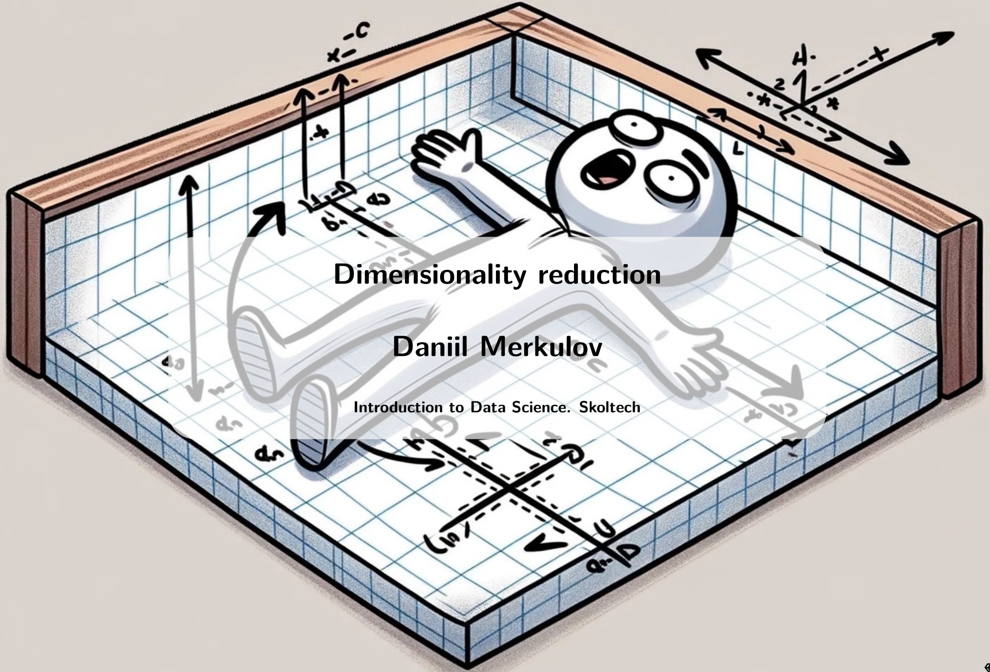


Dimensionality reduction

Daniil Merkulov

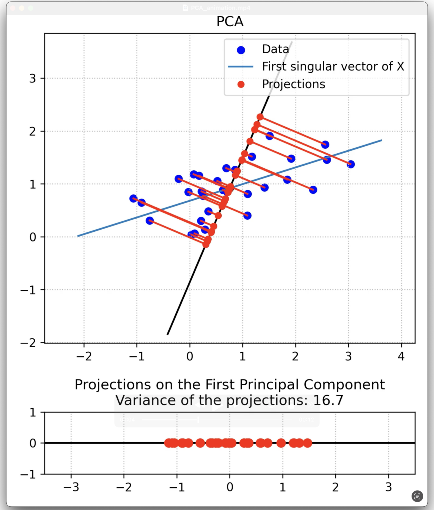
Introduction to Data Science. Skoltech

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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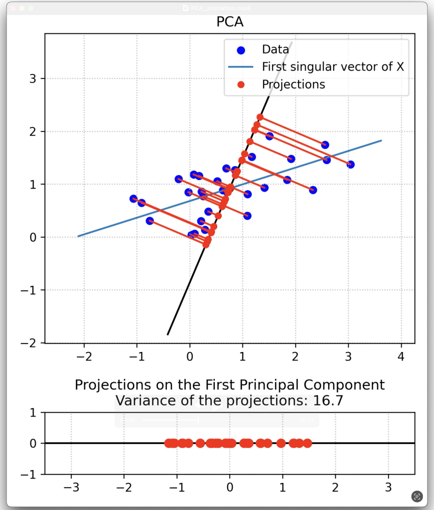

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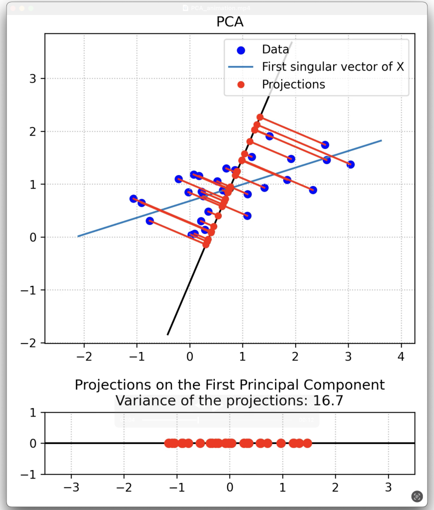

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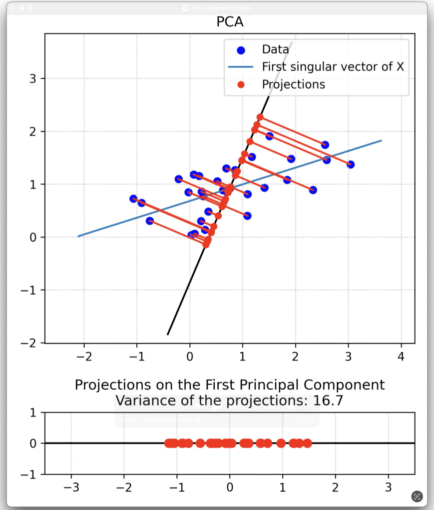

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since we are looking for the unit vector, we can reformulate the problem:

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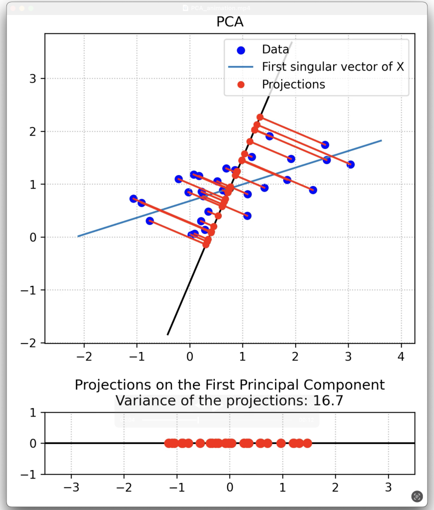

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It is known, that for the positive semidefinite matrix $A^\top A$ such vector is nothing else, but an eigenvector of $A^\top A$, which corresponds to the largest eigenvalue.

Algorithm derivation

So, we can conclude, that the following mapping:

$$\underset{n\times k}{\Pi} = \underset{n\times d}{A} \cdot \underset{d\times k}{W}$$

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 $A^\top A$.

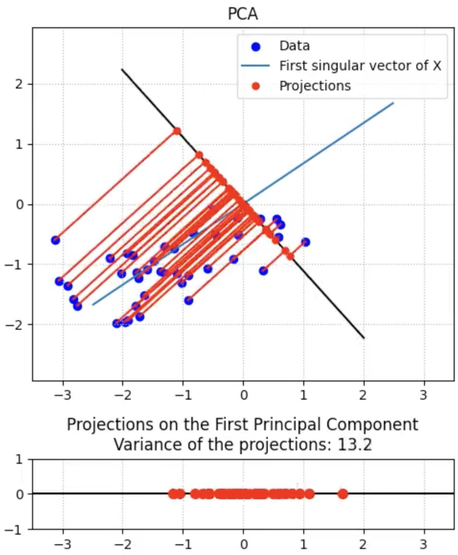
At the end:

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

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

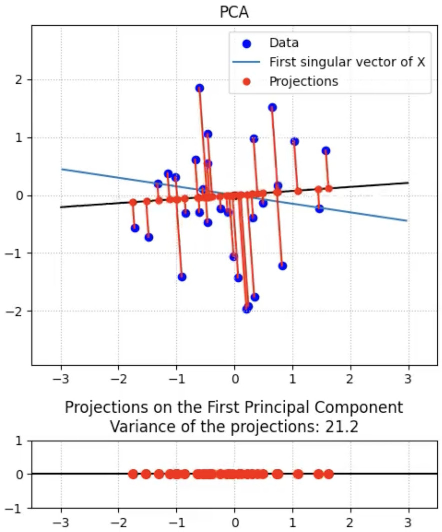
$$\Pi_r = U_r \Sigma_r$$

Exercise 1



What could be wrong with this PCA?

Exercise 2



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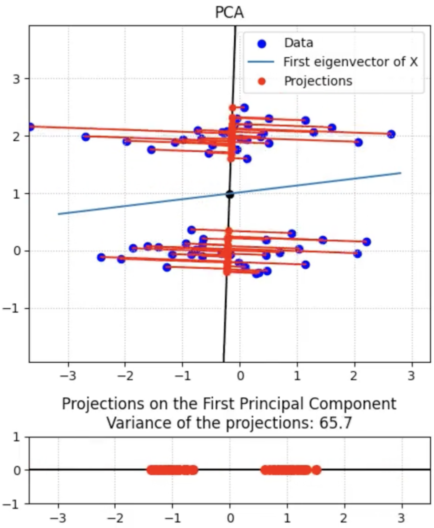


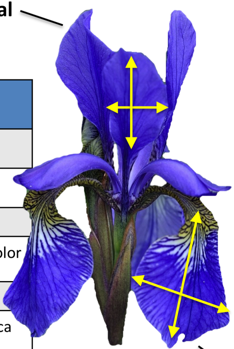
What could be wrong with this PCA?

Iris dataset variance

Samples
(instances, observations)

	Sepal length	Sepal width	Petal length	Petal width	Class label
1	5.1	3.5	1.4	0.2	Setosa
2	4.9	3.0	1.4	0.2	Setosa
...					
50	6.4	3.5	4.5	1.2	Versicolor
...					
150	5.9	3.0	5.0	1.8	Virginica

Petal

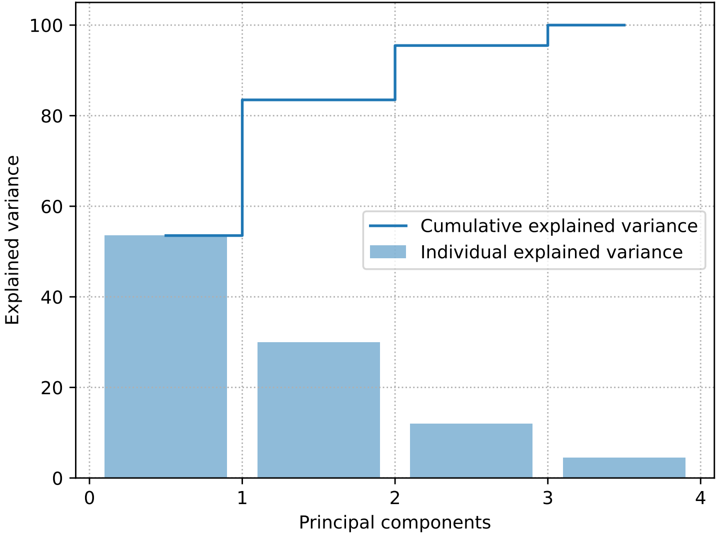


Sepal

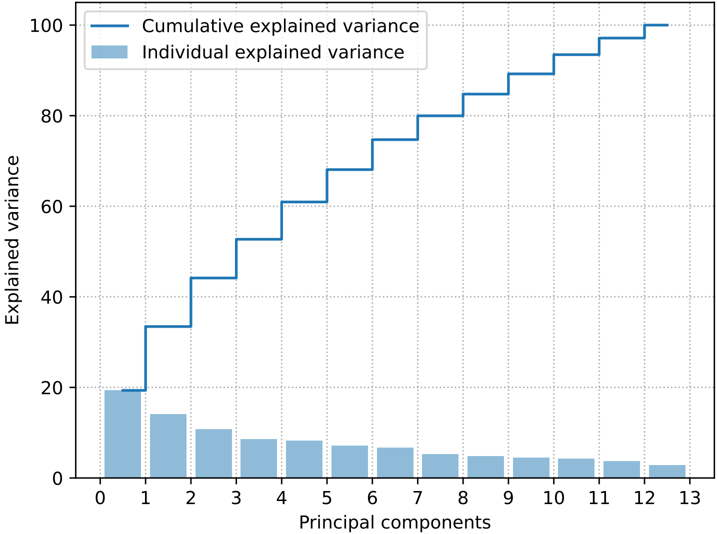
Features
(attributes, measurements, dimensions)

Class labels
(targets)

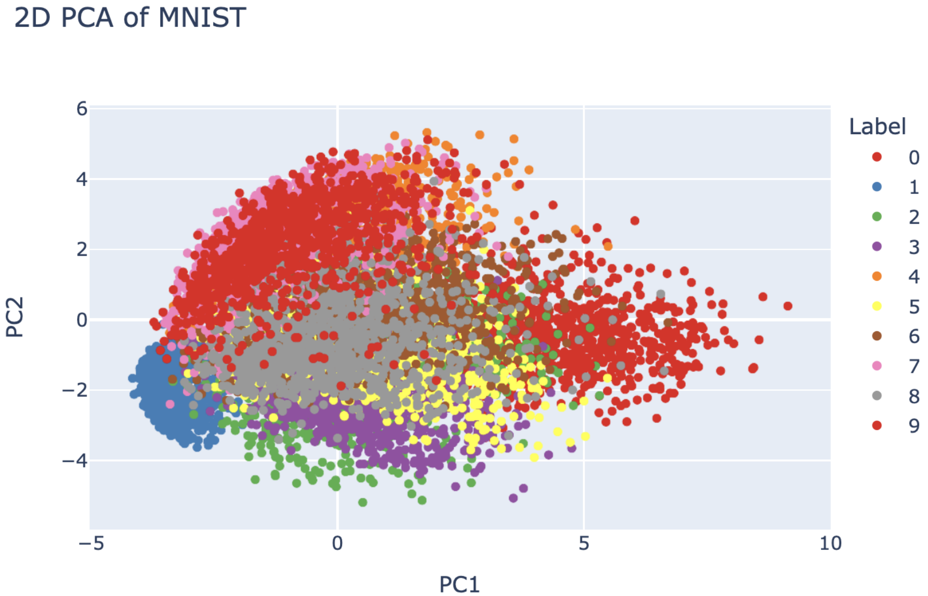
Iris dataset variance



Wine dataset variance



PCA on MNIST



Other methods

t-SNE

t-Distributed Stochastic Neighbor Embedding (t-SNE) is a nonlinear dimensionality reduction technique particularly well-suited for visualizing high-dimensional data in 2 or 3 dimensions.

- **Key Concepts:**

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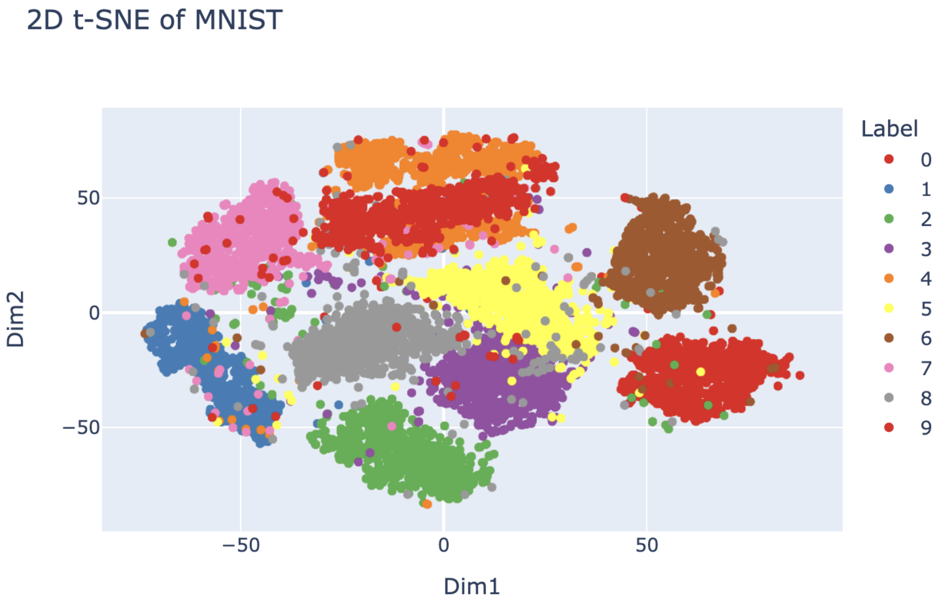
t-SNE on MNIST



UMAP

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  1. **Construct High-Dimensional Graph:** Use k-nearest neighbors to build the graph.
  2. **Compute Fuzzy Simplicial Sets:** Model the probability distribution of data relationships.
  3. **Optimize Low-Dimensional Embedding:** Apply stochastic gradient descent to minimize cross-entropy between high and low-dimensional graphs.
- **Advantages:**
  - **Speed:** Faster than t-SNE, suitable for large datasets.
  - **Preservation of Structure:** Maintains more global structure compared to t-SNE.
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UMAP

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  - **Manifold Learning:** Assumes data lies on a manifold in high-dimensional space.
  - **Topological Data Analysis:** Utilizes concepts from topology to model the manifold structure.
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UMAP on MNIST