Machine/Statistical Learning

PCA and Kernel PCA

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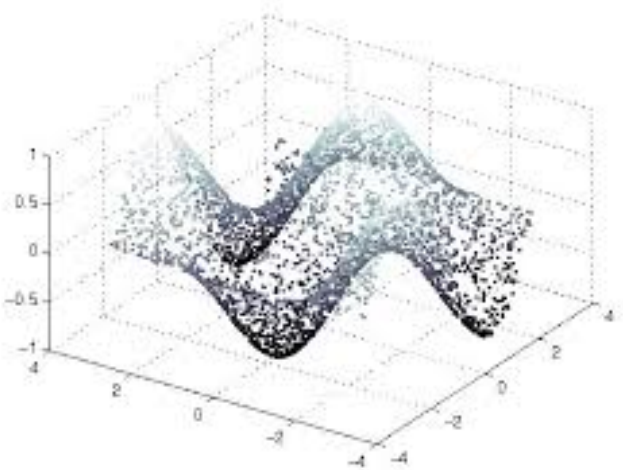
(material from Florent Chatelain, Olivier Michel)

ENSTA 2023

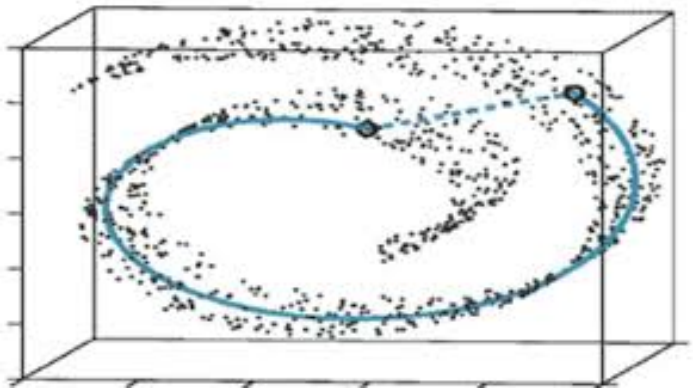
Dimension Reduction : motivation

- Compression : reduction of the size of the data
- Interpretability : which dimensions are important/linked for prediction, data visualization
- Curse of dimensionality : the amount of data to "fill" the space is exponential in the dimension. High dimensional spaces are mostly empty !
- Intrinsic dim. $\ll$ representation dim. : high-dim data often live in an (unknown) lower dimensional space
- dimension reduction $\rightarrow$ noise reduction : noise "visits" all possible dimensions



Extraction techniques (manifold learning)

- Physically based methods, k-NN graphs, geodesic distances...
- Statistical methods, dictionary learning
- Filtering (linear/non linear)
- Deep autoencoders...



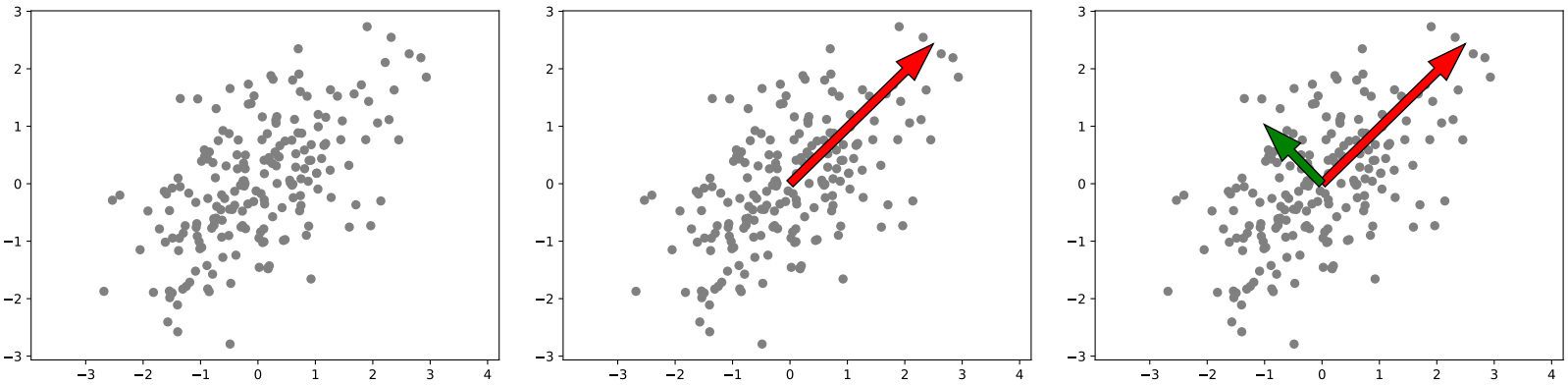
☞ Finding/learning **data representation** ("features extraction") is somehow the core of modern ML. **PCA is a foundational idea**.

Classical (non probabilistic) PCA

- PCA is a linear dimension reduction method
- Idea : find "directions" in the data such that :
  - the first explains **most the variation of the data**
  - the second most of the remaining variation (while being orthogonal to the first)
  - etc. (here $d = 2$ but usually d very high !)

Mathematically :

- Find p orthonormal vectors $v_1, \ldots, v_p$ where $p \ll d$ such that :
  - $v_1 = \arg\max_v [\mathrm{var}(\langle v, x \rangle)]$ s.t. $\|v\| = 1$
  - $v_2 = \arg\max_v [\mathrm{var}(\langle v, x \rangle)]$ s.t. $\|v\| = 1, \langle v, v_1 \rangle = 0$
  - $v_3 = \arg\max_v [\mathrm{var}(\langle v, x \rangle)]$ s.t. $\|v\| = 1, \langle v, v_1 \rangle = 0, \langle v, v_2 \rangle = 0$, etc



Computing PCA

- Find $v_1 = \arg\max_v [\mathrm{var}(\langle v, x \rangle)]$ s.t. $\|v\| = 1$: we have

$$\mathrm{var}(\langle v, x \rangle) = \mathbb{E}(\langle v, x - \mathbb{E}(x) \rangle)^2 = v^\top \mathbb{E}[(x - \mathbb{E}(x))(x - \mathbb{E}(x))^\top] v = v^\top \Sigma v$$

  where $\Sigma = \mathrm{Cov}(x)$.
- Form the Lagrangian (Recall : constrained optimization)

$$\mathcal{L}(v, \lambda) = v^\top \Sigma v + \lambda(1 - v^\top v)$$

- Compute the gradient wrt v

$$\nabla_v \mathcal{L} = 2\Sigma v - 2\lambda v$$

- v is an eigenvector of Σ, λ is an eigenvalue :

$$[\nabla \mathcal{L} = 0] \Leftrightarrow [\Sigma v = \lambda v]$$

- The variance is $v^\top \Sigma v = \lambda$.

☞ v_1 is the eigenvector that corresponds to the **maximum** eigenvalue of the covariance of the data

Let's do v_2 !

- Find $v_2 = \arg\max_v [\mathrm{var}(\langle v, x \rangle)]$ s.t. $\|v\| = 1, \langle v, v_1 \rangle = 0$
- Form the Lagrangian

$$\mathcal{L}(v, \lambda, \beta) = v^\top \Sigma v + \lambda(1 - v^\top v) + \beta(0 - v_1^\top v)$$

- Compute the gradient

$$\nabla \mathcal{L} = 2\Sigma v - 2\lambda v - \beta v_1 = 0$$

- Multiplying by $v_1^\top$, and using $v_1^\top v = 0, \|v_1\| = 1, \Sigma v_1 = \lambda_1 v_1$: $\beta = 0$
- Finally, $\Sigma v = \lambda v$: (λ, v) is again a pair eigval./eigvec., and thus $\lambda = \lambda_2$

☞ v_2 is the eigenvector that corresponds to the **second maximum** eigenvalue of the covariance of the data

☞ Same for $v_3, \ldots, v_p$

Computing PCA in practice

- Of course, for real data, we use the empirical covariance $\hat{\Sigma}$

Algorithm : PCA

1. Compute empirical mean : $\hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} x_i$ (cost $O(nd)$)
2. Compute empirical cov. matrix : $\hat{\Sigma} = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \hat{\mu})(x_i - \hat{\mu})^\top$ (cost $O(nd^2)$)
3. Compute the eigenvectors of the p largest eigenvalues of $\hat{\Sigma}$ (cost $O(d^3)$)

Remark : SVD

Taking X_c the matrix of centered data $x_i - \hat{\mu}$, such that $\hat{\Sigma} = X_c^\top X_c/(n-1)$, and the Singular Value Decomposition

$$X_c = U\Gamma V^\top \qquad \text{(cost } O(nd^2 + d^3)\text{)}$$

we have directly $\hat{\Sigma} = V\Gamma^2 V^\top/(n-1)$. SVD is often "more convenient" (more algorithms available, more stable, etc.)

PCA : remarks

Standardization matter

- Often center and "whiten" data to unit norm column $\tilde{x}_i = \text{diag}(1/\sigma_k)(x_i - \hat{\mu})$
- The low-dimensional representation of x is $z = [\tilde{x}^\top v_k]_k \in \mathbb{R}^p$. Don't forget the same pre-processing ! ! Scikit-learn does it automatically.

Computational cost

SVD is costly for high n or d, but **we need only the p first eigenvectors** ! There are strategies : power iterations/Lanczos, randomized SVD...

Model selection

Popular criterion : increase p until the "explained variance"

$$\frac{\sum_{k=1}^{p} \lambda_k}{\sum_{k=1}^{d} \lambda_k}$$

is close enough to 1. But computing full SVD may be too costly ! Myriad of other strategies.

PCA for high dimensional data ($n < d$)

- When d is high, we want to avoid the cost $O(d^3)$.
- Remember : the eigenvalue equation

$$\Sigma v = \frac{1}{n-1} X_c^\top X_c v = \lambda v$$

This can be written as

$$\frac{1}{n-1} X_c X_c^\top X_c v = \lambda X_c v \Leftrightarrow Su = \lambda u$$

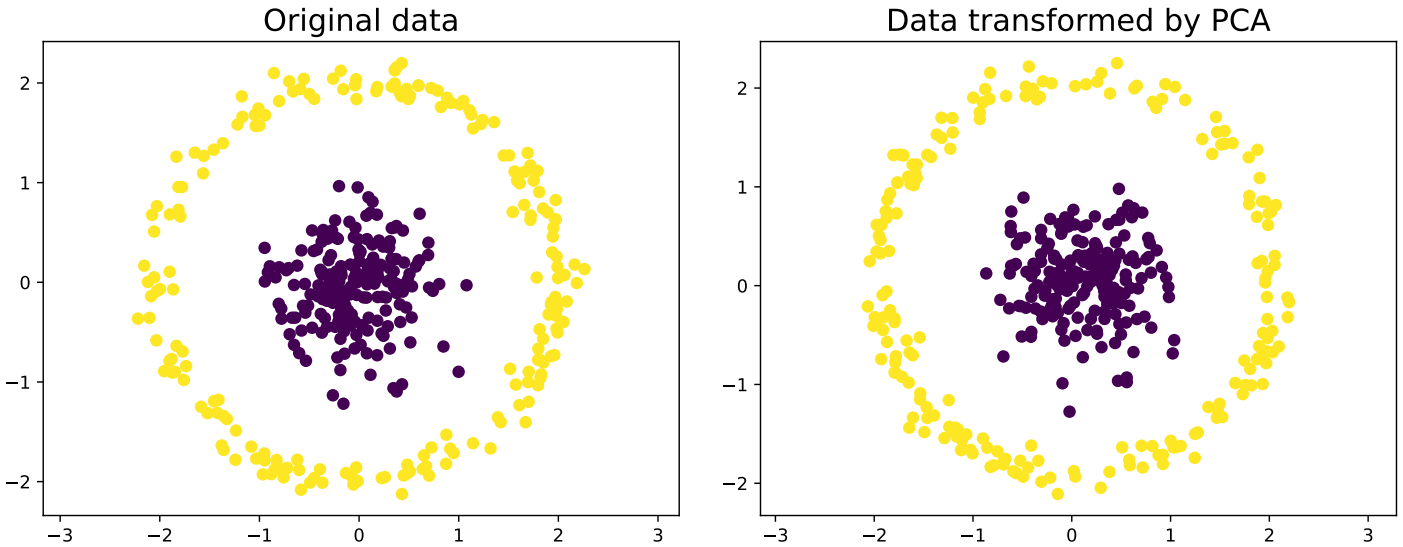
with $u = X_c v$, i.e. an eigenvalue problem on $S = \frac{1}{n-1} X_c X_c^\top$ instead.

- Properties :
  - the matrix Σ is rank $n < d$, it has only n non-zero eigenvalues.
  - Same non-zero eigenvalues as full-rank S.
  - Given v_i, $X_c v_i$ is an eigenvector of S, and given u_i, $X_c^\top v_i$ is an eigenvector of Σ. Not necessarily normalized ! !
- The decomposition can be done on S instead ! Cost $O(n^3)$. Given u_i with $\|u_i\| = 1$, v_i can be recovered (after normalization $\|v_i\| = 1$) as

$$v_i = \frac{1}{\sqrt{(n-1)\lambda_i}} X_c^T u_i$$

Kernel PCA

What to do when data are far from being linearly "oriented" ?



Kernel PCA

What to do when data are far from being linearly "oriented" ?

- Assume the data is centered $\hat{\mu} = 0$. Then $S_{ij} = \frac{1}{n-1} x_i^\top x_j$.

- (High-dim) PCA **depends only on the inner products between samples**.

- We can improve PCA by transforming the data into a higher-dimensional space $\Phi(x_i) \in \mathcal{H}$, as long as we know how to compute $\langle \Phi(x), \Phi(x') \rangle_{\mathcal{H}}$

Some properties of Kernel function

Definition (Positive semi-definite kernel)

A symmetric kernel $k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is said to be positive semi-definite (psd) iff

$$\forall n \in \mathbb{N}, \quad \forall \xi_1 \dots \xi_n \in \mathbb{R}, \quad \forall x_1 \dots x_n \in \mathbb{R}^d, \sum_{i,j}^{n} \xi_i \xi_j k(x_i, x_j) \geq 0$$

This is true for any inner product : $\sum_{i,j} \xi_i \xi_j \langle \phi(x_i), \phi(x_j) \rangle_{\mathcal{H}} = \| \sum_i \xi_i \phi(x_i) \|^2_{\mathcal{H}}$.
But the converse is also true ! !

Theorem (Mercer Theorem)

For every positive semi-definite kernel k, there exists a Hilbert space $\mathcal{H}$ and a feature map $\phi : \mathbb{R}^d \to \mathcal{H}$ such that $k(x, x') = \langle \phi(x), \phi(x') \rangle_{\mathcal{H}}$.

It is possible to choose $\mathcal{H}$ as a space of functions, such that $k(\cdot, x) \in \mathcal{H}$, and $\langle f, k(\cdot, x) \rangle_{\mathcal{H}} = f(x)$. It is called the Reproducing Kernel Hilbert Space (RKHS) associated to k.

Operations on kernels

Let k_1 and k_2 be psd, and $\lambda_{1,2} > 0$ then :

1. $\lambda_1 k_1$, (multiplication by a positive scalar)
2. $\lambda_1 k_1 + \lambda_2 k_2$, (sum of kernels),
3. $k_1 k_2$, (product of kernels),
4. $\exp(k_1)$, (exponential of kernel),
5. $(x_i, x_j) \mapsto g(x_i) g(x_j) k_1(x_i, x_j)$, with $g : \mathbb{R}^d \to \mathbb{R}$, (multiplication by a function)

are all positive semi-definite, hence valid kernels.

☞ These operations allow us to create more complicated kernels by combining simple ones.

Choosing the Kernel function

Usual kernel functions

- Linear kernel ($\mathcal{F} \equiv \mathbb{R}^d$) : $k(x, x') = x^T x'$
- Polynomial kernel (dimension of $\mathcal{F}$ increases with the order d)

$$k(x, x') = (x^T x')^d \quad \text{or} \quad (x^T x' + 1)^d$$

- Gaussian radial function ($\mathcal{F}$ with infinite dimension)

$$k(x, x') = \exp\left(-\gamma ||x - x'||^2\right)$$

- Neural net kernel ($\mathcal{F}$ with infinite dimension)

$$k(x, x') = \tanh\left(\kappa_1 x^T x' + \kappa_2\right)$$

☞ standard practice is to estimate the optimal kernel parameters by cross-validation

Kernel PCA

Idea

Replace $x_i^\top x_j$ with $k(x_i, x_j) = \langle \Phi(x_i), \Phi(x_j) \rangle_{\mathcal{H}}$...

☞ Just replace $S = \frac{1}{n-1} X_c X_c^\top$ with $S_K = \frac{1}{n-1} K$, where $K = [k(x_i, x_j)]_{ij}$.

- Compute the eigenvalues/eigenvectors (λ_k, u_k) of S_K.
- It is generally impossible to compute $v_k = \frac{\sum_i \Phi(x_i)(u_k)_i}{\sqrt{(n-1)\lambda_k}}$ since it is in $\mathcal{H}$...
- ... however for any x we can compute the projection on the components $\langle \Phi(x), v_k \rangle_{\mathcal{H}} = \frac{1}{\sqrt{(n-1)\lambda_k}} \sum_i k(x, x_i)(u_k)_i$

Centering

- Recall that we have assumed $\hat{\mu} = 0$, or equivalently, we work with $\tilde{x} = x - \hat{\mu}$.
- In the kernel space, we would like to work with $\tilde{\Phi}(x) = \Phi(x) - \frac{1}{n} \sum_i \Phi(x_i)$.
- The inner product becomes $\langle \tilde{\Phi}(x), \tilde{\Phi}(x') \rangle_{\mathcal{H}} = k(x, x') - \frac{1}{n} \sum_i [k(x, x_i) + k(x', x_i)] + \frac{1}{n^2} \sum_{ij} k(x_i, x_j)$

Kernel PCA summary

Kernel PCA

1. Construct the normalized Kernel Matrix

$$\tilde{K} = K - UK - KU + UKU$$

where $U = 1_{n\times n}/n$.

2. Solve the eigenvalue problem

$$S_{\tilde{K}} u_k = \lambda_k u_k$$

3. The projection of x is $z_k = \langle \tilde{\Phi}(x), v_k \rangle$ with $v_k = \frac{\sum_i (u_k)_i \tilde{\Phi}(x_i)}{\sqrt{\lambda_k (n-1)}}$, i.e.

$$z_k = \frac{\tilde{K}_x^\top u_k}{\sqrt{\lambda_k (n-1)}}$$

where $K_x = [k(x, x_i)]_i$ and $\tilde{K}_x = K_x - UK_x - K\frac{1_n}{n} + UK\frac{1_n}{n}$.

Example of KPCA