

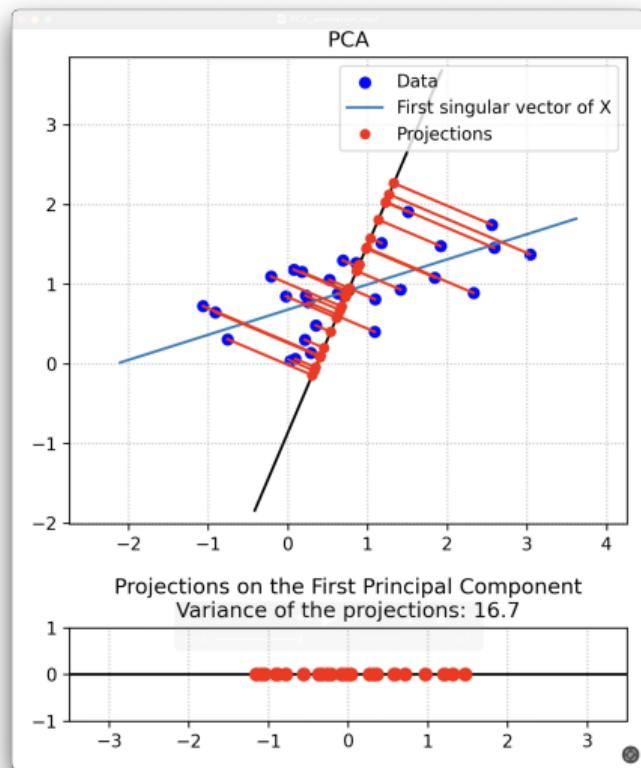


## Dimensionality reduction

## General idea

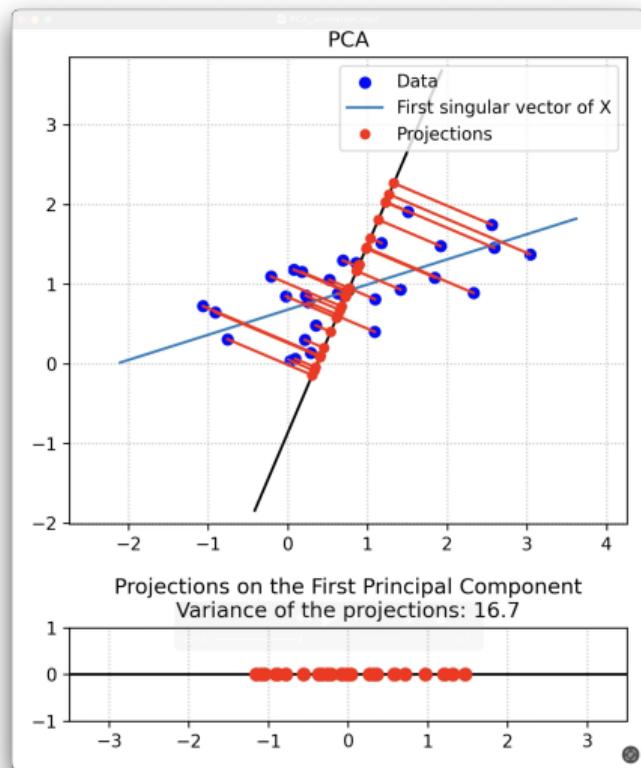
# PCA

## 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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$$\mathbf{w}_{(1)} = \arg \max_{\|\mathbf{w}\|=1} \left\{ \sum_i (\mathbf{a}_{(i)}^\top \cdot \mathbf{w})^2 \right\}$$

or

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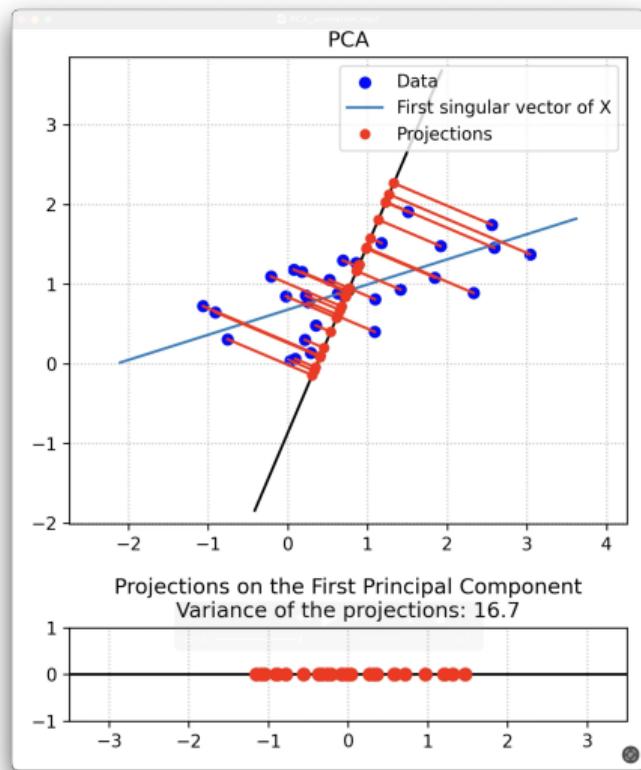
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since we are looking for the unit vector, we can reformulate the problem:

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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  $\Sigma^2$  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?

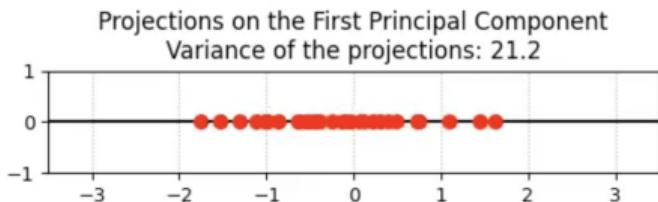


Projections on the First Principal Component  
Variance of the projections: 13.2



## Exercise 2

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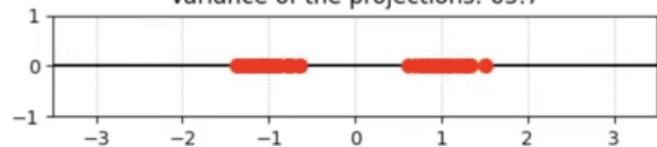


## Exercise 3

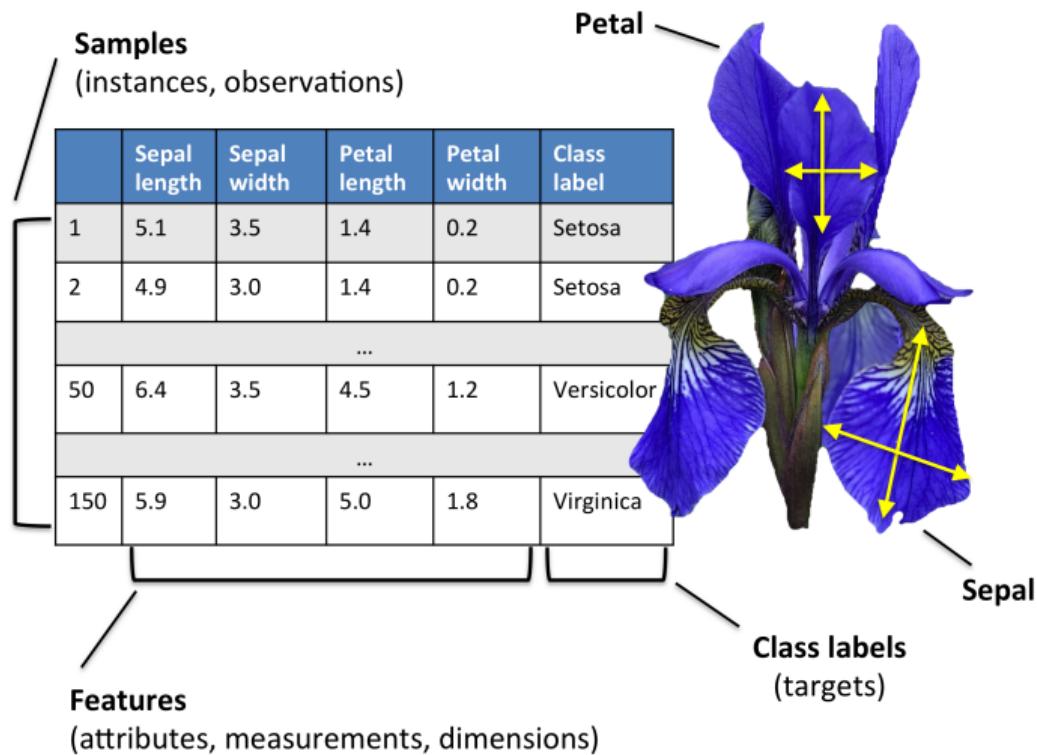
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Projections on the First Principal Component  
Variance of the projections: 65.7



# Iris dataset variance



## Iris dataset variance



## Wine dataset variance



# PCA on MNIST

## 2D PCA of MNIST



## Other methods

# t-SNE

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- Key Concepts:

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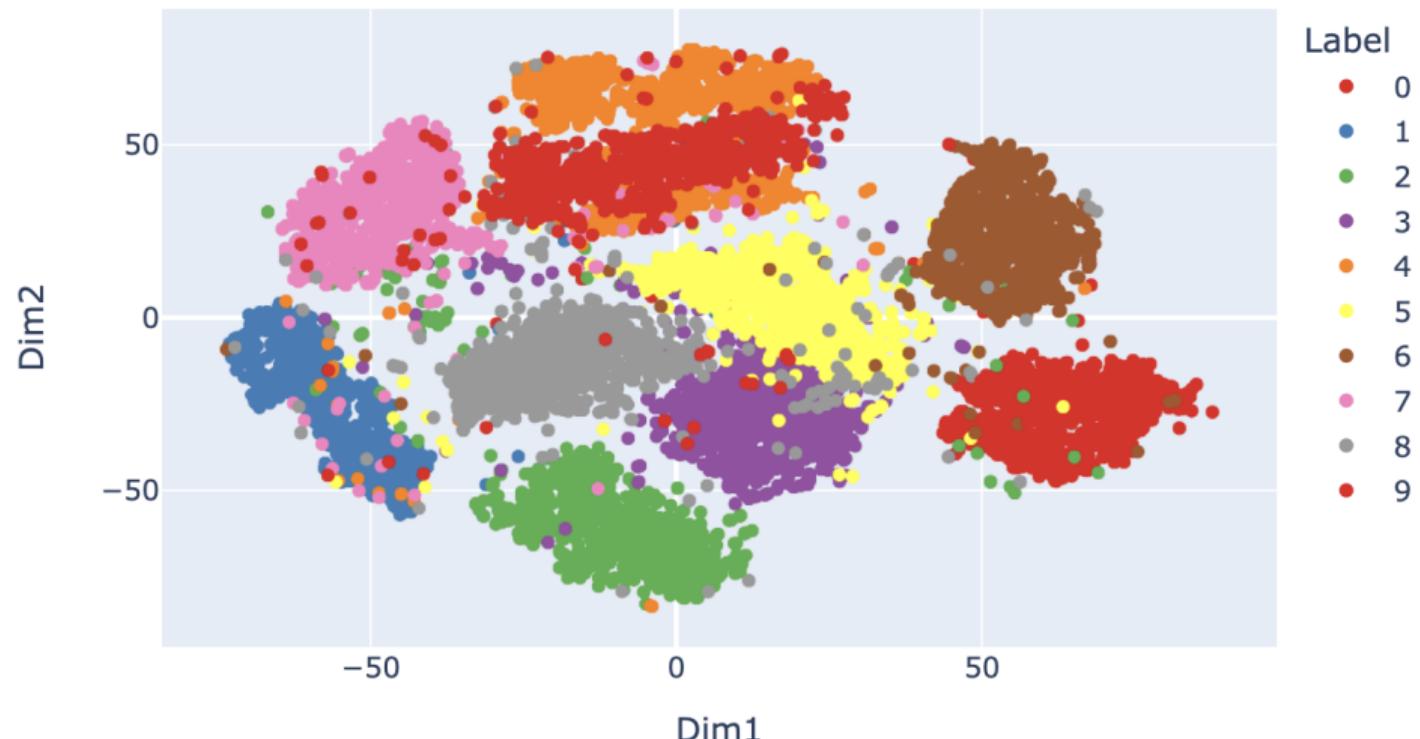
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- **Random Initialization:** Different runs may yield different results; multiple runs can help validate findings.

# t-SNE on MNIST

## 2D t-SNE of MNIST



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(UMAP) is a nonlinear dimensionality reduction technique that preserves both local and global data structure.

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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

