In The Name of Allah

Digital Media Laboratory
Sharif University of Technology

Statistical Pattern Recognition

Introduction to Kernel Methods

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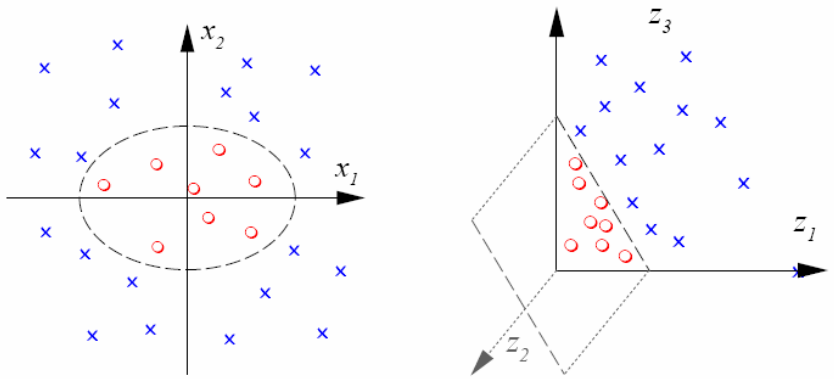
http://ce.sharif.edu/courses/90-91/2/ce725-1/

Agenda

- **Motivations**
- **Kernel Definition**
- **Mercer's Theorem**
- **Kernel Matrix**
- **Kernel Construction**

Motivations

- **Learning linear classifiers can be done effectively (SVM, Perceptron, …).**
  - **How to generalize existing efficient linear classifiers to non-linear ones.**
- **It may be hard to classify data points in the original feature space.**
  - **Use an appropriate high dimensional non-linear map to change the feature space.**



Kernel Definition

- Consider data x lying in R^n.
- Use a high dimensional mapping Φ: $R^n \rightarrow R^N$, with N>n.
- Define the kernel function $K(x,x') = \Phi(x)^T \Phi(x')$.
  - That is the kernel function is the dot product in the new feature space.
  - Dot product measures the similarity of two data points.
  - K(x,x') shows the similarity of x and x'.
  - It is efficient to use K instead of Φ if the dimensionality of Φ is high (Why?).

Kernel Definition

- **A simple example:**
  - **Consider x = (x_1, x_2) lies in 2 dimensional plane and $\Phi : R^2 \rightarrow R^3$ with the following definition**

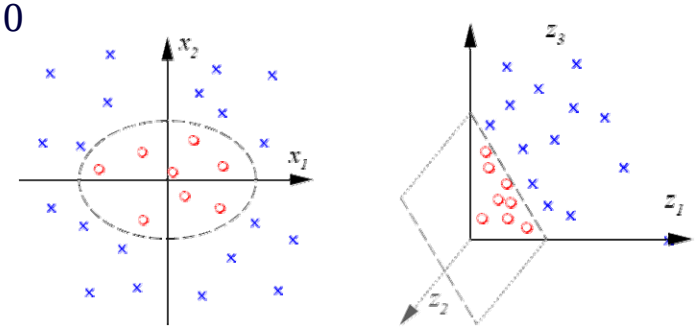
$$\Phi(x_1, x_2) = (z_1, z_2, z_3) = (x_1^2, \sqrt{2}x_1x_2, x_2^2)$$

  - **A linear classifier in new space will become (w' is a vector in new space):**

$$g(x) = w'^T x' + w'_0 = w'^T \Phi(x) + w'_0 = w'_1 x_1^2 + \sqrt{2} w'_2 x_1 x_2 + w'_3 x_2^2 + w'_0$$

  - **What will be the shape of separating curve in the original space?**

$$w'_1 x_1^2 + \sqrt{2} w'_2 x_1 x_2 + w'_3 x_2^2 + w'_0 = 0$$



Kernel Definition

- **What will be the kernel function in the previous example?**

$$K(u,v)=\Phi(u)^T\Phi(v)=\begin{pmatrix}u_1^2\\ \sqrt{2}u_1u_2\\ u_2^2\end{pmatrix}^T\begin{pmatrix}v_1^2\\ \sqrt{2}v_1v_2\\ v_2^2\end{pmatrix}$$

$$=(u_1v_1)^2+2(u_1v_1)(u_2v_2)+(u_2v_2)^2$$

$$=(u_1v_1+u_2v_2)^2=(u^Tv)^2$$

The dot product in the new space is squared of the dot product in the original space.

- **Can we construct an arbitrary conic section in original feature space? Why?**

We instead use $(u^Tv+1)^2$

Kernel Definition

- **Some typical kernels include :**
  - **Polynomial:** $K(u,v)=\left(u^T v+c\right)^d$
  - **Sigmoid:** $K(u,v)=\tanh\left(\kappa u^T v+\theta\right)$
  - **Gaussian RBF:** $K(u,v)=\exp\left\{-\|u-v\|^2/2\sigma^2\right\}$
- **Can any function K(u,v) be a valid kernel function?**
  - **That is, does there exist a function Φ with $K(u,v) = \Phi(u)^T \Phi(v)$?**
  - **In the case of Mercer's condition, it is a valid kernel function.**

Mercer's Theorem

- **If for any squared integrable function f(.), we have**

$$\int_{R^{2n}} K(x,x')f(x)f(x')dxdx' \geq 0$$

then the function K(x, x') is a valid kernel function.

- **In this case the components of the corresponding function Φ are proportional to the eigenfunctions of K(x, x'), that is**

$$\Phi(x) = \begin{pmatrix} \sqrt{\lambda_1}\varphi_1(x) \\ \sqrt{\lambda_2}\varphi_2(x) \\ \vdots \\ \end{pmatrix} \qquad \int_{R^n} K(u,v)\varphi_i(v)dv = \lambda_i\varphi_i(u)$$

In fact Mercer's theorem checks that if K(x, y) is positive semi-definite and hence all $\lambda_i \geq 0$.

Kernel Matrix

- **Restricting the kernel function to a set of points $\{x_1, \ldots, x_k\}$, the kernel function can be represented with a matrix :**

$$K = \begin{bmatrix} K(x_1,x_1) & K(x_1,x_2) & \cdots & K(x_1,x_k) \\ K(x_2,x_1) & \ddots & & \\ \vdots & & & \\ K(x_k,x_1) & & & K(x_k,x_k) \end{bmatrix}$$

- **A matrix K is a valid kernel matrix if it is a positive semi-definite matrix,**
  - **That is, all its eigenvalues are greater or equal to zero.**
  - **The eigenvectors multiplied by squared roots of eigenvalues will be the restrictions of φ_i to the set $\{x_1, \ldots, x_k\}$.**

Polynomial Kernel

- **2nd degree polynomial:**

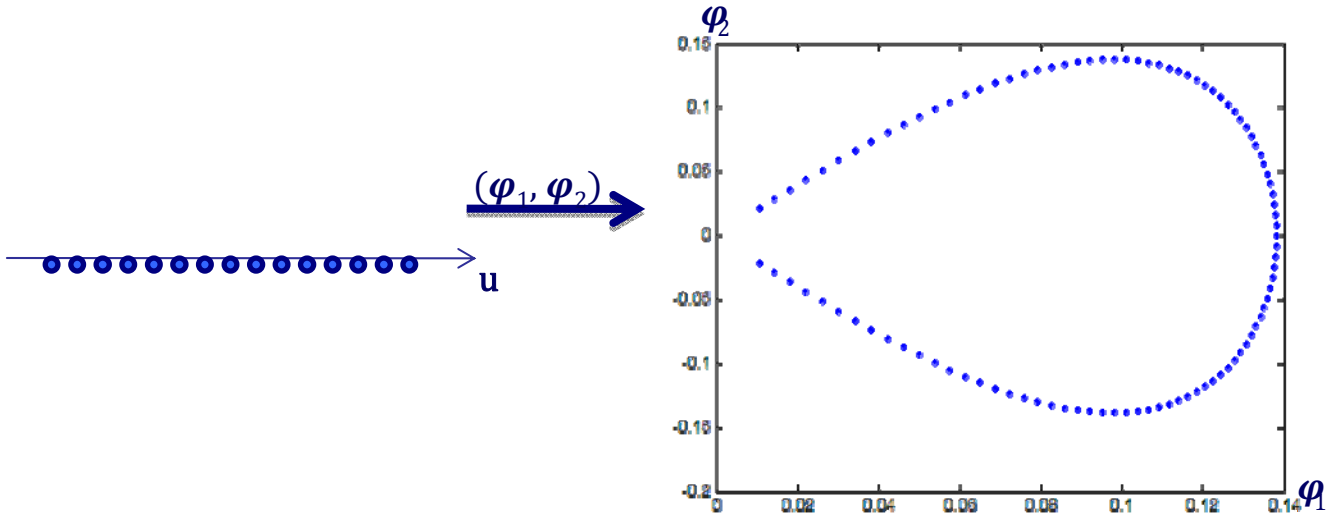
$$K(u,v)=\left(u^T v\right)^2=\left(u_1v_1+u_2v_2\right)^2$$
$$=\begin{pmatrix} u_1^2 \\ \sqrt{2}u_1u_2 \\ u_2^2 \end{pmatrix}^T \begin{pmatrix} v_1^2 \\ \sqrt{2}v_1v_2 \\ v_2^2 \end{pmatrix}$$

- **Up to 2nd degree polynomial:**
  - **Can construct any 2nd order function in original feature space**

$$K(u,v)=\left(u^T v+1\right)^2=\left(u_1v_1+u_2v_2+1\right)^2$$
$$=\begin{pmatrix} u_1^2 \\ \sqrt{2}u_1u_2 \\ \sqrt{2}u_1 \\ \sqrt{2}u_2 \\ u_2^2 \\ 1 \end{pmatrix}^T \begin{pmatrix} v_1^2 \\ \sqrt{2}v_1v_2 \\ \sqrt{2}v_1 \\ \sqrt{2}v_2 \\ v_2^2 \\ 1 \end{pmatrix}$$

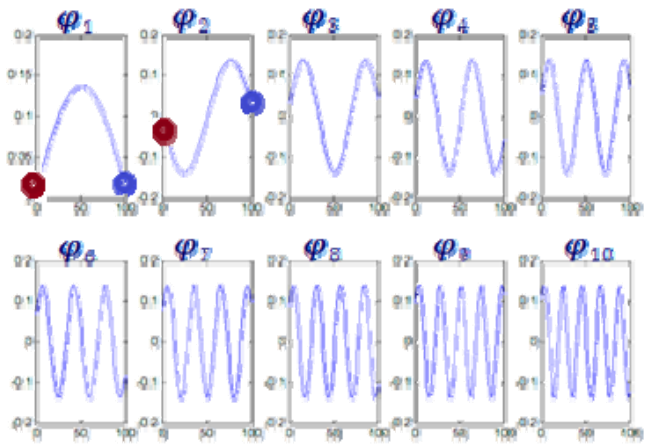
RBF Kernel

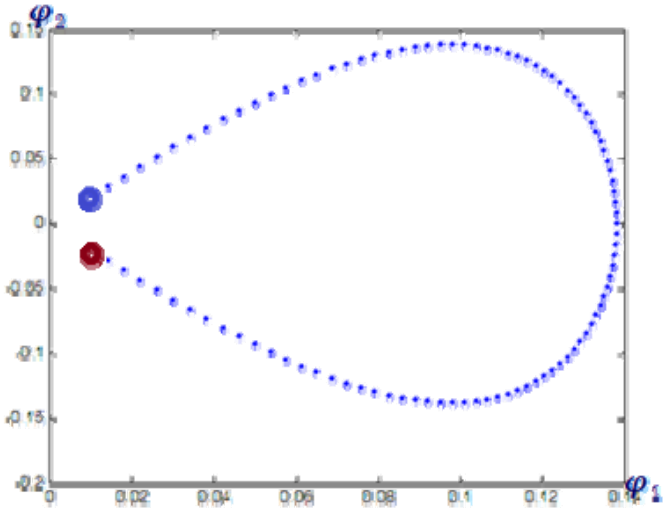
- **An example**
  - **That is the input space -5<u<5 will be mapped to a curve using only 2 dimensions of Φ.**



RBF Kernel

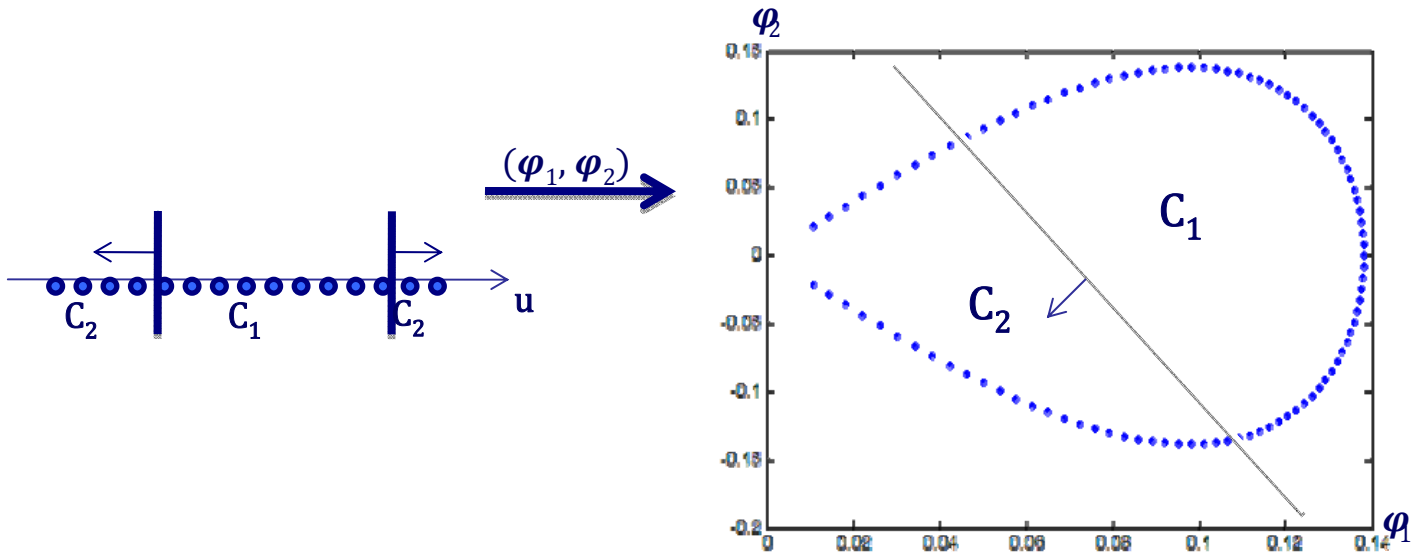
- **An example (cont.)**
  - **Consider the Gaussian kernel :** $K(u,v) = \exp\left\{-\|u-v\|^2 / 2\sigma^2\right\}$
    - Where u lies in a subset of R, -5<u<5.
    - The eigenfunctions of K are illustrated. $\Phi = (\boldsymbol{\varphi}_1, ..., \boldsymbol{\varphi}_{10}, ...)$.





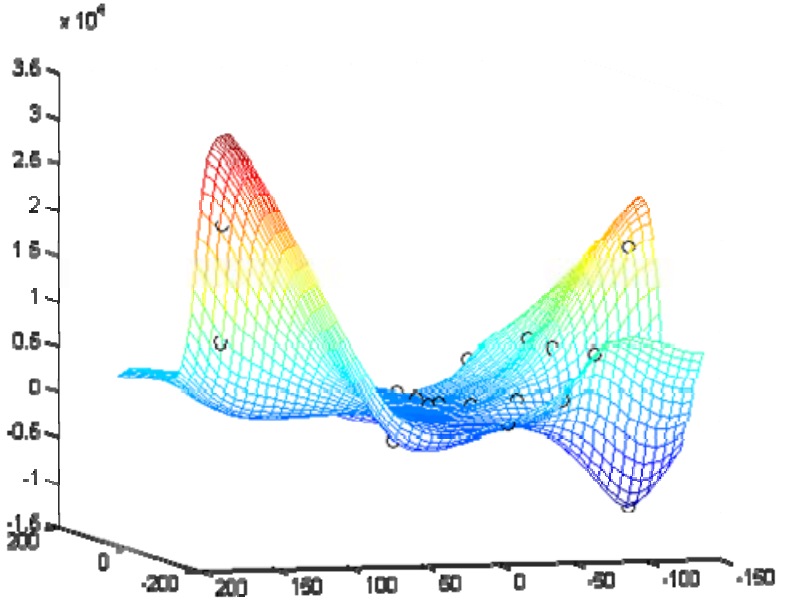
RBF Kernel

- **An example (cont.)**
  - **Consider a linear classifier in the new space.**
  - **The corresponding classifier in the u space is clearly non-linear in the original space.**



RBF Kernel

- RBF kernel considers a Gaussian around each data point.
- Linear discriminant function cuts through the surface in embedding function.
- Therefore any arbitrary set of points can be classified by RBF kernels.
- Training error is zero when $\sigma \rightarrow 0$.



Kernel Construction

- How to build valid kernels from existing kernels?
- According to Mercer's theorem if $c > 0$ and k_1, k_2 are valid kernels, and ψ is an arbitrary function, then following functions will also be valid kernels:
  - $K(u,v) = ck_1(u,v)$
  - $K(u,v) = k_1(u,v) + k_2(u,v)$
  - $K(u,v) = k_1(u,v)\, k_2(u,v)$
  - $K(u,v) = k_1(\psi(u), \psi(v))$

Kernel Construction

- **Construct kernels from probabilistic generative models (class conditional probabilities, HMM, …) and then use the kernel in a discriminative model (such as SVM or linear discriminant functions, …).**
- **K(x,x') = p(x)p(x') is clearly a valid kernel, which states that x and x' are similar if they both have high probability (Why it is valid?).**
- **A better kernel can be constructed in the same way :**

$$K(u,v) = \sum_{i=1}^{n} p(u \mid c_i) p(v \mid c_i) p(c_i)$$

  - **That is u and v are similar if they have high probabilities under same classes.**

Kernel Construction

- State of the arts methods tries to learn the kernel from (probably many) training points.
- The simplest one is the multiple kernel learning.
  - Consider $\{k_1, \ldots, k_n\}$ as n valid kernels.
  - Find an appropriate kernel, k(u,v), from the training data $K(u,v) = \sum_{i=1}^{n} c_i k_i(u,v),\ c_i \geq 0$
  - Minimize training loss (MSE) by changing c_i and simultaneously minimize trace of the kernel matrix on training data to avoid overfitting.
  - Many variations of the algorithm are developed.

Any Question?

End of Lecture 11

Thank you!

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