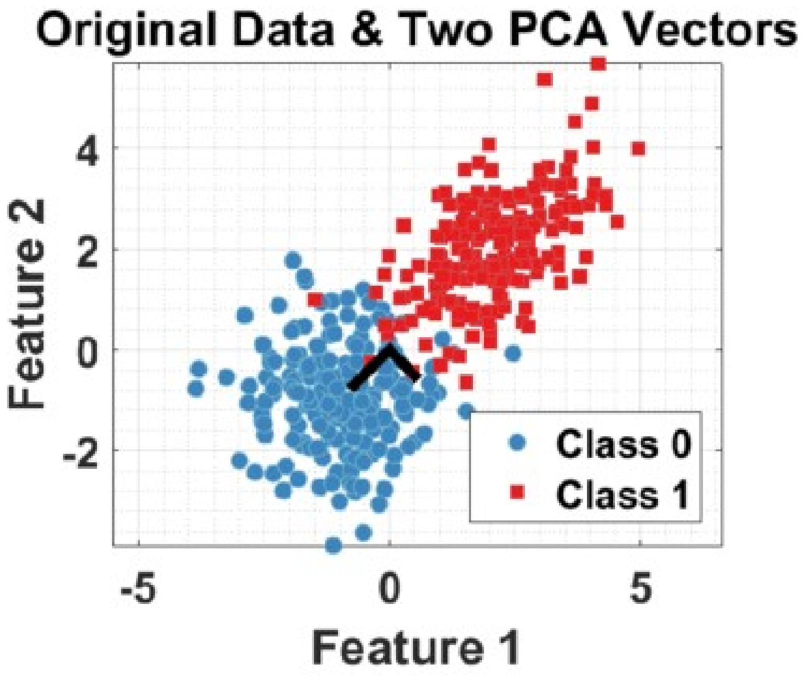
Dimensional reduction Generalities

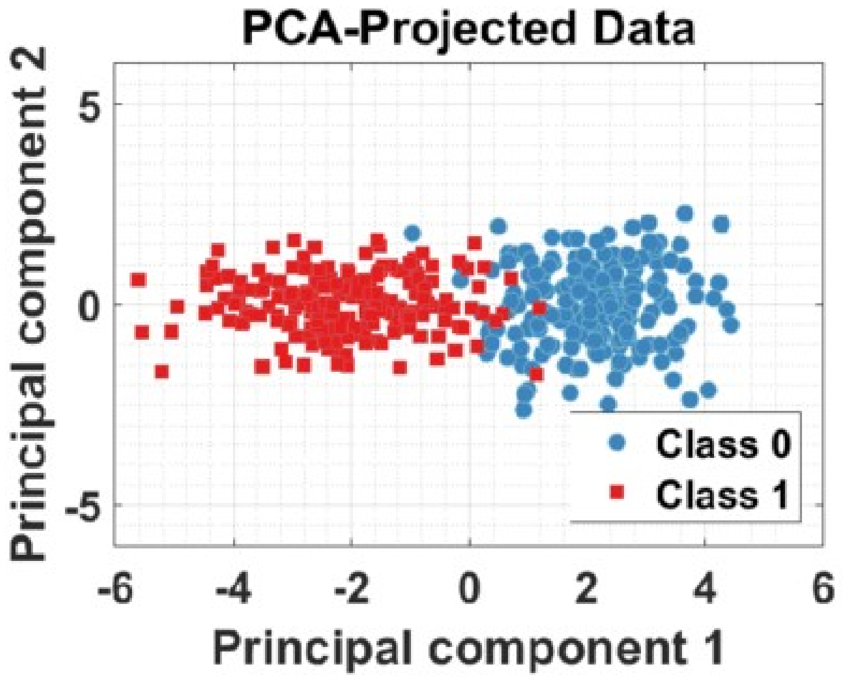
- Transform input features with a non-injective application : $\phi : \mathbb{R}^D \longrightarrow \mathbb{R}^p, p < D$
- Why would we do that?
- \- **eliminate redundancy** in the input information
  \- reduce “noise” (~ useless information)
  \- Avoid the « ***Curse of dimensionality*** » (large D)
  \- helps the learning:
    * **speed**: helps a lot
    * **performance**: it depends
  \- visualization (but there’s better, e.g. *t-SNE*)
- It’s a form of ***data compression***

Dimensional reduction
Principal Component Analysis

- Linear application towards a smaller subspace
  → projection on a hyper-plane



(3 dimensions, or more)



(2 dimensions shown)

PCA - first perspective: Maximize the Variance

- **Maximize** the **variance** of projected data along direction $\mathbf{u_i}$: Var = $\mathbf{u_i^T C u_i}$ with C the **covariance**

$$\mathbf{C} = \frac{1}{N}\sum_{n}^{N}(\vec{x}_n - \langle\vec{x}\rangle)(\vec{x}_n - \langle\vec{x}\rangle)^T$$

under the constraint : $\mathbf{u_i^T u_i} = 1$, we find:

$$\Rightarrow \mathbf{C u_i} = \lambda_i \mathbf{u_i}$$

$\rightarrow$ take the p first **eigenvectors** of the covariance matrix C

- Full proof: *Bishop book*, sec. 12.1.1, page 561-563

Proof

PCA
The “algorithm”

- Compute **covariance** matrix (centered data)

$$\mathbf{C} = \frac{1}{N}\sum_{n}^{N}(\vec{x}_n - \langle\vec{x}\rangle)(\vec{x}_n - \langle\vec{x}\rangle)^T$$

- Diagonalize C : $C = V\Lambda V^{-1}$

- Keep only the first p eigenmodes: $P = V[:p]$
(keep p columns.. be careful with *np.linalg*)

$$P = \left(\begin{pmatrix} \cdot \\ v_1 \\ \cdot \end{pmatrix} \begin{pmatrix} \cdot \\ v_2 \\ \cdot \end{pmatrix} \ \dots \ \begin{pmatrix} \cdot \\ v_p \\ \cdot \end{pmatrix} \right)_{D,p}$$

- transform: $\vec{x}_{n,transformed} = (\vec{x}_n - \langle\vec{x}\rangle) \cdot P$

PCA
inverse transform

- Transformation forward:

$$\vec{x}_{n,transformed} = (\vec{x}_n - \langle\vec{x}\rangle) \cdot P \tag{1}$$

$$X_{transformed} = (X - \langle X\rangle) \cdot P \tag{2}$$

- Backwards:

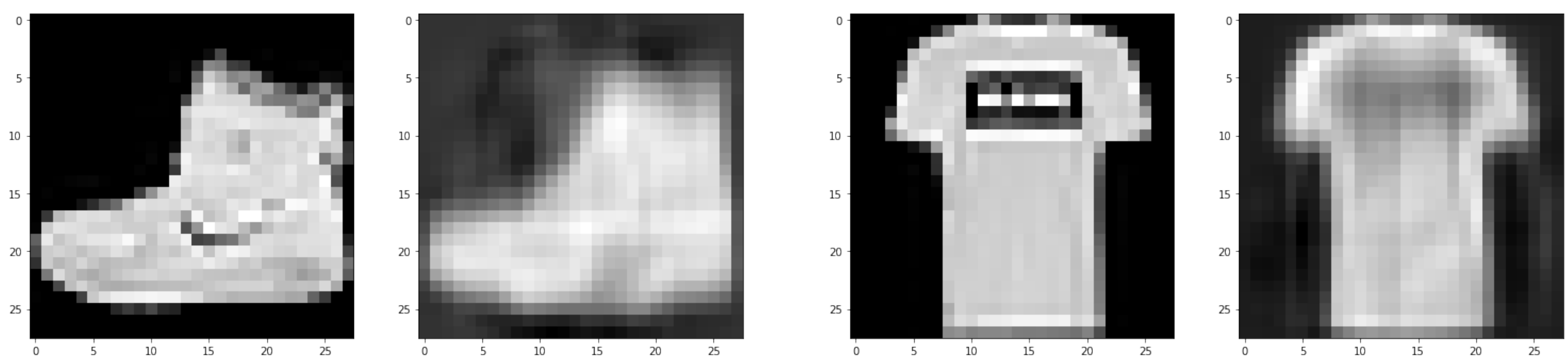
$$\begin{aligned}
\vec{x}_{n,decompressed} &= \vec{x}_{n,transformed} \cdot P^T + \langle\vec{x}\rangle && (1)\\
&= (\vec{x}_n - \langle\vec{x}\rangle) \cdot P \cdot P^T + \langle\vec{x}\rangle && (2)\\
&= \vec{x}_n \cdot P \cdot P^T + const && (3)
\end{aligned}$$

- Information is lost since $P.P^T$ is of rank p
- Hence, reconstruction error is defined as: (quadratic reconstruction loss)
- $$E_n = ||\vec{x}_n - \vec{x}_{n,decompressed}||_2^2$$

PCA
Concretely

- Full diagonalization: takes time $O(D^3)$,
  but iterative solution in time $O(pD^2)$
  Approximate solutions are faster, but slightly random

- Fashion-MNIST $(D{=}784,\ p{=}30)$:



→ `TP5.2-PCA-from-scratch+overfitting.ipynb`

- Interactive PCA, to build your intuition:
  http://setosa.io/ev/principal-component-analysis/

Dimensional reduction

- PCA: **minimizes reconstruction error** (can be proven)
- PCA limitation: reduces the representation dimensionality, **independently from the labels** (class or target value) of examples
- *Independent Component Analysis* ***(ICA)***: deals with correlations of order > 2
- ***Auto Encoders*** *(AE) and*
  Variational Auto Encoders (VAE)
  → also compress, and make generative models

Key concepts

- Curse of dimensionality
- PCA, variance, covariance, projection, reconstruction error
- Limits of PCA

New definition of what is Machine Learning: building a *model* of the data