

Dimensionality reduction

General idea

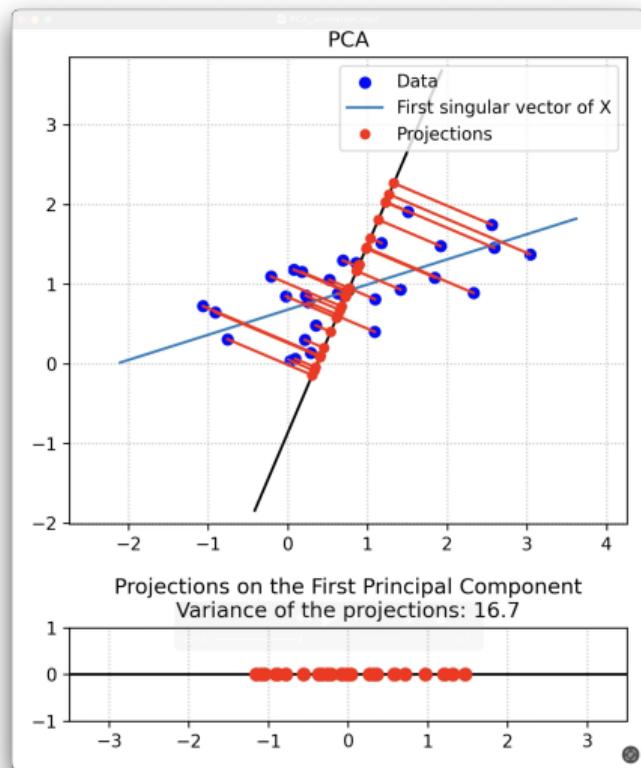
PCA

PCA optimization problem



The first component should be defined in order to maximize the projection variance. Suppose, we've already normalized the data, i.e. $\sum_i a_i = 0$, then sample variance will become the sum of all squared projections of data points to our vector $\mathbf{w}_{(1)}$, which implies the following optimization problem:

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since we are looking for the unit vector, we can reformulate the problem:

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It is known, that for the positive semidefinite matrix $\mathbf{A}^\top \mathbf{A}$ such vector is nothing else, but an eigenvector of $\mathbf{A}^\top \mathbf{A}$, which corresponds to the largest eigenvalue.

Algorithm derivation

So, we can conclude, that the following mapping:

$$\Pi_{n \times k} = A_{n \times d} \cdot W_{d \times k}$$

describes the projection of data onto the k principal components, where W contains first (by the size of eigenvalues) k eigenvectors of $A^\top A$.

Now we'll briefly derive how SVD decomposition could lead us to the PCA.

Firstly, we write down SVD decomposition of our matrix:

$$A = U \Sigma W^\top$$

and to its transpose:

$$\begin{aligned} A^\top &= (U \Sigma W^\top)^\top \\ &= (W^\top)^\top \Sigma^\top U^\top \\ &= W \Sigma^\top U^\top \\ &= W \Sigma U^\top \end{aligned}$$

Then, consider matrix AA^\top :

$$\begin{aligned} A^\top A &= (W \Sigma U^\top)(U \Sigma V^\top) \\ &= W \Sigma I \Sigma W^\top \\ &= W \Sigma \Sigma W^\top \\ &= W \Sigma^2 W^\top \end{aligned}$$

Which corresponds to the eigendecomposition of matrix $A^\top A$, where W stands for the matrix of eigenvectors of $A^\top A$, while Σ^2 contains eigenvalues of $A^\top A$.

At the end:

$$\begin{aligned} \Pi &= A \cdot W = \\ &= U \Sigma W^\top W = U \Sigma \end{aligned}$$

The latter formula provide us with easy way to compute PCA via SVD with any number of principal components:

$$\Pi_r = U_r \Sigma_r$$

Exercise 1

What could be wrong with this PCA?



Projections on the First Principal Component
Variance of the projections: 13.2

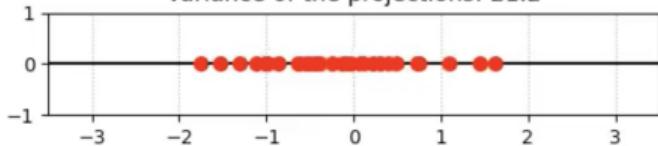


Exercise 2

What could be wrong with this PCA?



Projections on the First Principal Component
Variance of the projections: 21.2

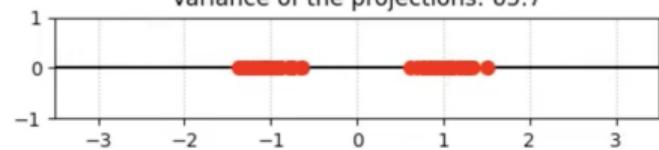


Exercise 3

What could be wrong with this PCA?



Projections on the First Principal Component
Variance of the projections: 65.7



Iris dataset variance



Iris dataset variance



Wine dataset variance



PCA on MNIST

2D PCA of MNIST



Other methods

t-SNE

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is a nonlinear dimensionality reduction technique
particularly well-suited for visualizing high-dimensional
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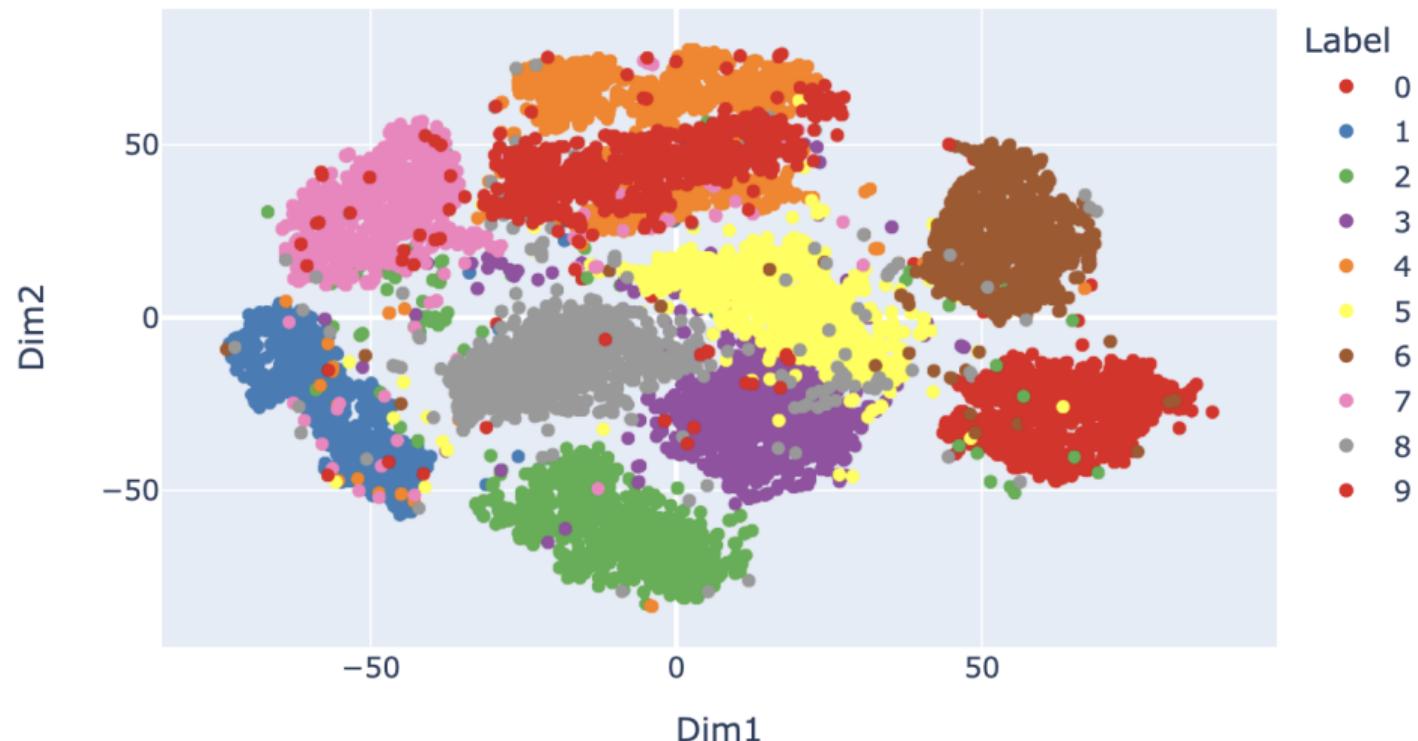
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- **Computational Complexity:** Can be slow for large datasets due to pairwise computations.
- **Random Initialization:** Different runs may yield different results; multiple runs can help validate findings.

t-SNE on MNIST

2D t-SNE of MNIST



UMAP

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- **Minimum Distance (min_dist):** Dictates how tightly points are packed in the low-dimensional space.

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2D UMAP of MNIST

