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# AUTO-ASSOCIATIVE MODELS AND GENERALIZED PRINCIPAL COMPONENT ANALYSIS

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## Outline

1. Principal Component Analysis, 2 points of view,
2. Generalized PCA, theoretical aspects,
3. Implementation aspects,
4. Illustration on simulated datasets,
5. Illustration on real datasets.

## 1. Principal Component Analysis

- **Background:** Multidimensional data analysis ( $n$  observations in a  $p$ - dimensional space)
- **Goal:** Dimension reduction.
  - Data visualization (dimension less than 3),
  - To find which variables are important,
  - Compression.
- **Method:** Projection on low  $d$ - dimensional linear subspaces.

## PCA: Geometrical interpretation

### Problem

- Let  $X$  be a centered random vector in  $\mathbb{R}^p$ .
- Estimate the  $d$ -dimensional linear subspace  $d \in \{0, \dots, p\}$  minimizing the mean distance to  $X$ .
- Minimize with respect to  $a^1, \dots, a^d$  (orthonormal):

$$\mathbb{E} \left[ \left\| X - \sum_{k=1}^d \langle X, a^k \rangle a^k \right\|^2 \right].$$

### Explicit solution

- $a^1, \dots, a^d$  are the eigenvectors associated to the  $d$  largest eigenvalues of  $\mathbb{E}[X^t X]$ , the covariance matrix of  $X$ .
- The  $a^k$ 's are called principal axes, the  $Y^k = \langle X, a^k \rangle$  the principal variables.
- The associated residual is defined by

$$R^d = X - \sum_{k=1}^d \langle X, a^k \rangle a^k,$$

and it can be shown that  $\|R^d\| \leq \|R^{d-1}\|$ .

## PCA: Projection Pursuit interpretation

### Equivalent problem

- Estimate the  $d$ - dimensional linear subspace  $d \in \{0, \dots, p\}$  maximizing the projected variance.
- Maximize iteratively with respect to  $a^1, \dots, a^d$  (orthonormal):

$$\text{Var} [\langle X, a^1 \rangle], \dots, \text{Var} [\langle X, a^d \rangle].$$

## Algorithm

- For  $j = 0$ , let  $R^0 = X$ .
- For  $j = 1, \dots, d$  :
  - [A] Estimation of a projection axis.  
Determine  $a^j = \arg \max_{x \in \mathbb{R}^p} \mathbb{E} \left[ \langle x, R^{j-1} \rangle^2 \right]$  such that  $\|a^j\| = 1$  and  $\langle a^j, a^k \rangle = 0, 1 \leq k < j$ .
  - [P] Projection.  
Compute the principal variable  $Y^j = \langle a^j, R^{j-1} \rangle$ .
  - [R] Linear regression.  
Determine  $b^j = \arg \min_{x \in \mathbb{R}^p} \mathbb{E} \left[ \|R^{j-1} - Y^j x\|^2 \right]$  such that  $\langle b^j, a^j \rangle = 1$  and  $\langle b^j, a^k \rangle = 0, 1 \leq k < j$ . The solution is  $b^j = a^j$ , and let the regression function be  $s^j(t) = ta^j$ .
  - [U] Residual update.  
Compute  $R^j = R^{j-1} - s^j(Y^j)$ .

**Algorithm output.** After  $d$  iterations, we have the following expansion:

$$X = \sum_{k=1}^d s^k(Y^k) + R^d, \quad (1)$$

with  $s^k(t) = ta^k$  and  $Y^k = \langle a^k, X \rangle$ , or equivalently

$$X = \sum_{k=1}^d \langle a^k, X \rangle a^k + R^d.$$

This equation can be rewritten as

$$F(X) = R^d \quad (2)$$

where we have defined

$$F(x) = x - \sum_{k=1}^d \langle a^k, x \rangle a^k.$$

The equation  $F(x) = 0$  defines a  $d$ - dimensional linear subspace, spanned by  $a^1, \dots, a^d$ . Equation (2) defines a  $d$ - dimensional linear auto-associative model for  $X$ .



## Goals of a generalized PCA

1. To keep an expansion similar to (2):

$$F(X) = R^d,$$

but with a non necessarily linear function  $F$ , such that the equation  $F(x) = 0$  could model more general subspaces.

2. To keep an expansion “principal variables + residual” similar to (1):

$$X = \sum_{k=1}^d s^k(Y^k) + R^d,$$

but with non necessarily linear functions  $s^k$ .

3. To benefit from the “nice” theoretical properties of PCA.
4. To keep a simple iterative algorithm.

## 2. Generalized PCA, theoretical aspects

We adopt the Projection Pursuit point of view. The steps [A] and [R] are generalized:

### [A] Estimation of a projection axis.

Introduction of an index  $I$  which measures the quality of the projection axis. For instance:

- Dispersion,
- Deviation from normality,
- Clusters detection,
- Outliers detection,...

### [R] Regression.

Estimation of the regression function from  $\mathbb{R}$  to  $\mathbb{R}^p$  in a given set:

- Linear functions,
- Splines, kernels,...

**New algorithm.**

- For  $j = 0$ , let  $R^0 = X$ .
- For  $j = 1, \dots, d$  :
  - [A] Estimation of a projection axis.  
Determine  $a^j = \arg \max_{x \in \mathbb{R}^p} I(\langle x, R^{j-1} \rangle)$  such that  $\|a^j\| = 1$  and  $\langle a^j, a^k \rangle = 0$ ,  $1 \leq k < j$ .
  - [P] Projection.  
Compute the principal variable  $Y^j = \langle a^j, R^{j-1} \rangle$ .
  - [R] Regression.  
Determine  $s^j = \arg \min_{s \in \mathcal{S}(\mathbb{R}, \mathbb{R}^p)} \mathbb{E} \left[ \|R^{j-1} - s(Y^j)\|^2 \right]$  such that  $P_{a^j} \circ s^j = \text{Id}_{\mathbb{R}}$  and  $P_{a^k} \circ s^j = 0$ ,  $1 \leq k < j$ .
  - [U] Residual update  
Compute  $R^j = R^{j-1} - s^j(Y^j)$ .

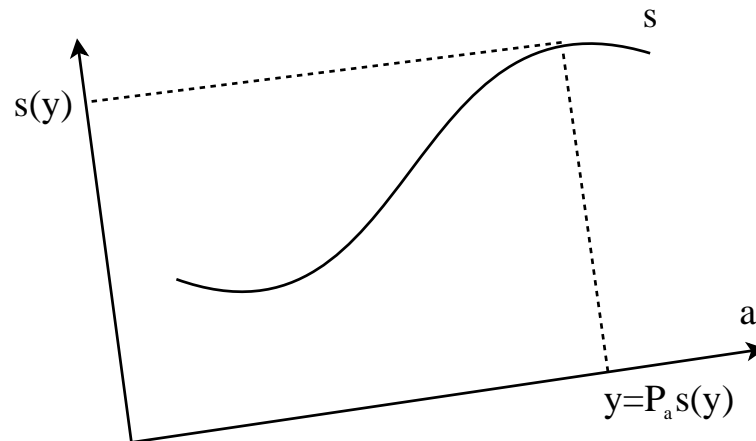
**Remark:** At the end of iteration  $j$ , the residual is given by

$$\begin{aligned}
 R^j &= R^{j-1} - s^j (Y^j) \\
 &= R^{j-1} - s^j (\langle a^j, R^{j-1} \rangle) \\
 &= R^{j-1} - s^j \circ P_{a^j} (R^{j-1}) \\
 &= (\text{Id}_{\mathbb{R}^p} - s^j \circ P_{a^j}) (R^{j-1}) \\
 &= (\text{Id}_{\mathbb{R}^p} - s^j \circ P_{a^j}) \circ (\text{Id}_{\mathbb{R}^p} - s^{j-1} \circ P_{a^{j-1}}) (R^{j-2}) \\
 &= \dots \\
 &= (\text{Id}_{\mathbb{R}^p} - s^j \circ P_{a^j}) \circ \dots \circ (\text{Id}_{\mathbb{R}^p} - s^1 \circ P_{a^1}) (R^0) \\
 &= (\text{Id}_{\mathbb{R}^p} - s^j \circ P_{a^j}) \circ \dots \circ (\text{Id}_{\mathbb{R}^p} - s^1 \circ P_{a^1}) (X).
 \end{aligned}$$

Auto-associative composite model.

**Remark:** The constraint  $P_{a^j} \circ s^j = \text{Id}_{\mathbb{R}}$ .

- Natural constraint.



- Important consequence: At the end of iteration  $j$ , the residual is given by  $R^j = (\text{Id}_{\mathbb{R}^p} - s^j \circ P_{a^j}) (R^{j-1})$ , and thus is projection on  $a^j$  is

$$\begin{aligned} P_{a^j} R^j &= (P_{a^j} - P_{a^j} \circ s^j \circ P_{a^j}) (R^{j-1}) \\ &= (P_{a^j} - P_{a^j}) (R^{j-1}) \\ &= 0. \end{aligned}$$

Thus, iteration  $(j + 1)$  can be performed on the linear subspace orthogonal to  $(a^1, \dots, a^j)$ , which is of dimension  $(p - j)$ .

**Goal 1.** After  $d$  iterations:

- One always has an auto-associative model

$$F(X) = R^d,$$

with

$$F = (\text{Id}_{\mathbb{R}^p} - s^d \circ P_{a^d}) \circ \dots \circ (\text{Id}_{\mathbb{R}^p} - s^1 \circ P_{a^1}) = \prod_{k=d}^1 (\text{Id}_{\mathbb{R}^p} - s^k \circ P_{a^k}),$$

and  $P_{a^j}(x) = \langle a^j, x \rangle$ .

- The equation  $F(x) = 0$  defines a  $d$ - dimensional manifold.

**Goal 2.** After  $d$  iterations:

- One always has the expansion “principal variables + residual” similar to (1):

$$X = \sum_{k=1}^d s^k(Y^k) + R^d,$$

and the functions  $s^k$  are non necessarily linear.

- For  $d = p$ , the expansion is exact:  $R^p = 0$ .
- We can still define principal axes  $a^k$  and principal variables  $Y^k$ .
- The residuals are centered:  $\mathbb{E}[R^k] = 0, k = 0, \dots, d$ .

**Goal 3.** After  $d$  iterations, we have:

- Some orthogonality properties

$$\langle a^k, a^j \rangle = 0, \quad 1 \leq k < j \leq d,$$

$$\langle a^k, R^j \rangle = 0, \quad 1 \leq k \leq j \leq d,$$

$$\langle a^k, s^j(Y^j) \rangle = 0, \quad 1 \leq k < j \leq d.$$

- Since the norm of the residuals is decreasing, we can define, similarly to the PCA case, the information ratio represented by the  $d$ -dimensional model as

$$Q_d = 1 - \mathbb{E} \left[ \|R^d\|^2 \right] / \text{Var} \left[ \|X\|^2 \right].$$

One can show that  $Q_0 = 0$ ,  $Q_p = 1$  and  $(Q_d)$  is increasing.

**Remark.** Except in particular cases, the non-correlation of the principal variables is lost:

$$\mathbb{E} [Y^k Y^j] \neq 0, \quad 1 \leq k < j \leq d.$$



## Goal 4.

- We still have an iterative algorithm. It converges at most in  $p$  steps.
- Its complexity depends on the two steps [A] et [R].

[A] Estimation of a projection axis.

Determine  $a^j = \arg \max_{x \in \mathbb{R}^p} I(\langle x, R^{j-1} \rangle)$  such that  $\|a^j\| = 1$  and  $\langle a^j, a^k \rangle = 0$ ,  $1 \leq k < j$ .

[R] Regression.

Determine  $s^j = \arg \min_{s \in \mathcal{S}(\mathbb{R}, \mathbb{R}^p)} \mathbb{E} \left[ \|R^{j-1} - s(Y^j)\|^2 \right]$  such that  $P_{a^j} \circ s^j = \text{Id}_{\mathbb{R}}$  and  $P_{a^k} \circ s^j = 0$ ,  $1 \leq k < j$ .

- Note that the above theoretical properties do not depend on these steps.

### 3. Implementation aspects, step [A]

- **Contiguity index.** Measure of the neighborhood preservation. Points which are neighbor in  $\mathbb{R}^p$  should stay neighbor on the axis.

$$I(\langle x, R^{j-1} \rangle) = \frac{\sum_{i=1}^n \langle x, R_i^{j-1} \rangle^2}{\sum_{k=1}^n \sum_{\ell=1}^n m_{k\ell} \langle x, R_k^{j-1} - R_\ell^{j-1} \rangle^2},$$

where  $M = (m_{k\ell})$  is the contiguity matrix defined by  $m_{k\ell} = 1$  if  $R_\ell^{j-1}$  is the closest neighbor of  $R_k^{j-1}$ ,  $m_{k\ell} = 0$  otherwise.

- **Optimization.** Explicit solution.

[A]  $a^j$  is the eigenvector associated to the largest eigenvalue of  $V_j^* V_j^{-1}$ , where

$$V_j = \sum_{k=1}^n {}^t R_k^{j-1} R_k^{j-1}, \quad V_j^* = \sum_{k=1}^n \sum_{\ell=1}^n m_{k\ell} {}^t (R_k^{j-1} - R_\ell^{j-1}) (R_k^{j-1} - R_\ell^{j-1})$$

are proportional to the covariance and local covariance matrices of  $R^{j-1}$ .

## Implementation aspects, step [R]

- **Set of  $L^2$  functions.** The regression step reduces to estimating the conditional expectation:

$$[R] \quad s^j(Y_j) = \mathbb{E} [R^{j-1} | Y_j].$$

- **Estimation of the conditional expectation.**

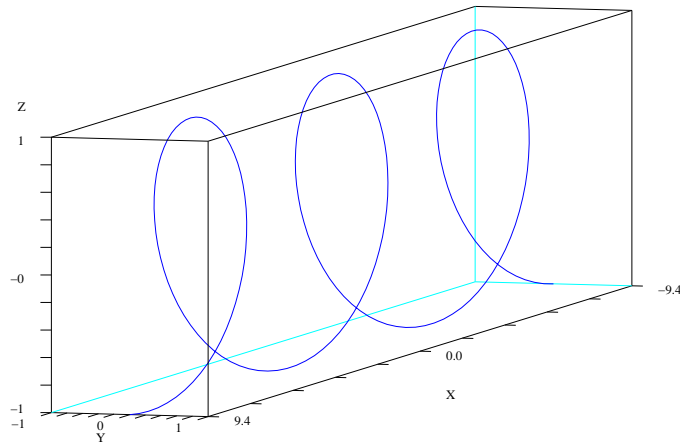
- Classical problem since the constraints  $P_{a^j} \circ s^j = \text{Id}$  and  $P_{a^k} \circ s^j = \text{Id}$ ,  $1 \leq k < j$  are easily taken into account in the  $a^k$ 's basis. Step [R] reduces to  $(p - j)$  independent regressions from  $\mathbb{R}$  to  $\mathbb{R}$ .
- Numerous estimates are available: splines, local polynomials, kernel estimates, ...
- For instance, for the coordinate  $k \in \{j + 1, \dots, p\}$ , the kernel estimate of  $s^j(u)$  can be written as

$$\tilde{s}_k^j(u) = \frac{\sum_{i=1}^n \tilde{R}_{i,k}^{j-1} K_h(u - Y_i^j)}{\sum_{i=1}^n K_h(u - Y_i^j)},$$

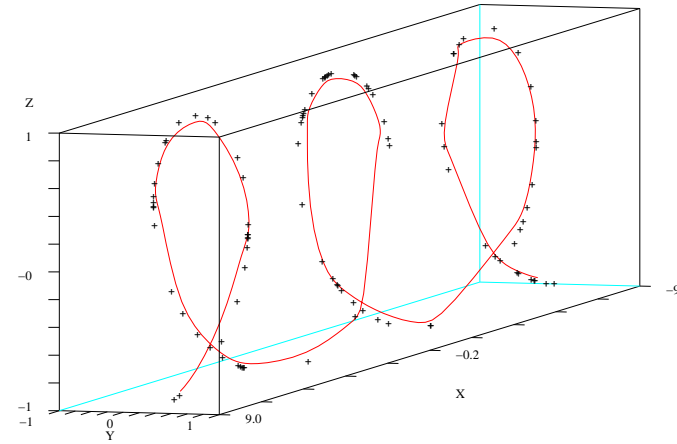
where  $h$  is a smoothing parameter (the bandwidth).

#### 4. First illustration on a simulated dataset

- $n = 100$  points in  $\mathbb{R}^3$  randomly chosen on the curve  $x \rightarrow (x, \sin x, \cos x)$ .
- One iteration  $h = 0.3 \rightarrow Q_1 = 99.97\%$ .



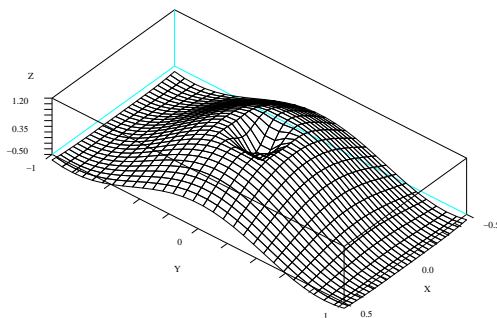
Theoretical curve



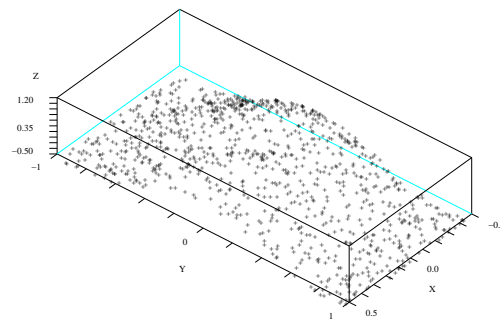
Estimated 1– dimensional manifold

## Second illustration on a simulated dataset

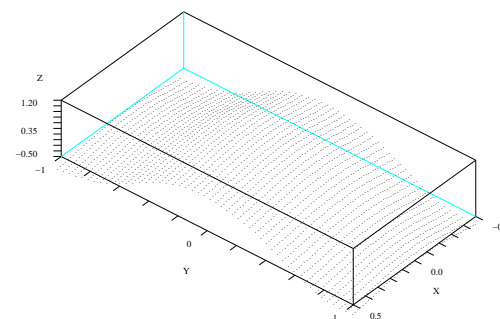
- $n = 1000$  points in  $\mathbb{R}^3$  randomly chosen on the surface  
 $(x, y) \rightarrow (x, y, \cos(\pi\sqrt{x^2 + y^2})(1 - \exp\{-64(x^2 + y^2)\}))$ .
- Two iterations:  $Q_1 = 84.1\%$  et  $Q_2 = 97.6\%$ .



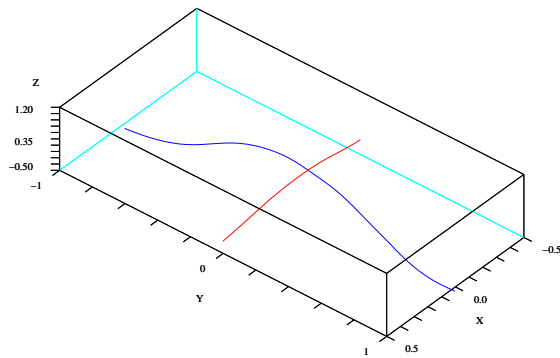
Theoretical surface



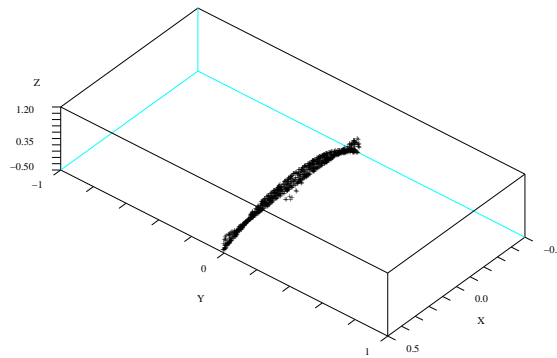
Simulated points



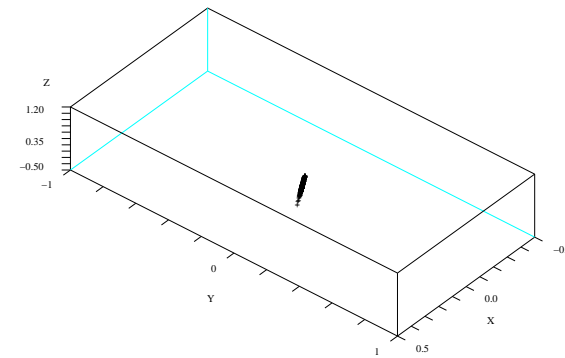
Estimated 2– dimensional manifold



$s^1$  (blue) and  $s^2$  (red)



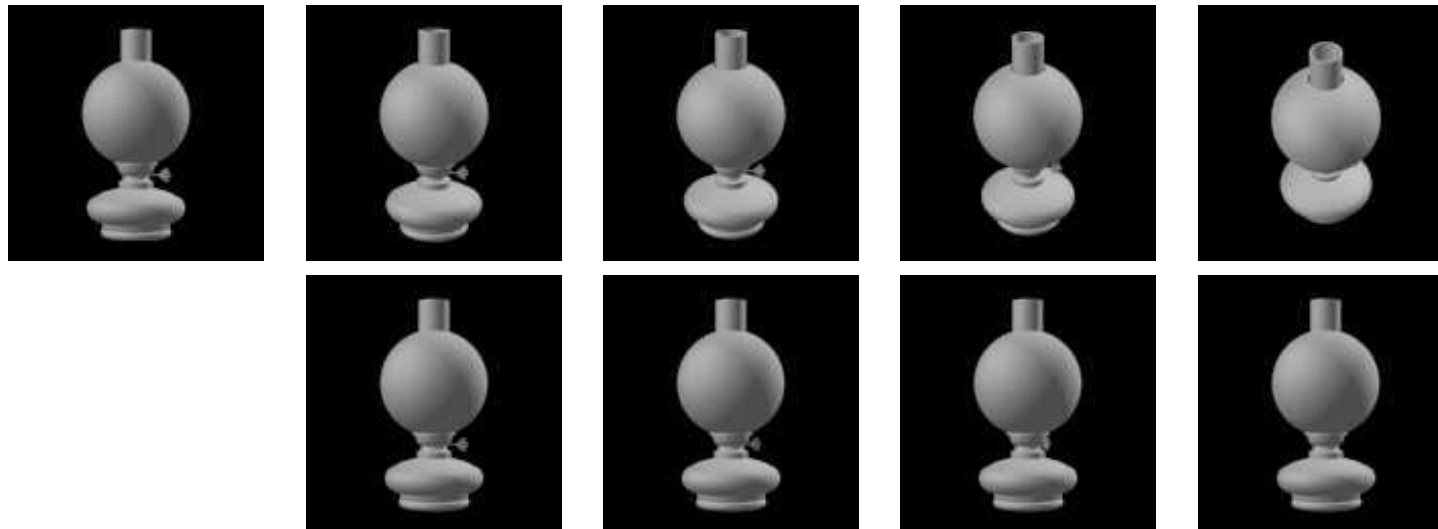
Residuals  $R_i^1$



Residuals  $R_i^2$

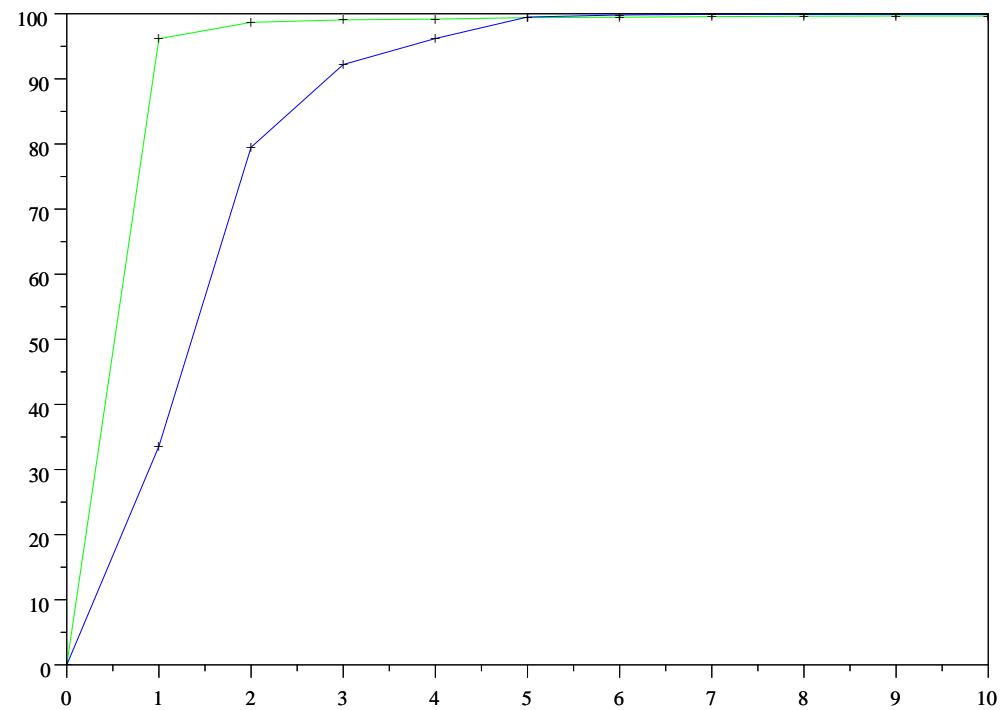
## 5. First illustration on a real dataset

- Set of  $n = 45$  images of size  $256 \times 256$ .



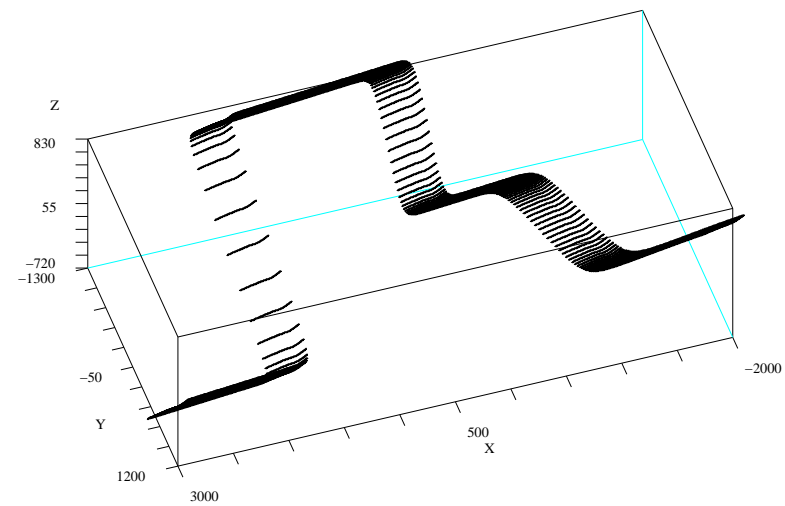
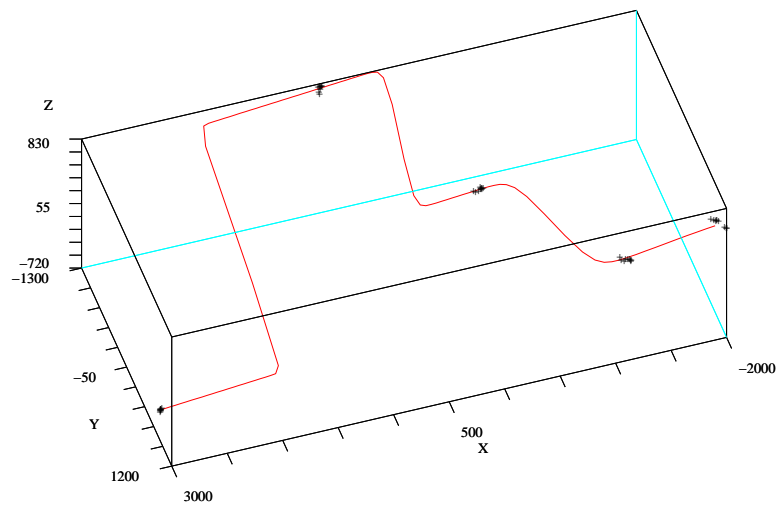
- Interpretation :  $n = 45$  points in dimension  $p = 256^2$ .
- Rotation :  $n = 45$  points in dimension  $p = 44$ .

- Information ratio  $Q_d$  as a function of  $d$  (blue: classical PCA, green: generalized PCA).



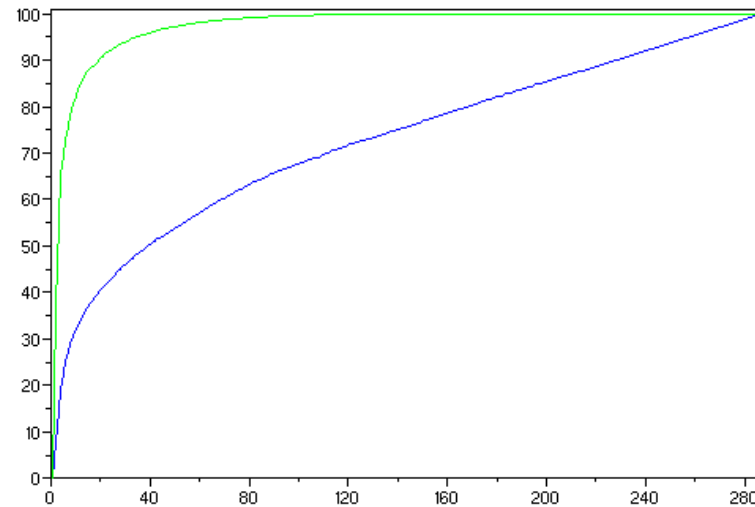


- Projection on the 3 first PCA axes of the estimated manifolds (dimension 1 & dimension 2).

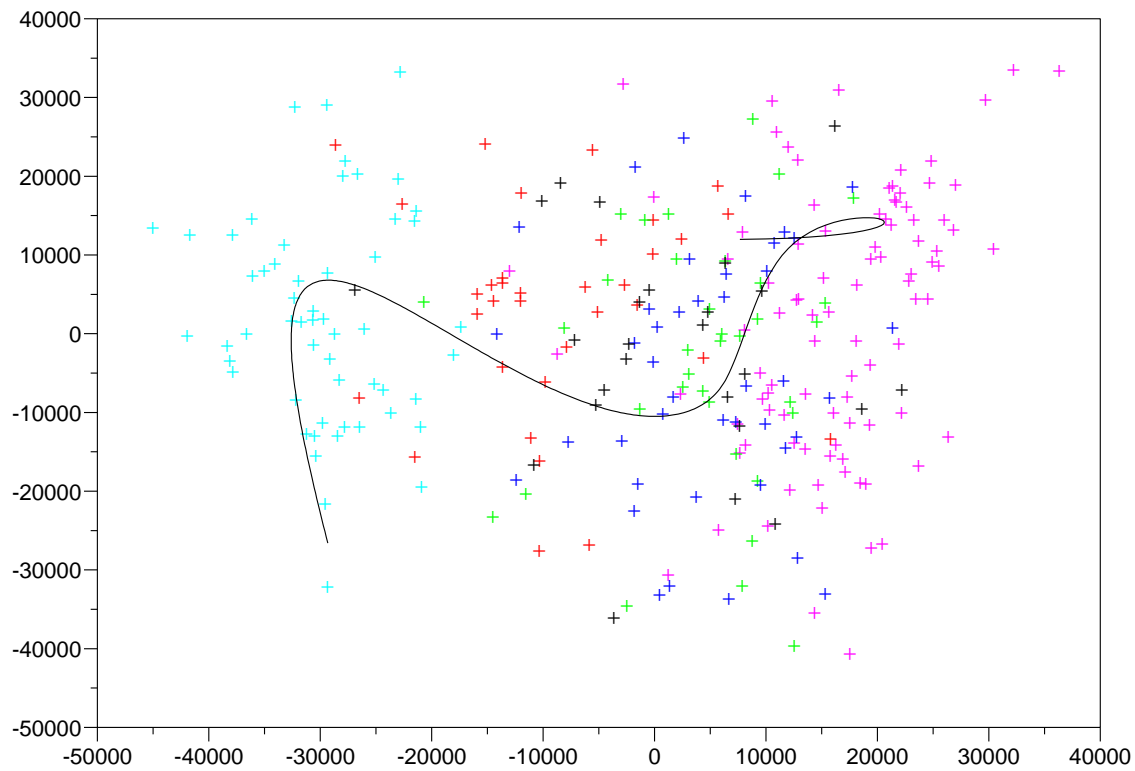


## Second illustration on a real dataset

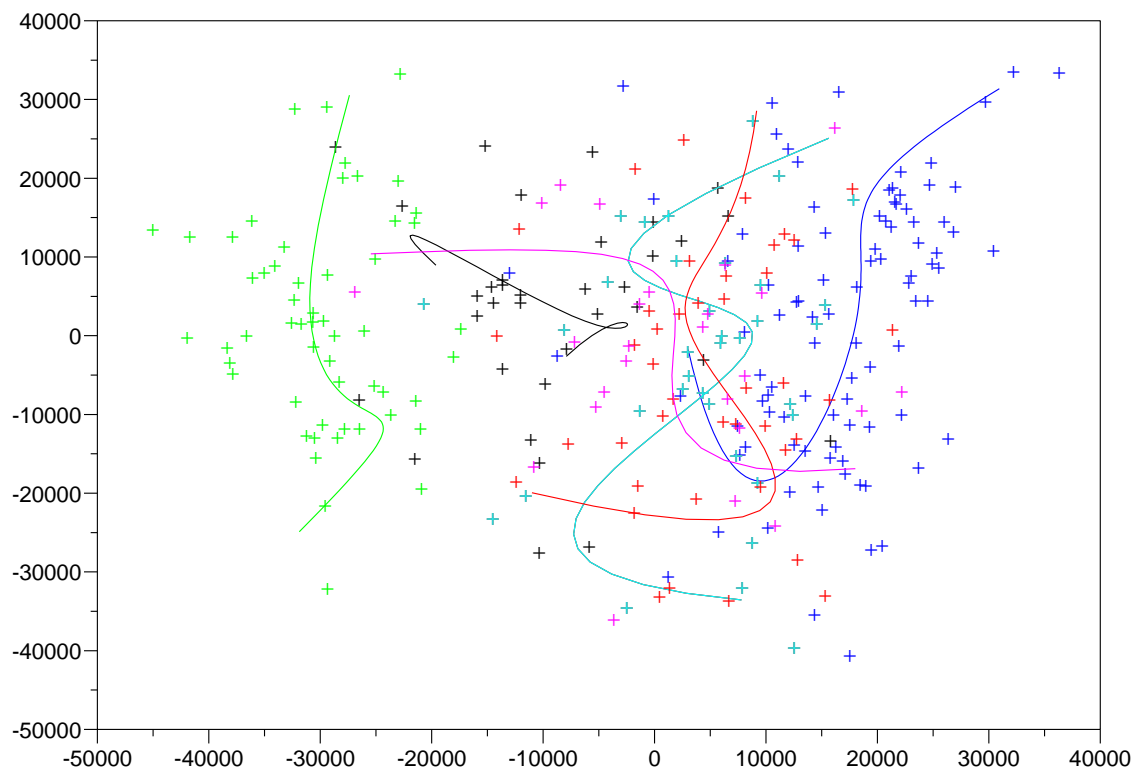
- Dataset I, five types of breast cancer.
- Set of  $n = 286$  samples in dimension  $p = 17816$ .
- Rotation :  $n = 286$  points in dimension  $p = 285$ .
- Forgetting the labels, information ratio  $Q_d$  as a function of  $d$  (blue: classical PCA, green: generalized PCA).



Estimated 1– dimensional manifold projected on the principal plane.



Estimated 1– dimensional manifolds projected on the principal plane, for each type of cancer.



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