

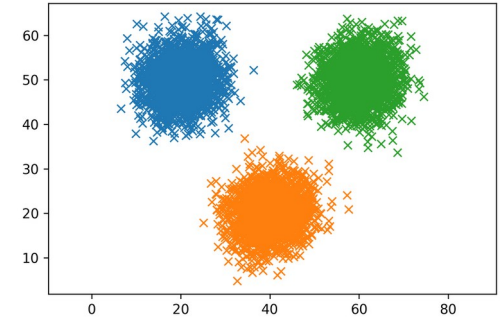
PCA, kernel PCA, Laplacian eigenmaps

- Feature selection / generation without using labels

PCA

(Karhunen-Loève transform)

$$\begin{array}{c}
 \xleftarrow{\text{Samples}} \\
 \mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ \vdots \end{pmatrix} = \begin{pmatrix} x_1(1) & x_1(2) & \dots & x_1(N) \\ x_2(1) & x_2(2) & \dots & \cdot \\ \cdot & \cdot & \dots & \cdot \\ \cdot & \cdot & \dots & x_K(N) \end{pmatrix} \xrightarrow{\text{Features}}
 \end{array}$$



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

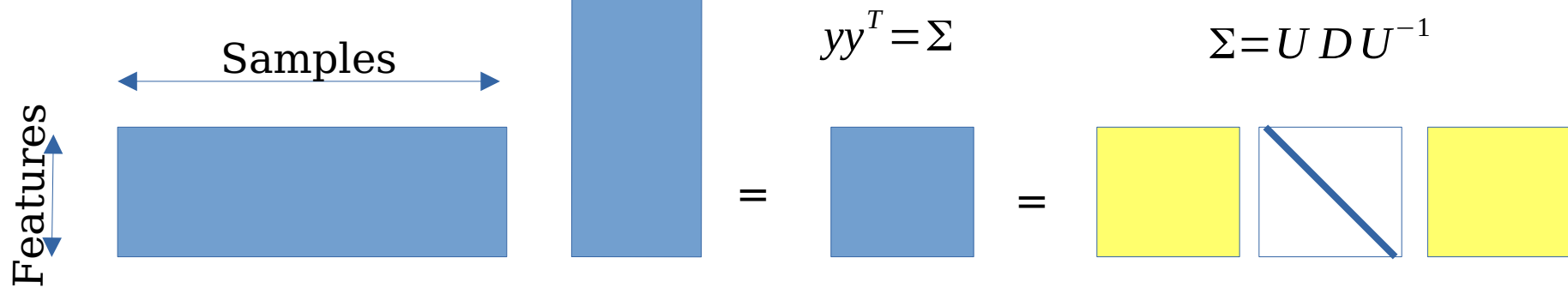
$$yy^T = \Sigma$$

Diagonalize the covariance matrix

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

Note: no label information used

PCA



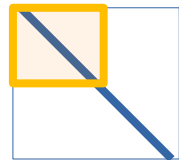
PCA

$$Y = A^T X$$

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: $\underset{w}{argmax} \frac{w^T M w}{w^T w}$

Solution: w eigenvector of M with largest eigenvalue

Min-max (Courant-Fisher-Weyl) theorem

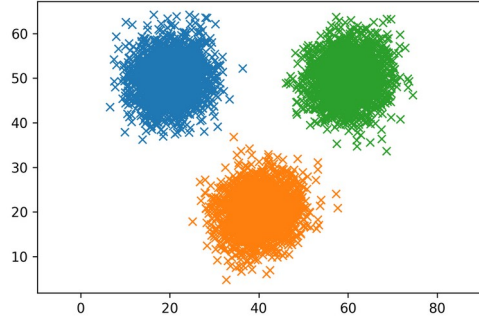
PCA

- Some visual examples

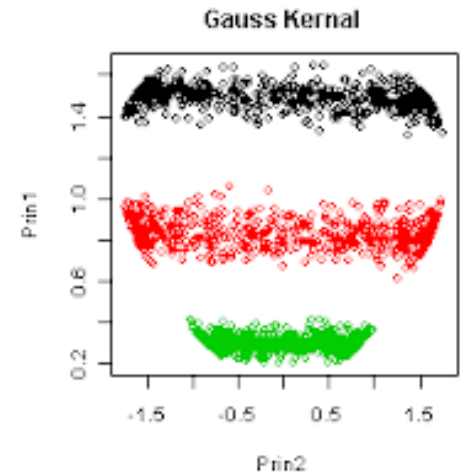
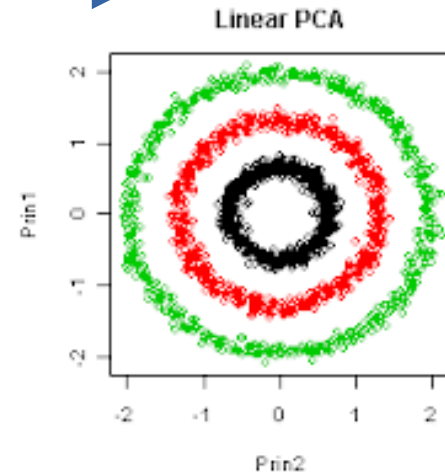
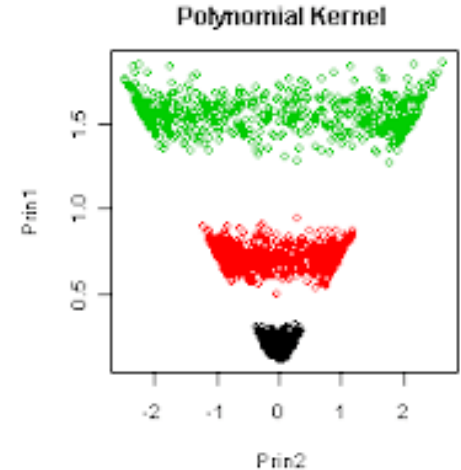
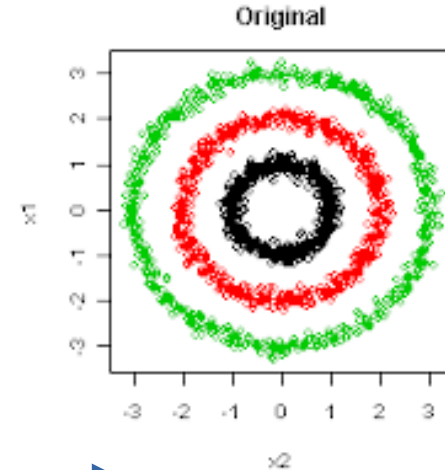
LDA & PCA

- 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

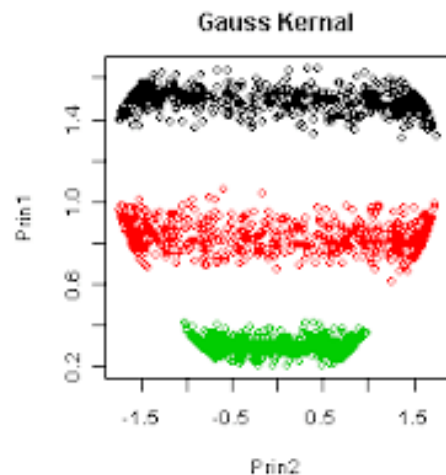
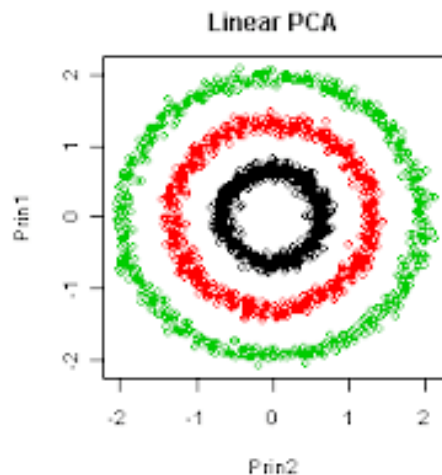
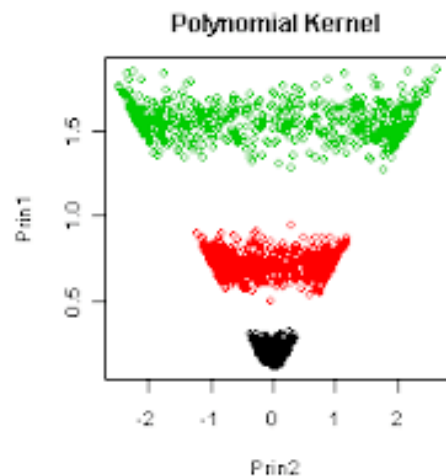
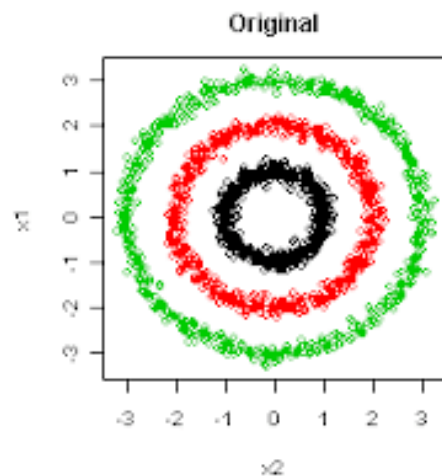
$$Y = A^T X$$

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

Nonlinear transformation + high dimensional

$$\begin{aligned}\phi: \mathbb{R}^n &\rightarrow \mathbb{R}^d \\ \phi: x &\rightarrow \phi(x)\end{aligned}$$

PCA in the high dimensional space ?
→ No, untractable



Going in high dimension



$$XX^T$$

A diagram showing the matrix product XX^T . It consists of a small blue rectangle, followed by a taller blue rectangle, an equals sign, and a small blue square.

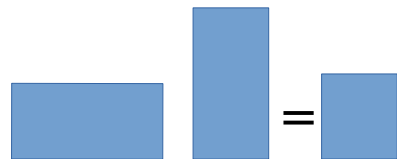
$$X^T X$$

A diagram showing the matrix product $X^T X$. It consists of a tall blue rectangle, followed by a small blue rectangle, an equals sign, and a blue square.

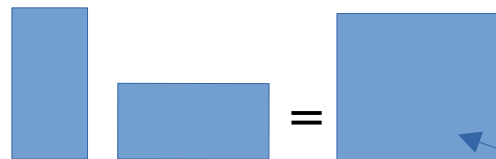
Singular Value Decomposition (SVD):
Same non-zero eigenvalues

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

Going in high dimension

$$X^T X$$


A diagram illustrating the multiplication of two matrices. On the left, a wide blue rectangle (representing X^T) is followed by a tall blue rectangle (representing X). An equals sign follows, and then a small blue square (representing the resulting $X^T X$ matrix).

$$X X^T$$


A diagram illustrating the multiplication of two matrices. On the left, a tall blue rectangle (representing X) is followed by a wide blue rectangle (representing X^T). An equals sign follows, and then a large blue square (representing the resulting $X X^T$ matrix).

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

Eigenvector v

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

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

Eigenvector $u = X v$ of the covariance matrix!

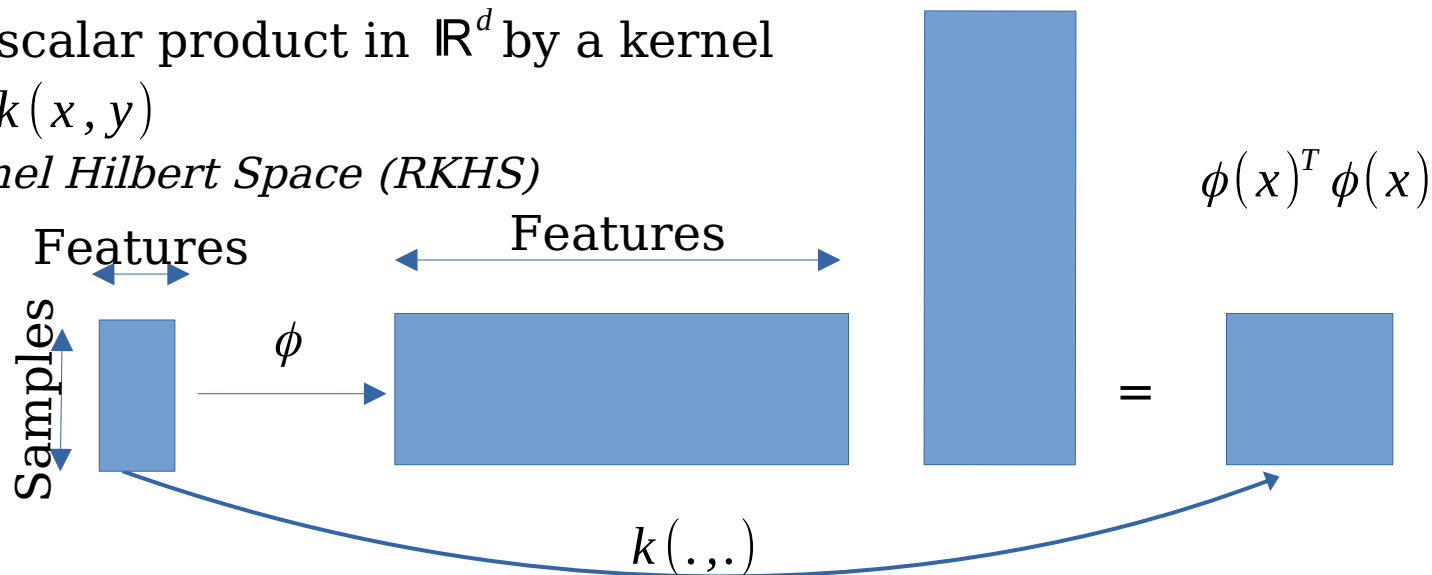
$$X X^T u = \lambda u$$

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

$$K(x, y) = (x^T y + c)^d$$

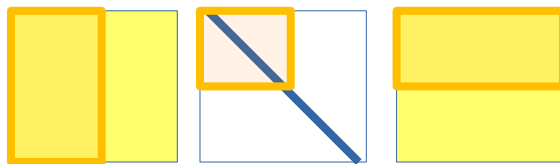
See Moore-Aronszajn theorem for conditions on k

The kernel trick!

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

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!

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

In the high dim space

Replace by kernel

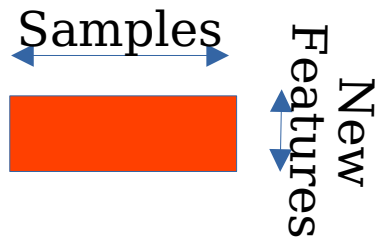
In the original space

Projection

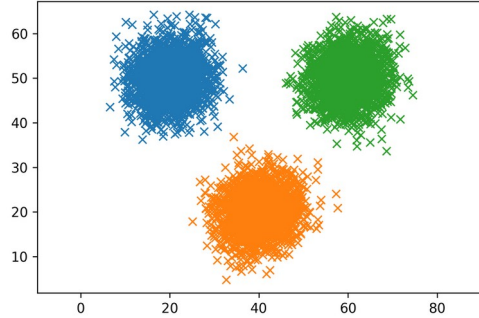
$$v_k(i)$$

$$k(x_i, x_j)$$

=



Kernel PCA



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