_1 = \boldsymbol{c}_1^{\intercal} S \boldsymbol{c}_1 = \lambda_1 \boldsymbol{c}_1^{\intercal} \boldsymbol{c}_1 = \lambda_1$$

Practice: PCA

Given a dataset that consists of the following points below:

A=(2, 3), B=(5, 5), C=(6, 6), D=(8,9)

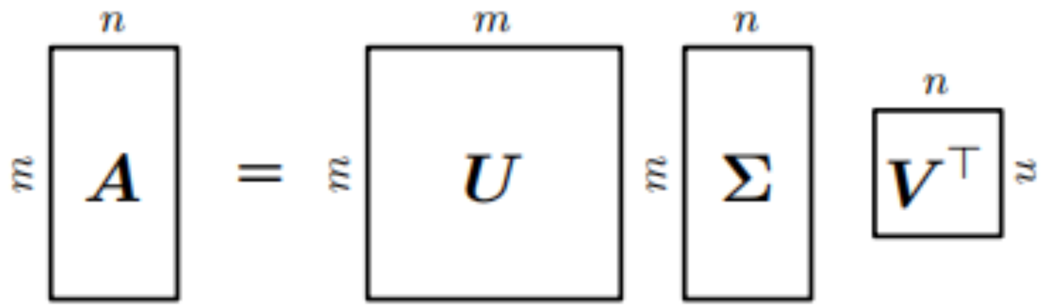
1. Calculate the covariance matrix for the dataset.

2. Calculate the eigenvalues and eigenvectors of the covariance matrix.

PCA

Singular Value Decomposition (SVD)

Theorem: Let $A \in R^{m*n}$ be a rectangular matrix of rank r ∈ [0, min(m, n)]. The SVD of A is a decomposition of the form



-$U \in R^{m*m}$ is an orthogonal matrix with column vectors $u_i, i = 1, \ldots m$,

- $V \in R^{n*n}$ an orthogonal matrix with column vectors $v_j, j = 1, \ldots n$.

- Σ is an m × n matrix with $\Sigma_{ii} = \sigma_i \geq 0$ and $\Sigma_{ij} = 0, i \neq j$

- $\boldsymbol{The\ singular\ value\ matrix\ \Sigma\ is\ unique}$

PCA

Singular Value Decomposition (SVD)

$$A = [x_1 \quad \cdots \quad x_n]_{m*n} = U\Sigma V^{\top} = [u_1 \quad \cdots \quad u_m]_{m*m} \begin{bmatrix} \sigma_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \sigma_n \\ 0 & \dots & 0 \\ \vdots & & \vdots \\ 0 & \dots & 0 \end{bmatrix}_{m*n} [v_1 \quad \dots \quad v_n]_{n*n}^{\top}$$

V contains the unit vectors that define all the principal components that we are looking for.

```
X_centered = (X - X.mean(axis=0))/X.std(axis=0)
U, s, Vt = np.linalg.svd(X_centered)
c1 = Vt.T[:, 0]
c2 = Vt.T[:, 1]
```

Principal Component Analysis (PCA)

Principal components matrix

$$\mathbf{V} = \begin{pmatrix} | & | & & | \\ \mathbf{c}_1 & \mathbf{c}_2 & \cdots & \mathbf{c}_n \\ | & | & & | \end{pmatrix}$$

$\boldsymbol{c}_1$, $\boldsymbol{c}_2$ … $\boldsymbol{c}_n$ are orthogonal

Projecting Down to d Dimension:

$$X_{d-proj} = XV_d$$

V_d is the first d eigen vectors of data covariance matrix

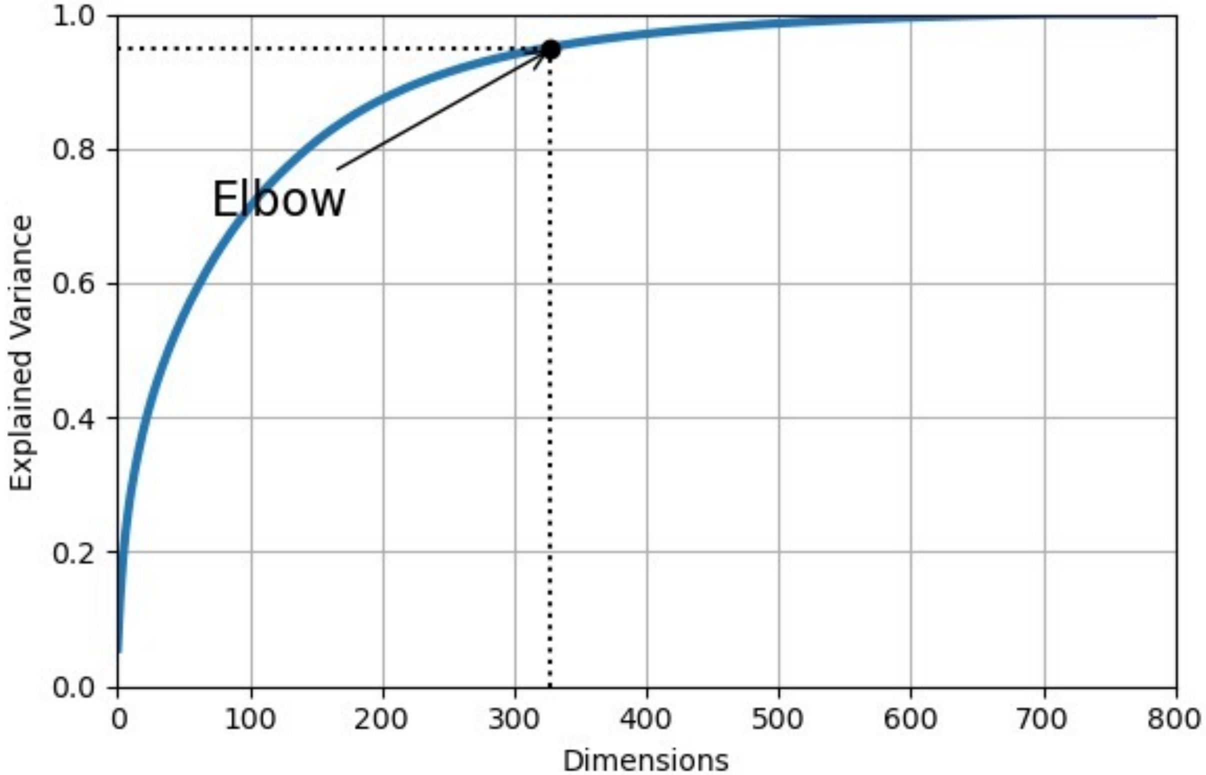
Explained Variance Ratio

$\frac{\lambda_1}{\lambda_1+\lambda_2 \ldots +\lambda_n}$ (eigenvalue/ total eigenvalue)

PCA

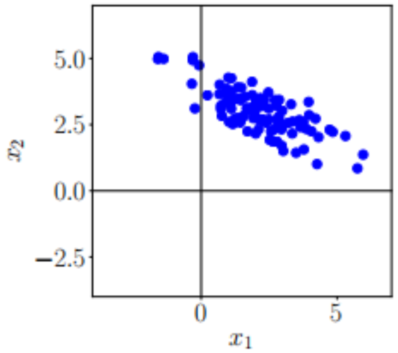
Choosing the Right Number of Dimensions:

- Choose the number of dimensions that add up to sufficiently large portion of the variance (e.g., 95%)
- $\frac{\lambda_1+\cdots+\lambda_d}{\lambda_1+\lambda_2\ldots+\lambda_n}$>95%

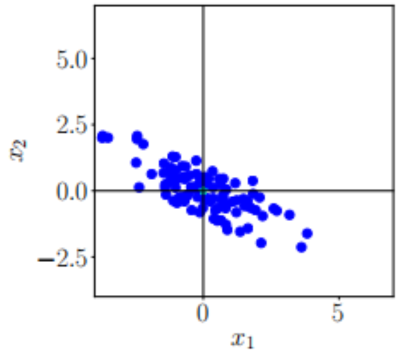


PCA

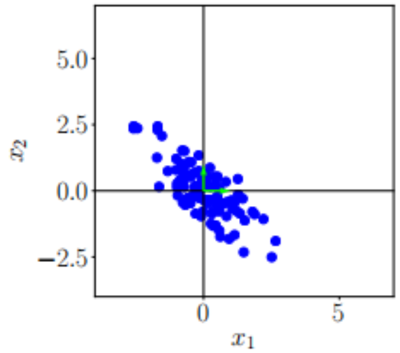
Key steps of PCA in practice



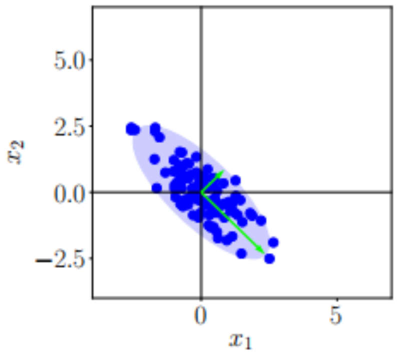
(a) Original dataset.



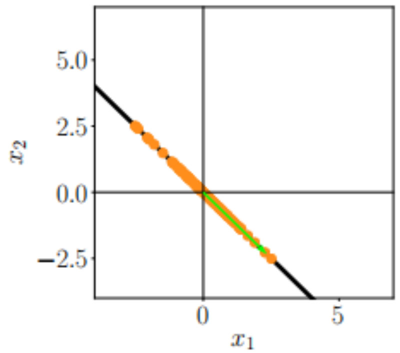
(b) Step 1: Centering by subtracting the mean from each data point.



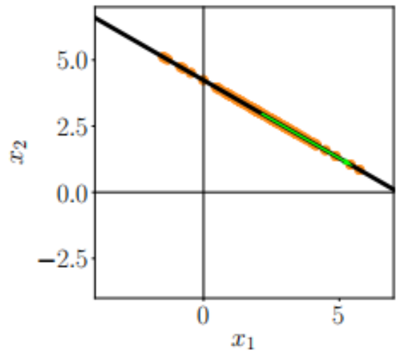
(c) Step 2: Dividing by the standard deviation to make the data unit free. Data has variance 1 along each axis.



(d) Step 3: Compute eigenvalues and eigenvectors (arrows) of the data covariance matrix (ellipse).



(e) Step 4: Project data onto the principal subspace.



(f) Undo the standardization and move projected data back into the original data space from (a).

PCA

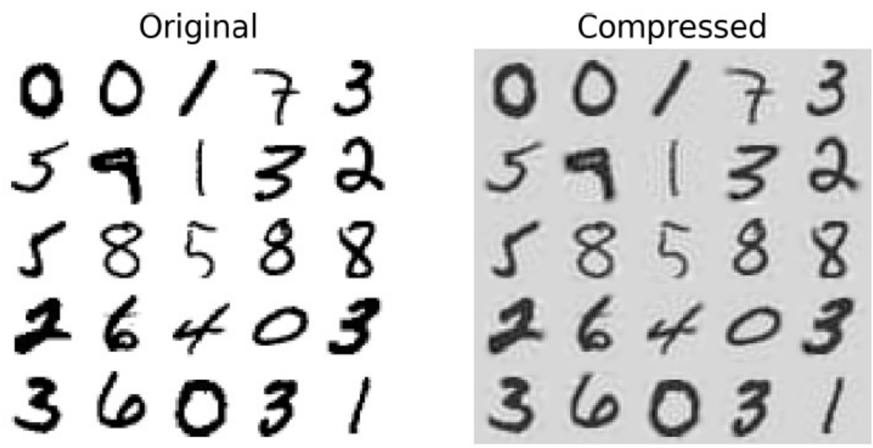
PCA for Compression

- Projecting Down to d Dimension

$$X_{d-proj} = XV_d$$

- PCA inverse transformation, back to the original number of dimensions

$$X_{recovered} = X_{d-proj}V_d^{\intercal}$$

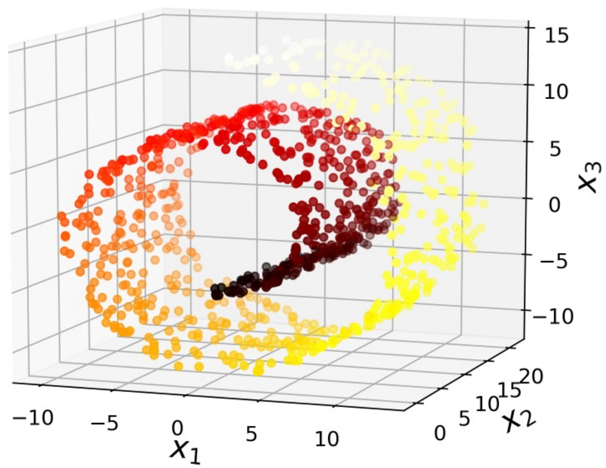


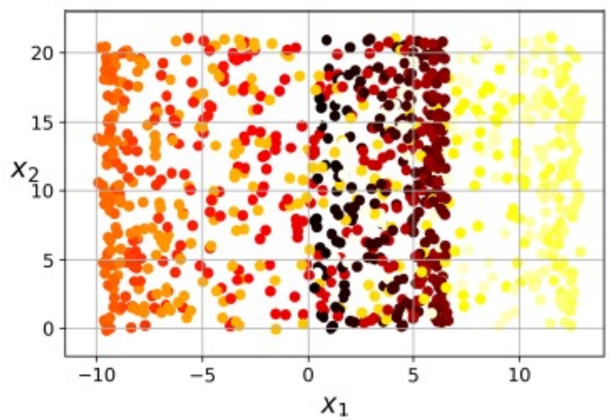
(Example MNIST data: 40% original size preserves 95% variance)

Approaches for Dimensionality Reduction

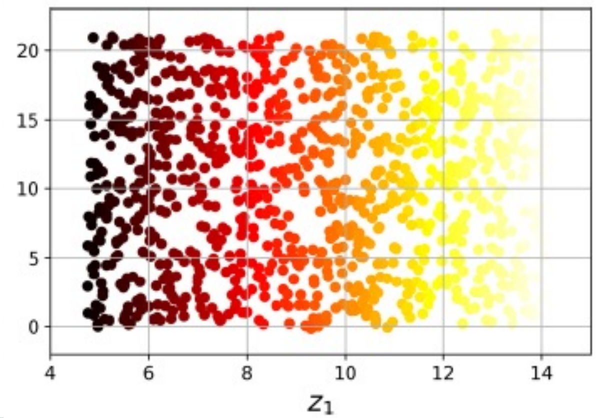
Manifold Learning

- Data lies on d-dimensional manifold is a part of an n-dimensional space (where d < n)





Simply projecting onto a plane



Unrolling the Swiss roll

Locally Linear Embedding (LLE)

LLE is a powerful *nonlinear dimensionality reduction* (NLDR) technique.
It is a Manifold Learning technique that does not rely on projections

Step one: Linearly modeling local relationships

$$\widehat{\mathbf{W}} = \underset{\mathbf{W}}{\operatorname{argmin}} \sum_{i=1}^{m} \left(\mathbf{x}^{(i)} - \sum_{j=1}^{m} w_{i,j} \mathbf{x}^{(j)} \right)^2$$

$$\text{subject to} \begin{cases} w_{i,j} = 0 & \text{if } \mathbf{x}^{(j)} \text{ is not one of the } k \text{ c.n. of } \mathbf{x}^{(i)} \\ \sum_{j=1}^{m} w_{i,j} = 1 & \text{for } i = 1, 2, \cdots, m \end{cases}$$

Step two: Reducing dimensionality while preserving relationships

$$\widehat{\mathbf{Z}} = \underset{\mathbf{Z}}{\operatorname{argmin}} \sum_{i=1}^{m} \left(\mathbf{z}^{(i)} - \sum_{j=1}^{m} \widehat{w}_{i,j} \mathbf{z}^{(j)} \right)^2$$

Locally Linear Embedding (LLE)

```
from sklearn.manifold import LocallyLinearEmbedding

lle = LocallyLinearEmbedding(n_components=2, n_neighbors=10)
X_reduced = lle.fit_transform(X)
```

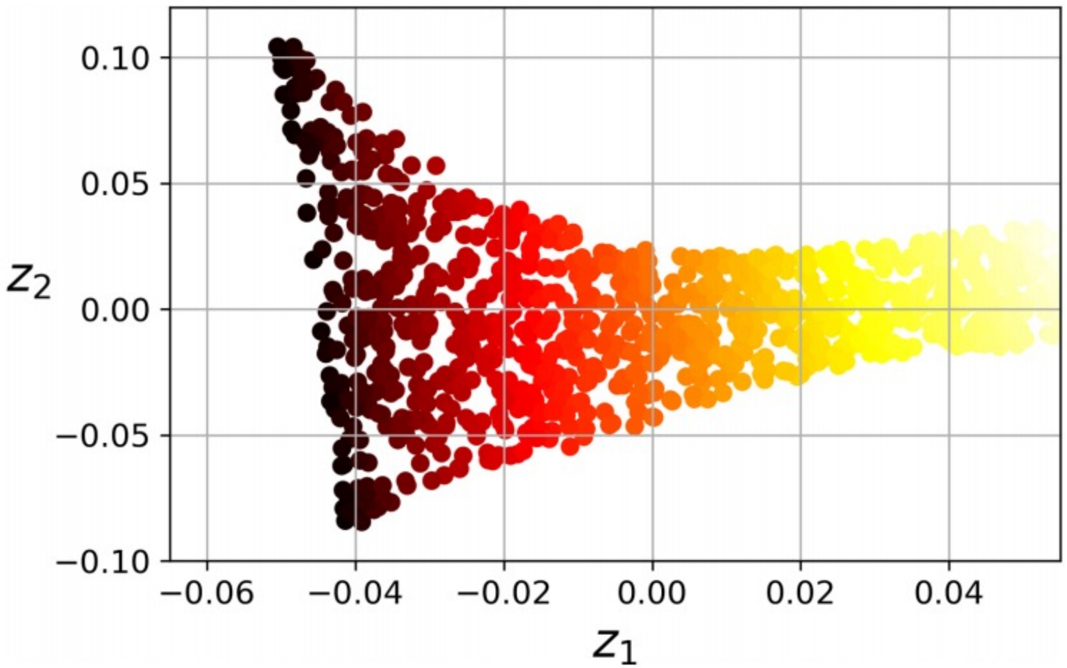


Figure 8-12. Unrolled Swiss roll using LLE

Other Techniques

- Multidimensional Scaling (MDS)

  Trying to preserve the distances between the instances.
- Isomap

  Trying to preserve the geodesic distances between the instances.
- t-Distributed Stochastic Neighbor Embedding (t-SNE)

  Trying to keep similar instances close and dissimilar instances apart.