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Designing Kernel Functions Using the Karhunen-Loève Expansion

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Learning with Kernels

- Kernel methods:
  Approximate unknown function $f(x)$ by

$$\hat{f}(x) = \sum_{i=1}^{n} \alpha_i K(x, x_i)$$

α_i : Parameters
$K(x, x')$: Kernel function
x_i : Training points

- Kernel methods are known to generalize very well, given appropriate kernel function.
- Therefore, how to choose (or design) kernel function is critical in kernel methods.

Recent Development in Kernel Design

- Recently, a lot of attention have been paid to designing kernel functions for non-vectorial structured data.

  e.g., strings, sequence, trees, graphs.
- In this talk, however, we discuss the problem of designing kernel functions for standard vectorial data.

Choice of Kernel Function

- A kernel function is specified by
  - A family of functions (Gaussian, polynomial, etc.)
  - Kernel parameters (width, order, etc.)
- We usually focus on a particular family (say Gaussian), and optimize kernel parameters by, e.g., cross-validation.
- In principle, it is possible to optimize the family of kernels by CV.
- However, this does not seem so common because of too many degrees of freedom.

Goal of Our Research

- We propose a method for finding optimal family of kernel functions using some prior knowledge on problem domain.
- We focus on
  - Regression (squared-loss)
  - Translation-invariant kernel

$$K(x,x') = K(x - x')$$

- We do not assume kernel is positive semi-definite, since “kernel trick” is not needed in some regression methods (e.g. ridge).

Outline of The Talk

- A general method for designing translation-invariant kernels.
- Example of kernel design for binary regression.
- Implication of the results.

Specialty of Learning with Translation-Invariant Kernels

- Ordinary linear models:

$$\hat{f}(x) = \sum_{i=1}^{p} \alpha_i \varphi_i(x)$$

α_i : Parameters

$\varphi_i(x)$: Basis function

- Kernel models:

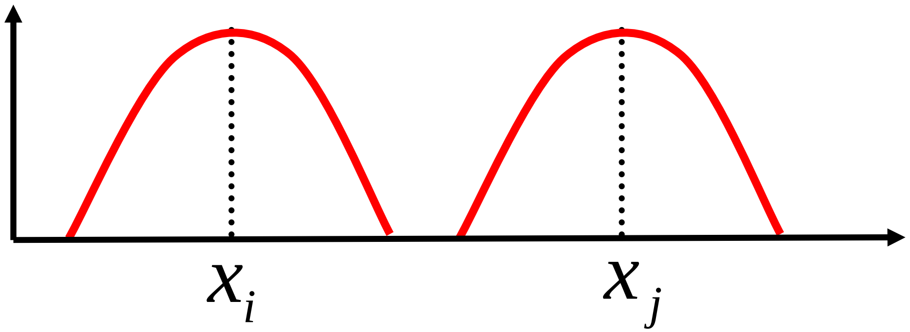
$$\hat{f}(x) = \sum_{i=1}^{n} \alpha_i K(x - x_i)$$

$K(x - x')$
: Translation-invariant kernel

- x_i is center of kernels.
- All basis functions have same shape!

Local Approximation by Kernels

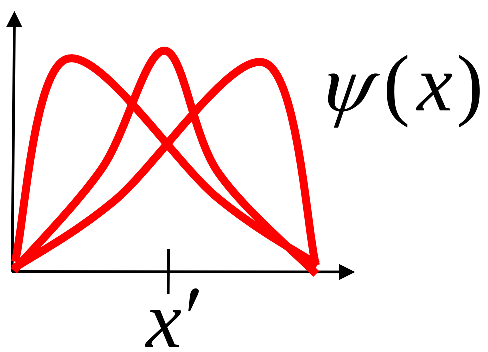
- Intuitively, each kernel function is responsible for local approximation in the vicinity of each training input point.

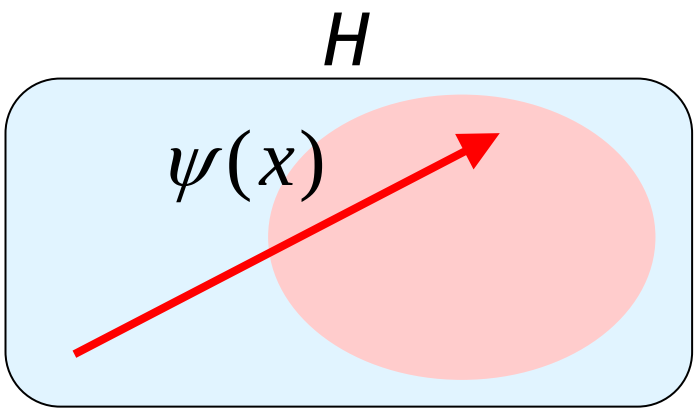


- Therefore, we consider the problem of approximating a function locally by a single kernel function.

Set of Local Functions and Function Space

- $\psi(x)$: A local function centered at x'
- Ψ : Set of all local functions
- H : A functional Hilbert space which contains Ψ (i.e., space of local functions)
- Suppose $\psi(x)$ is a probabilistic function.





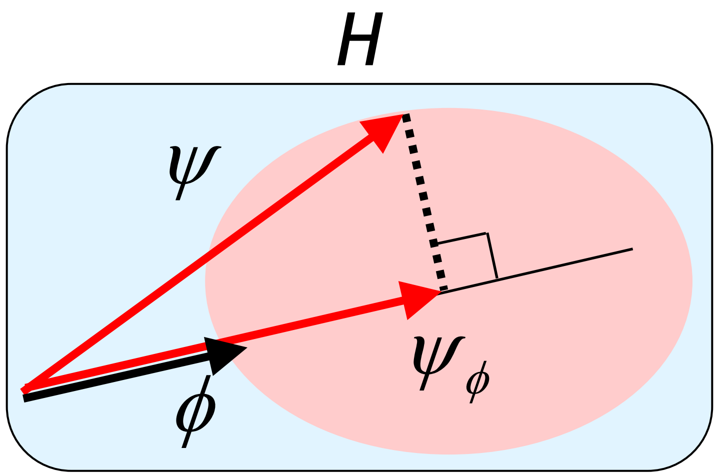
Optimal Approximation to Set of Local Functions

- We are looking for the optimal approximation to the set Ψ of local functions $\psi(x)$.
- Since we are interested in optimizing the family of functions, scaling is not important.
- We search the optimal direction ϕ_{opt} in H.

$$\phi_{opt} = \underset{\phi \in H}{\arg\min}\, E\left\|\psi - \psi_{\phi}\right\|^2$$

E : Expectation over ψ

ψ_{ϕ} : Projection of ψ onto ϕ



Karhunen-Loève Expansion

$$\phi_{opt} = \arg\min_{\phi \in H} E\left\| \psi - \psi_{\phi} \right\|^2$$

- R : Correlation operator of local functions

$$R\varphi = E\left[\langle \varphi, \psi \rangle \psi\right]$$

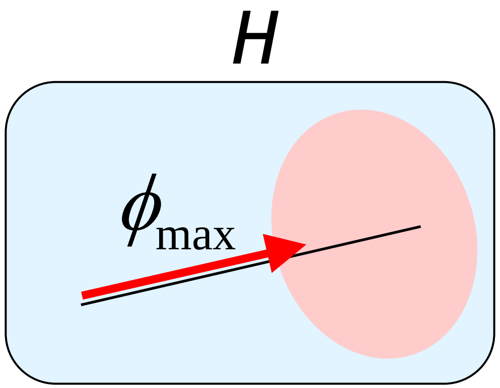
$\langle \cdot, \cdot \rangle$: Inner product in H

If ψ is vector,

$$R = E\left[\psi \psi^T\right]$$

- Optimal direction ϕ_{opt} is given by the eigenfunction $\phi_{\max}$ associated with the largest eigenvalue $\lambda_{\max}$ of R.

$$R\phi_{\max} = \lambda_{\max}\phi_{\max}$$



- Similar to PCA, but $E[\psi] \neq 0$.

Principal Component Kernel

- Using ϕ_{opt}, we define the kernel function by

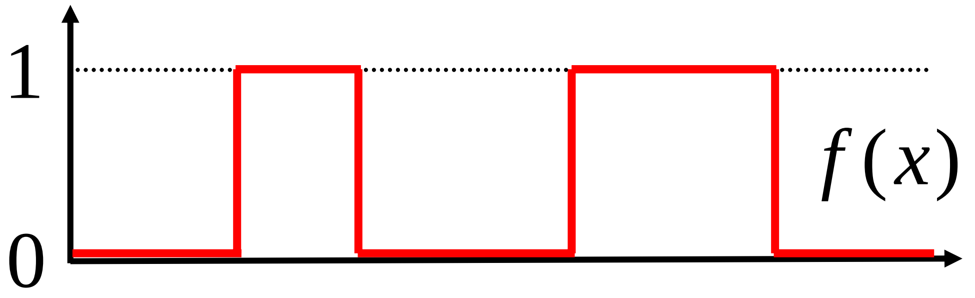
$$K(x, x') = \phi_{opt}\left(\frac{\|x - x'\|}{c}\right)$$

x': Center
c : Width

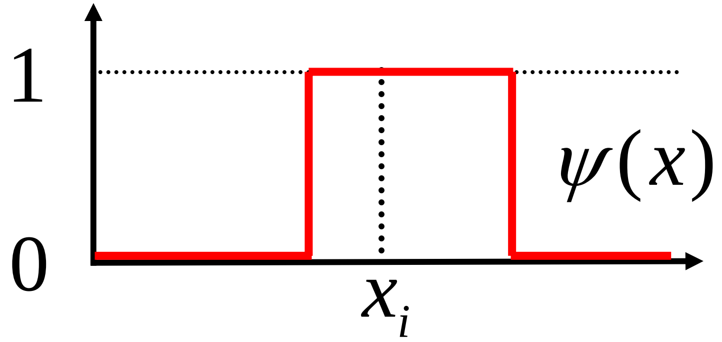
- Since the above kernel consists of the principal component of the correlation operator, we call it the principal component (PC) kernel.

Example of Kernel Design: Binary Regression Problem

- Learning target function is binary.



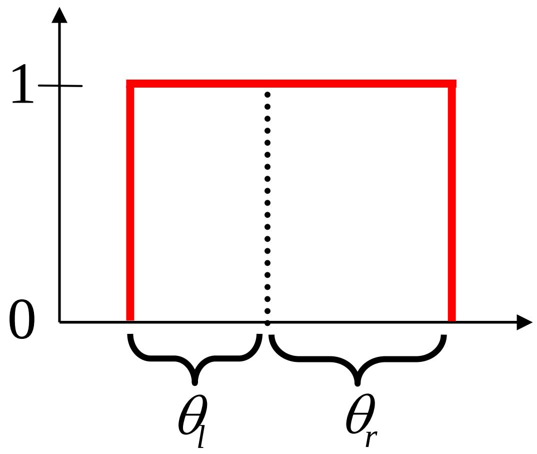
- The set of local functions is a set of rectangular functions with different width.



Widths of Rectangular Functions

- We assume that the width of rectangular functions is bounded (and normalized).
- Since we do not have prior knowledge on the width, we should define its distribution in an "unbiased" manner.
- We use uniform distribution for the width since it is non-informative.

$$\theta_l, \theta_r \sim U(0,1)$$



Eigenvalue Problem

- We use L_2 -space as a function space H .
- Considering the symmetry, the eigenvalue problem $R\phi = \lambda\phi$ is expressed as

$$\int_0^1 r(x,y)\phi(y)dy = \lambda\phi(x)$$

$$r(x,y) = 1 - \max(x,y)$$

- The principal component is given by

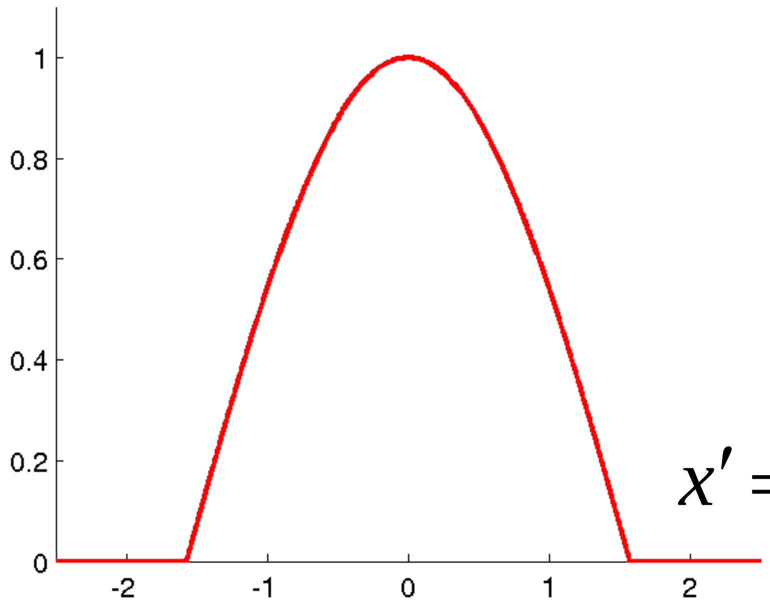
$$\phi_{\max}(x) = \sqrt{2}\cos\left(\frac{\pi}{2}x\right)$$

PC Kernel for Binary Regression

$$K(x,x') = \begin{cases} \cos\left(\dfrac{x-x'}{c}\right) & if \ \dfrac{|x-x'|}{c} \le \dfrac{\pi}{2} \\ 0 & otherwise \end{cases}$$

x' : Center

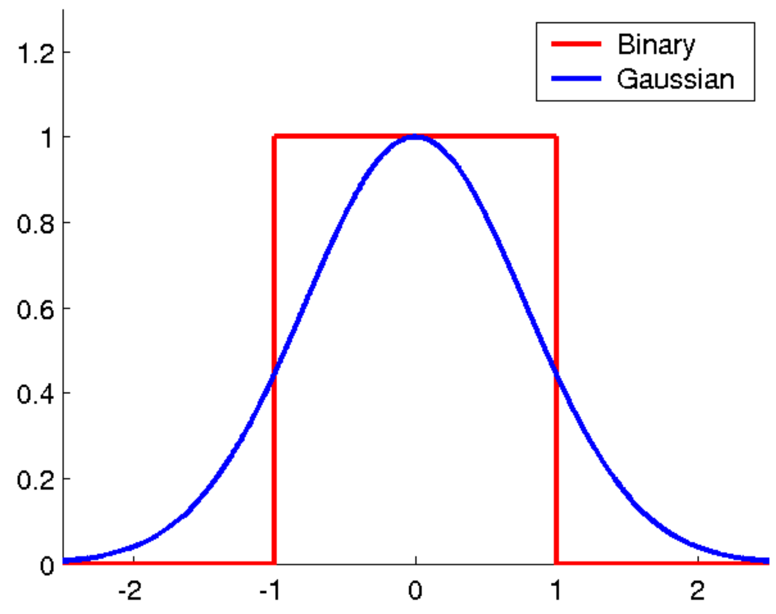
c : Width



$x' = 0, c = 1$

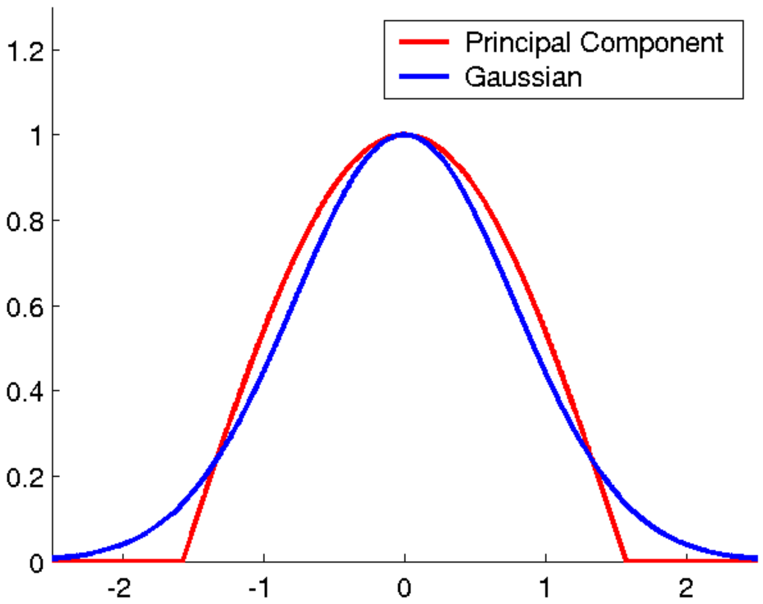
Implication of The Result

- Binary classification is often solved as binary regression with squared-loss (e.g., regularization networks, least-squares SVMs).
- Although binary function is not smooth at all, smooth Gaussian kernel often works very well in practice.
- Why?



Implication of The Result (cont.)

- By proper scaling, it can be confirmed that the shape of the obtained PC kernel is similar to Gaussian kernel.
- Both kernels work similarly in experiments.



Datasets	PC kernel	Gauss kernel
Banana	10.8±0.6	11.4±0.9
B.Cancer	27.1±4.6	27.1±4.9
Diabetes	23.2±1.8	23.3±1.7
F.Solar	33.6±1.6	33.5±1.6
Heart	16.1±3.3	16.2±3.4
Ringnorm	2.9±0.3	6.7±0.9
Thyroid	6.4±3.0	6.1±2.9
Titanic	22.7±1.4	22.7±1.0
Twonorm	2.6±0.2	3.0±0.2
Waveform	10.1±0.7	10.0±0.5

Implication of The Result (cont.)

- This implies that Gaussian-like bell-shaped function approximates binary functions very well.
- This partially explains why smooth Gaussian kernel is suitable for non-smooth classification tasks.

Conclusions

- Optimizing the family of kernel functions is a difficult task because it has infinitely many degrees of freedom.
- We proposed a method for designing kernel functions in regression scenarios.
- The optimal kernel shape is given by the principal component of correlation operator of local functions.
- We can beneficially use prior knowledge on problem domain (e.g., binary)