Machine/Statistical Learning

PCA and Kernel PCA

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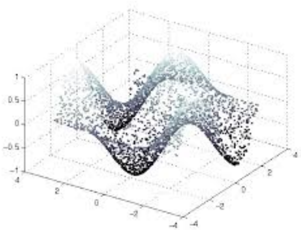
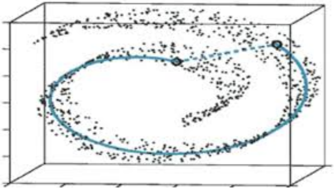
Dimension Reduction : motivation

- 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 → 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...



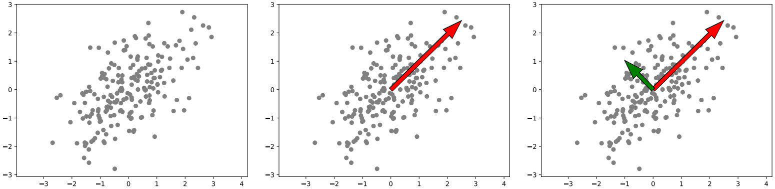
☞ Finding/learning **data representation** ("features extraction") is somehow the core of modern ML. **PCA is a foundational idea**.

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 $v_1 = \arg\max_v \left[\mathrm{var}(\langle v, x\rangle)\right]$ 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)

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

- 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

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

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 $\tilde{x}_i = \mathrm{diag}(1/\sigma_k)(x_i - \hat{\mu})$
- 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

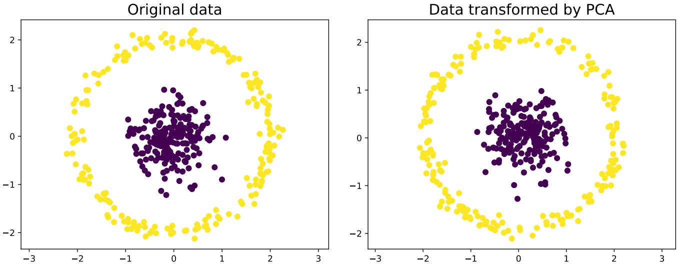
  $$\frac{1}{n-1} X_c X_c^\top X_c v = \lambda X_c v \Leftrightarrow Su = \lambda u$$

  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"?



Original data

Data transformed by PCA

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

$$\forall n \in \mathbb{N}, \quad \forall \xi_1 \dots \xi_n \in \mathbb{R}, \quad \forall \mathrm{x}_1 \dots \mathrm{x}_n \in \mathbb{R}^d, \sum_{i,j}^{n} \xi_i \xi_j k(\mathrm{x}_i, \mathrm{x}_j) \geq 0$$

This is true for any inner product : $\sum_{i,j} \xi_i \xi_j \langle \phi(\mathrm{x}_i), \phi(\mathrm{x}_j) \rangle_{\mathcal{H}} = \| \sum_i \xi_i \phi(\mathrm{x}_i) \|_{\mathcal{H}}^2$.
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. $(\mathrm{x}_i, \mathrm{x}_j) \mapsto g(\mathrm{x}_i) g(\mathrm{x}_j) k_1(\mathrm{x}_i, \mathrm{x}_j)$, 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

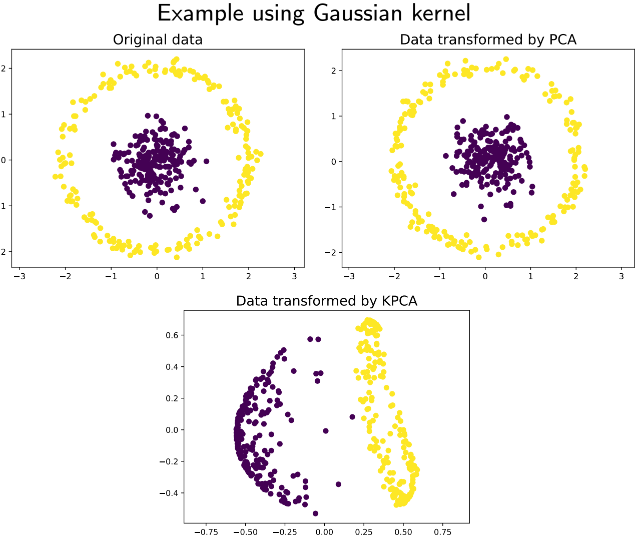
$$S_{\tilde{K}} u_k = \lambda_k u_k$$

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


Example using Gaussian kernel
Original data
Data transformed by PCA
Data transformed by KPCA