PCA, kernel PCA, Laplacian eigenmaps

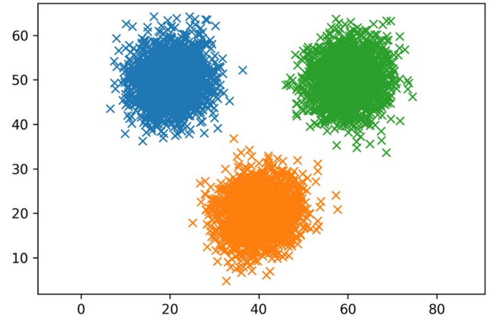
- Feature selection / generation without using labels

PCA
(Karhunen-Loève transform)

Samples

$$x=\begin{pmatrix} x_1 \\ x_2 \\ . \\ . \end{pmatrix}=\begin{pmatrix} x_1(1) & x_1(2) & \dots & x_1(N) \\ x_2(1) & x_2(2) & \dots & . \\ . & . & \dots & . \\ . & . & \dots & x_K(N) \end{pmatrix}$$

Features



Normalize the samples and write the covariance matrix $y_i = x_i - \mu_i$

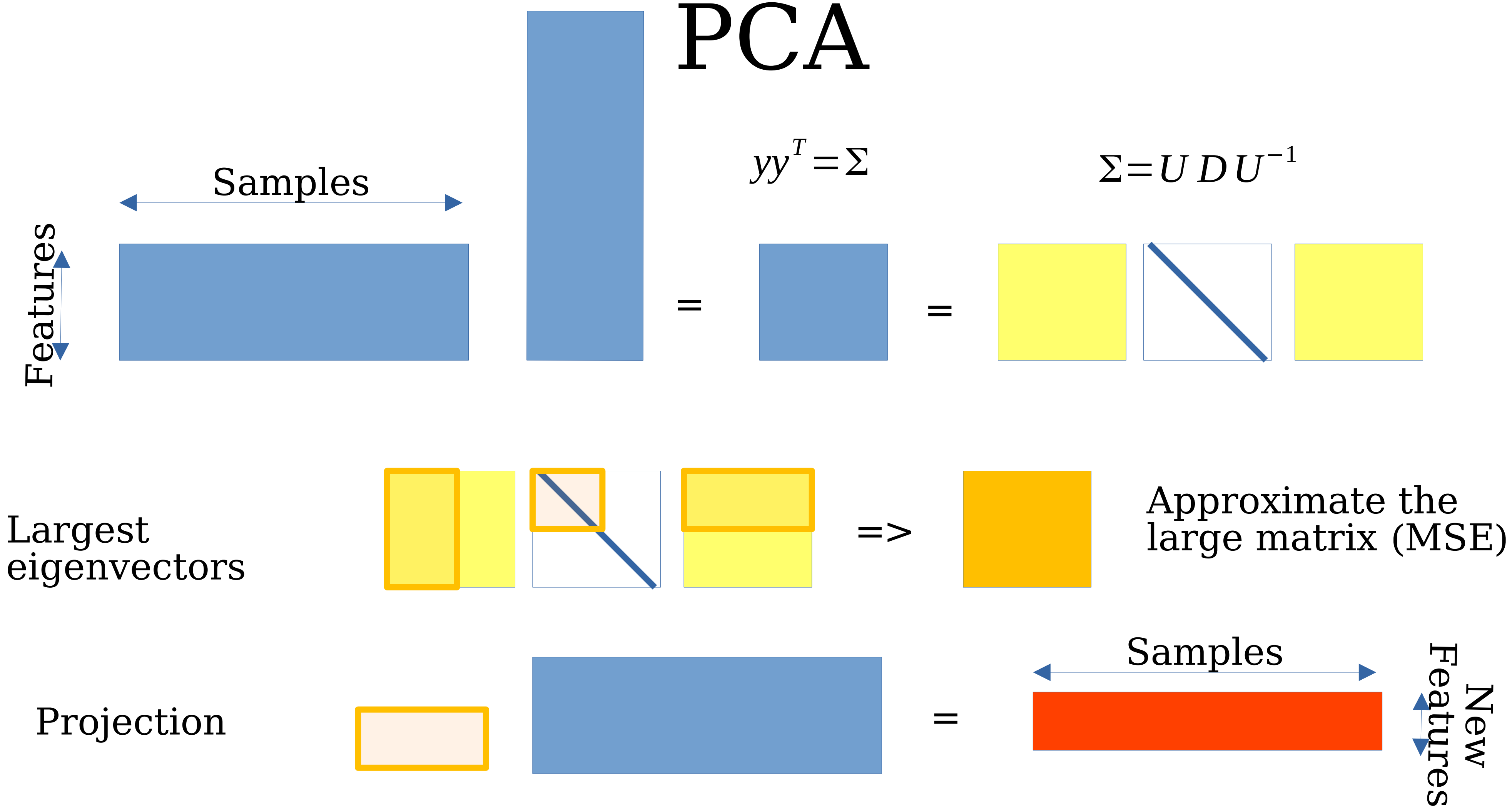
$$yy^T = \Sigma$$

Diagonalize the covariance matrix

$$\Sigma = U\,D\,U^{-1}$$

Note: no label information used

PCA

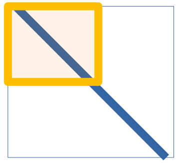

Samples
Features
$yy^T = \Sigma$
$\Sigma = U\,D\,U^{-1}$
=
=
Largest eigenvectors
=>
Approximate the large matrix (MSE)
Projection
=
Samples
New Features

PCA

$$Y = A^T X$$

Maximizing the covariance

$$YY^T = \Sigma_y = A^T XX^T A = A^T \Sigma_x A$$

If $A = U$ Matrix of eigenvectors, $\Sigma_y =$ 

- Zero covariance,
- maximal variance with largest eigenvalues

Note: $\underset{w}{argmax} \dfrac{w^T Mw}{w^T w}$ Solution: w eigenvector of M with largest eigenvalue

Min-max (Courant-Fisher-Weyl) theorem

PCA

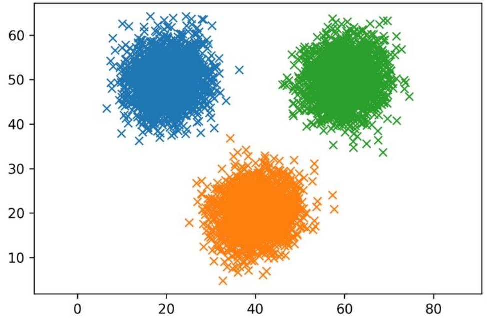
- Some visual examples

LDA & PCA

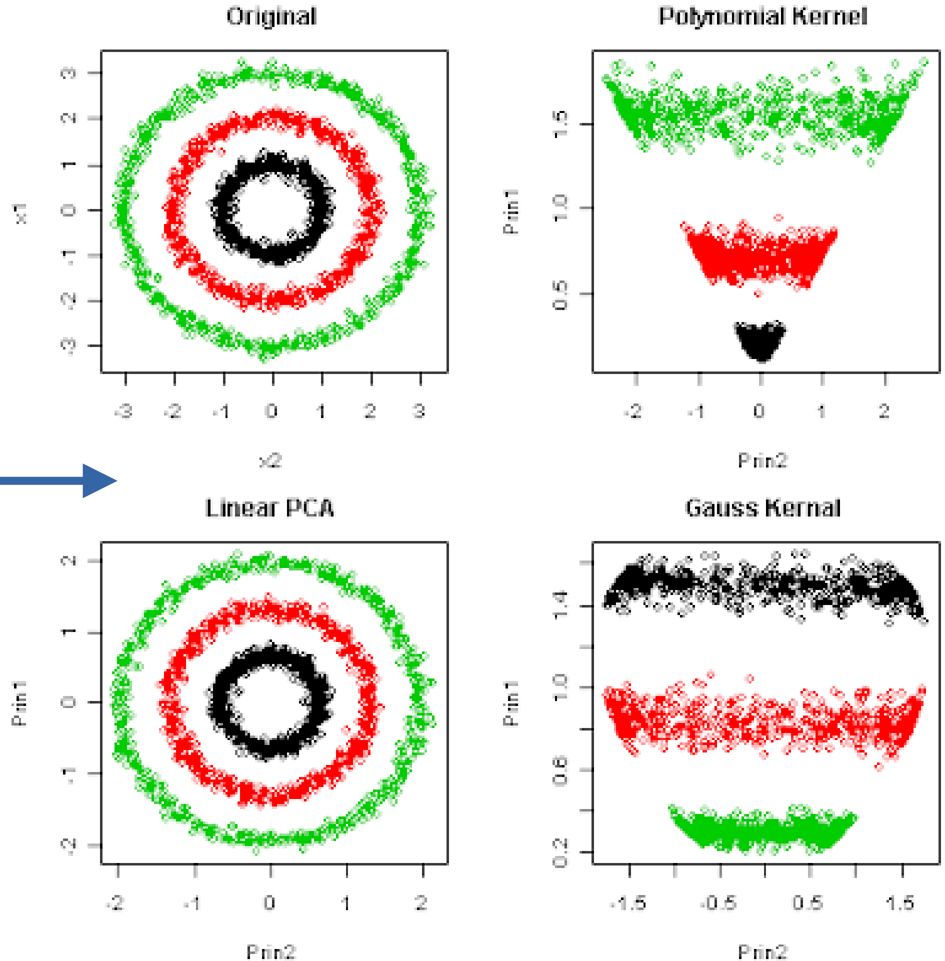
- Remarks: complex mix of initial features, can loose interpretability / explainability

  what the important features? Difficult to answer
- Only linear separability

Kernel PCA



Data not linearly separable:
Send the data in a higher dimensional space, nonlinearly



Kernel PCA

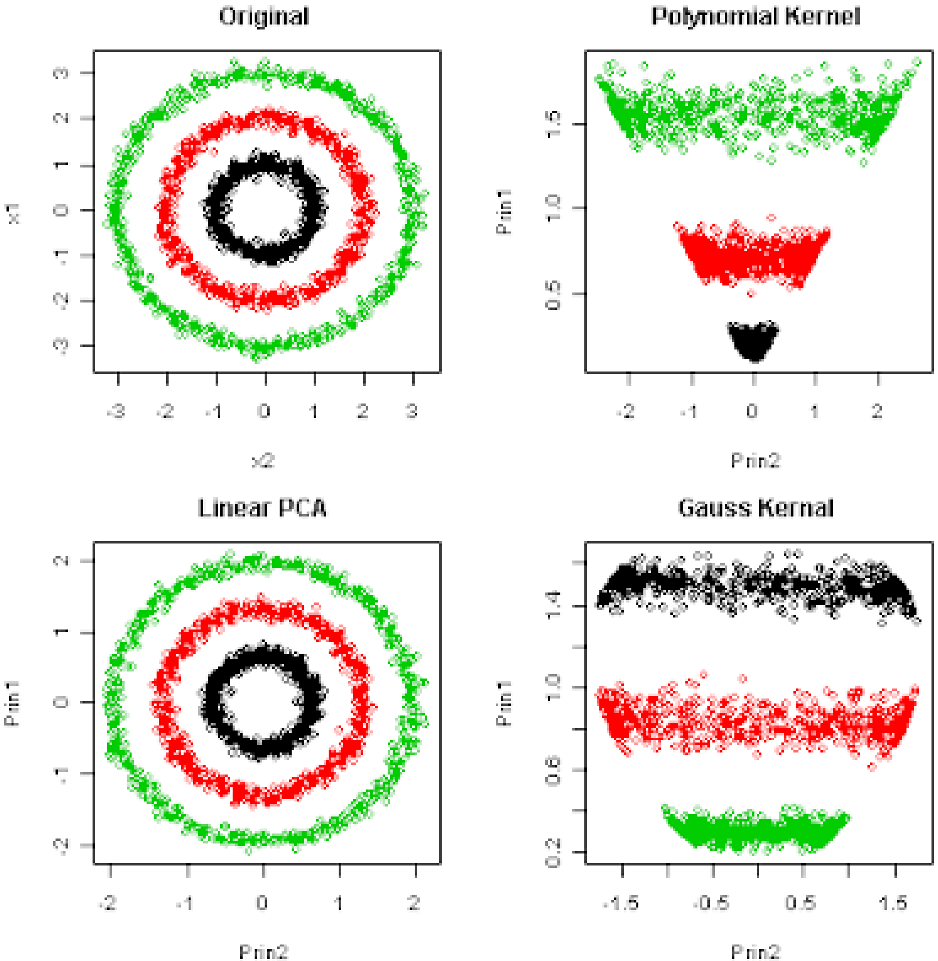
$$Y = A^T X$$

Matrix, linear transformation:
Rotation, translation, reflection, shear

Nonlinear transformation + high dimensional

$$\phi : \mathbb{R}^n \rightarrow \mathbb{R}^d$$
$$\phi : x \rightarrow \phi(x)$$

PCA in the high dimensional space ?
→ No, untractable



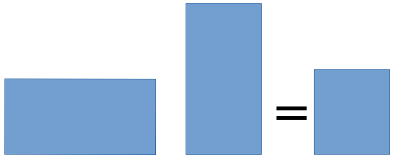
Going in high dimension

Singular Value Decomposition (SVD):
Same non-zero eigenvalues

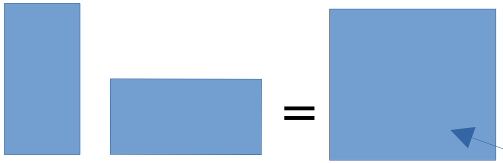
$$X = U \Lambda V^H$$

Going in high dimension

$X^T X$



XX^T



Covariance matrix,
Correlation matrix,
Gram matrix
In high dim space

Eigenvector v

$$X^T X v = \lambda v \qquad XX^T X v = \lambda X v$$

Eigenvector $u = Xv$ of the covariance matrix!

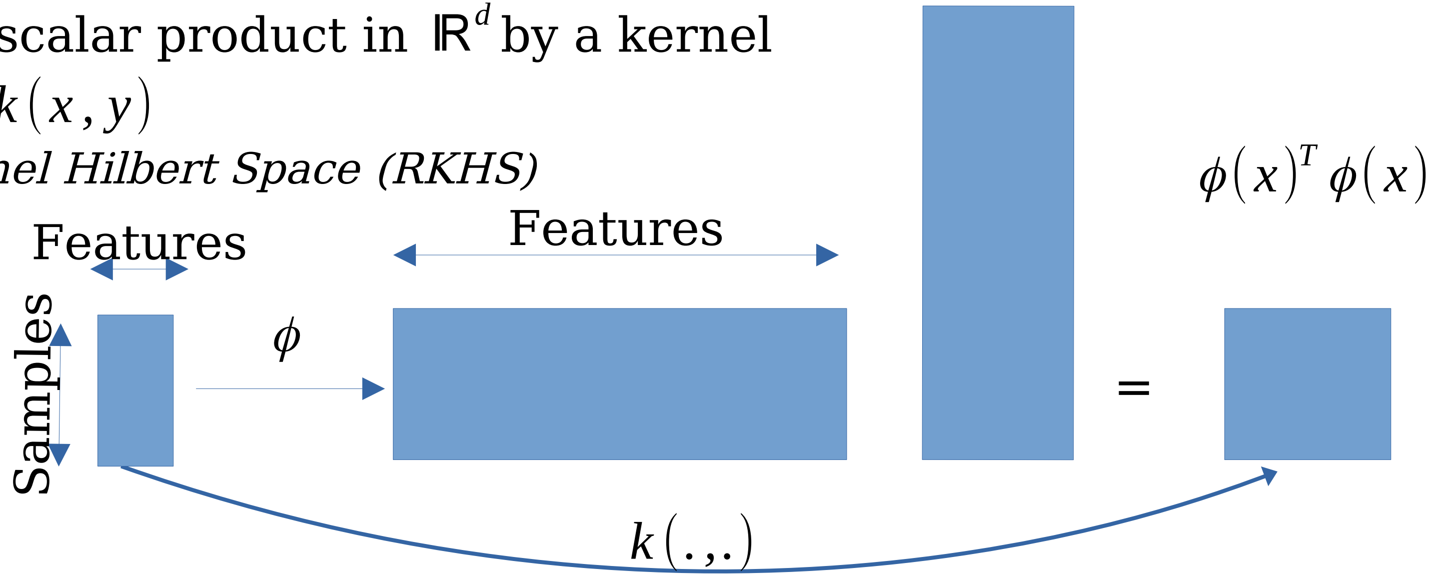
$$XX^T u = \lambda u$$

The kernel trick!

We replace the scalar product in $\mathbb{R}^d$ by a kernel

$$(\phi(x), \phi(y)) = k(x, y)$$

Reproducible Kernel Hilbert Space (RKHS)



Examples:

Gaussian kernel (RBF) $K(\mathbf{x}, \mathbf{y}) = \exp\left(-\frac{\|\mathbf{x}-\mathbf{y}\|^2}{2\sigma^2}\right).$

Polynomial kernel $K(x, y) = (x^\mathsf{T} y + c)^d$

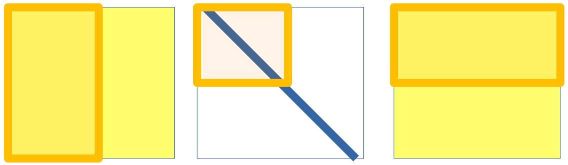
See Moore-Aronszajn theorem for conditions on k

The kernel trick!

$$\phi(x)^T \phi(x) = \begin{pmatrix} k(x_1, x_1) & k(x_1, x_2) & \dots \\ k(x_2, x_1) & k(x_2, x_2) & \dots \\ \vdots & . & . \\ . & . & k(x_N, x_N) \end{pmatrix}$$

Let us diagonalize this matrix!

Largest eigenvectors



$$\phi(x)^T \phi(x) v_k = \lambda_k v_k$$

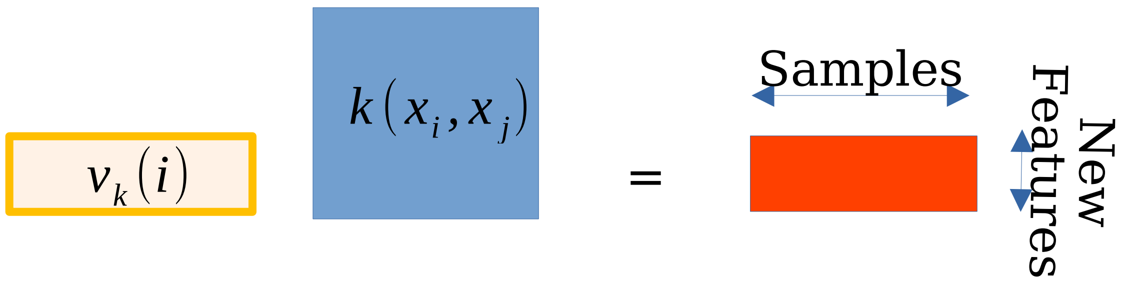
$$u_k = \phi(x) v_k$$

BUT: we cannot directly project, we have to pass through the high dim. space

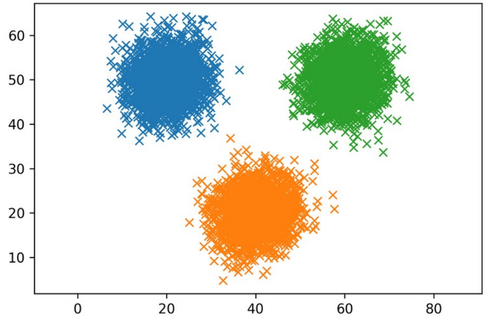
The kernel trick!

$$\underbrace{(u_k, \phi(x))}_{\text{In the high dim space}} = (\phi(x) v_k, \phi(x)) = v_k^T \underbrace{\phi(x)^T \phi(x)}_{\text{Replace by kernel}} = \sum_{i=1}^{N} \underbrace{v_k(i) k(x_i, x)}_{\text{In the original space}}$$

Projection



Kernel PCA



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