Nonliner PCA and manifold approximation

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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):

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

Explicit solution

- $a^1, \dots, a^d$ are the eigenvectors associated to the d largest eigenvalues of $\mathbb{E}\left[X^t X\right]$, the covariance matrix of X.

- The a^k 's are called principal axes, the $Y^k = \left\langle X, a^k \right\rangle$ the principal variables.

- The associated residual is defined by

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

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

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):

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

Algorithm

- For $j = 0$, let $R^0 = X$.

- For $j = 1, \dots, d$:

[A] Estimation of a projection axis.
Determine $a^j = \arg\max_{x\in\mathbb{R}^p} \mathbb{E}\left[\left\langle x, R^{j-1}\right\rangle^2\right]$ such that $\left\|a^j\right\| = 1$ and $\left\langle a^j, a^k\right\rangle = 0$, $1 \leq k < j$.

[P] Projection.
Compute the principal variable $Y^j = \left\langle a^j, R^{j-1}\right\rangle$.

[R] Linear regression.
Determine $b^j = \arg\min_{x\in\mathbb{R}^p} \mathbb{E}\left[\left\|R^{j-1} - Y^j x\right\|^2\right]$ such that $\left\langle b^j, a^j\right\rangle = 1$ and $\left\langle b^j, a^k\right\rangle = 0$, $1 \leq k < j$. 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:

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

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

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

This equation can be rewritten as

$$F(X) = R^d \tag{2}$$

where we have defined

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

The equation $F(x) = 0$ defines a $d-$ dimensional linear subspace, spanned by $a^1, \ldots, a^d$. 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 $j = 1, \ldots, d$:

  [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 $\left\| a^j \right\| = 1$ and $\langle a^j, a^k \rangle = 0$, $1 \le k < j$.

  [P] Projection.
  Compute the principal variable $Y^j = \langle a^j, R^{j-1} \rangle$.

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

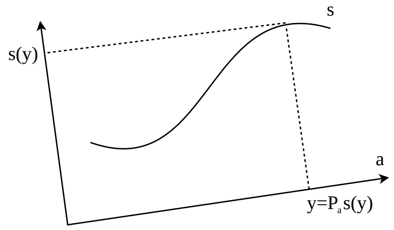
  [U] Residual update
  Compute $R^j = R^{j-1} - s^j(Y^j)$.

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

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

Auto-associative composite model.

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



- Natural constraint.

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

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

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

Goal 1. After d iterations:

- One always has an auto-associative model

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

  with

$$F = \left(\mathrm{Id}_{\mathbb{R}^p} - s^d \circ P_{a^d}\right) \circ \ldots \circ \left(\mathrm{Id}_{\mathbb{R}^p} - s^1 \circ P_{a^1}\right) = \coprod_{k=d}^{1} \left(\mathrm{Id}_{\mathbb{R}^p} - s^k \circ P_{a^k}\right),$$

  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 as 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: $\mathbb{E}\left[R^k\right] = 0$, $k = 0, \ldots, d$.

Goal 3. After d iterations, we have:

- Some orthogonality properties

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

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

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

- 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

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

  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:

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

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 $\left\|a^j\right\| = 1$ and $\left\langle a^j, a^k \right\rangle = 0,\ 1 \leq k < j.$

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

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

where $M = (m_{k\ell})$ is the contiguity matrix defined by
$m_{k\ell} = 1$ if R_ℓ^{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 $V_j^\star V_j^{-1}$, where

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

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

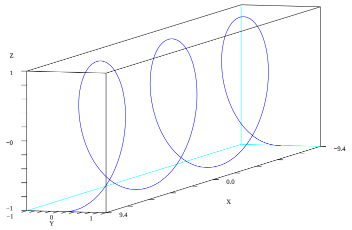
- **Estimation of the conditional expectation.**
  - Classical problem since the constraints $P_{a^j} \circ s^j = \mathrm{Id}$ and $P_{a^k} \circ s^j = \mathrm{Id}$, $1 \le k < j$ are easily taken into account in the a^k 's basis. Step [R] reduces to $(p-j)$ independent regressions from $\mathbb{R}$ 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

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

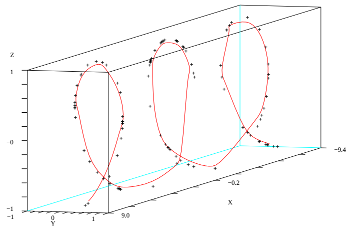
where h is a smoothing parameter (the bandwidth).

4. First illustration on a simulated dataset

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



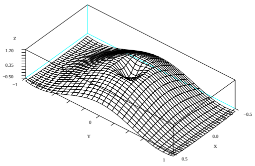
Theoretical curve



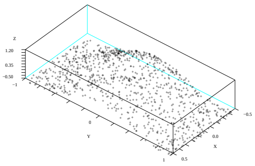
Estimated $1-$ dimensional manifold

Second illustration on a simulated dataset

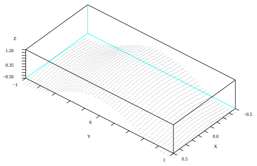
- $n = 1000$ points in $\mathbb{R}^3$ randomly chosen on the surface $(x, y) \to (x, y, \cos(\pi\sqrt{x^2 + y^2})(1 - \exp\{-64(x^2 + y^2)\}))$.
- Two iterations: $Q_1 = 84.1\%$ et $Q_2 = 97.6\%$.



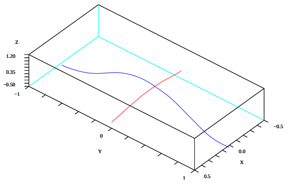
Theoretical surface



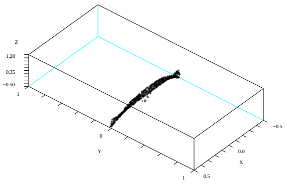
Simulations



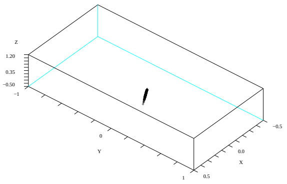
Estimated $2D$ manifold



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



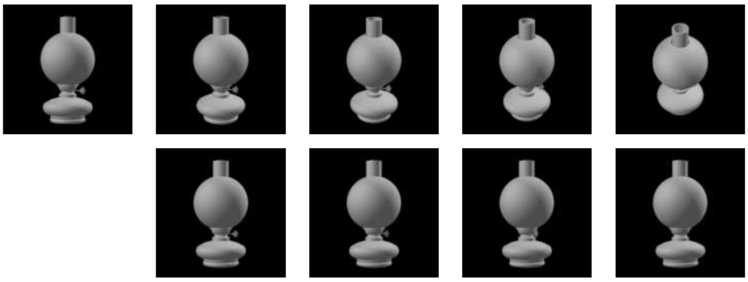
Residuals R_i^1



Residuals R_i^2

5. First illustration on a real dataset

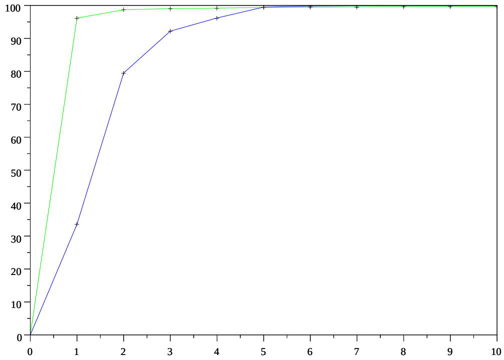
- Set of $n = 45$ images of size 256×256.



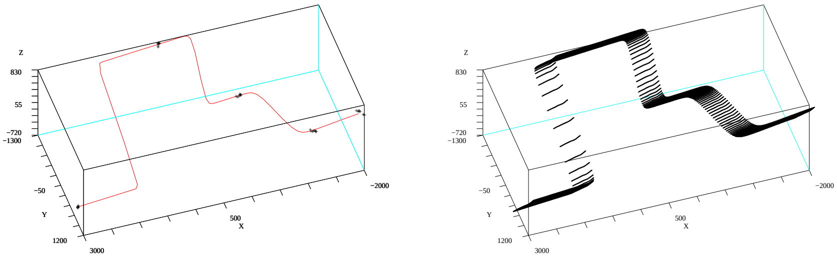
- Interpretation : $n = 45$ points in dimension $p = 256^2$.

- Rotation : $n = 45$ points in dimension $p = 44$.

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

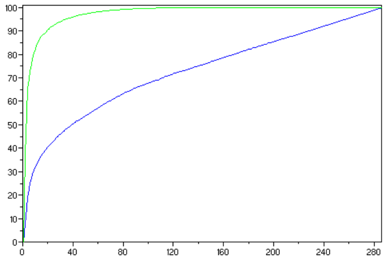


- Projection on the 3 first PCA axes of the estimated manifolds (dimension 1 & dimension 2).

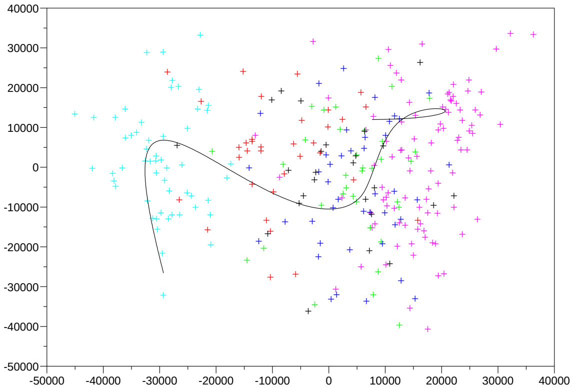


Second illustration on a real dataset

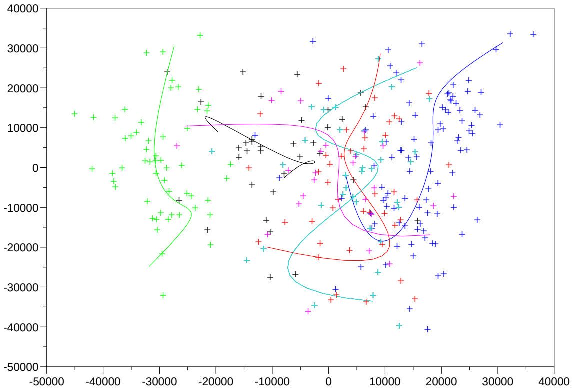
- Dataset I, five types of breast cancer.
- Set of $n = 286$ samples in dimension $p = 17816$.
- Rotation : $n = 286$ points in dimension $p = 285$.
- Forgetting the labels, information ratio Q_d as a function of d (blue: classical PCA, green: generalized PCA).



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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