Kernels

CS478 – Machine Learning
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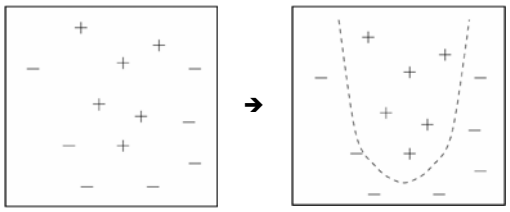
Reading: Schoelkopf/Smola Chapter 7.4, 7.6, 7.8
Cristianini/Shawe-Taylor 3.1, 3.2, 3.3.2, 3.4

Outline

- **Transform a linear learner into a non-linear learner**
- **Kernels can make high-dimensional spaces tractable**
- **Kernels can make non-vectorial data tractable**

Non-Linear Problems

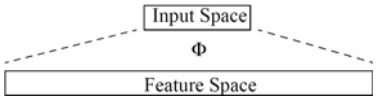


Problem:
- some tasks have non-linear structure
- no hyperplane is sufficiently accurate

How can SVMs learn non-linear classification rules?

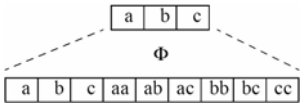
Extending the Hypothesis Space

Idea: add more features



➔ Learn linear rule in feature space.

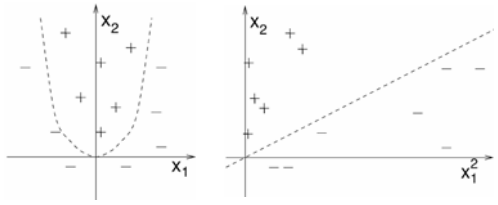
Example:



➔ The separating hyperplane in feature space is degree two polynomial in input space.

Example

- **Input Space:** $\vec{x} = (x_1, x_2)$ **(2 attributes)**
- **Feature Space:** $\Phi(\vec{x}) = (x_1^2, x_2^2, \sqrt{2}x_1, \sqrt{2}x_2, \sqrt{2}x_1x_2, 1)$ **(6 attributes)**



Dual SVM Optimization Problem

- **Primal Optimization Problem**

$$\begin{array}{ll} \text{minimize:} & P(\vec{w}, b, \vec{\xi}) = \frac{1}{2}\vec{w}\cdot\vec{w} + C\sum_{i=1}^{n}\xi_i \\ \text{subject to:} & \forall_{i=1}^{n} : y_i[\vec{w}\cdot\vec{x}_i + b] \geq 1 - \xi_i \\ & \forall_{i=1}^{n} : \xi_i > 0 \end{array}$$

- **Dual Optimization Problem**

$$\begin{array}{ll} \text{maximize:} & D(\vec{\alpha}) = \sum_{i=1}^{n}\alpha_i - \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} y_i y_j \alpha_i \alpha_j (\vec{x}_i \cdot \vec{x}_j) \\ \text{subject to:} & \sum_{i=1}^{n} y_i \alpha_i = 0 \\ & \forall_{i=1}^{n} : 0 \leq \alpha_i \leq C \end{array}$$

- **Theorem:** If w^* is the solution of the Primal and α^* is the solution of the Dual, then $\vec{w}^* = \sum_{i=1}^{n} \alpha_i^* y_i \vec{x}_i$

Kernels

Problem: Very many Parameters! Polynomials of degree *p* over *N* attributes in input space lead to $O(N^p)$ attributes in feature space!

Solution: [Boser et al.] The dual OP depends only on inner products => Kernel Functions

$$K(\vec{a},\vec{b}) = \Phi(\vec{a}) \cdot \Phi(\vec{b})$$

Example: For $\Phi(\vec{x}) = (x_1^2, x_2^2, \sqrt{2}x_1, \sqrt{2}x_2, \sqrt{2}x_1x_2, 1)$ calculating $K(\vec{a},\vec{b}) = [\vec{a}\cdot\vec{b}+1]^2$ computes inner product in feature space.

➔ no need to represent feature space explicitly.

SVM with Kernel

Training:

maximize: $D(\vec{\alpha}) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} y_i y_j \alpha_i \alpha_j K(\vec{x}_i, \vec{x}_j)$

subject to: $\sum_{i=1}^{n} y_i \alpha_i = 0$

$\forall_{i=1}^{n} : 0 \le \alpha_i \le C$

Classification: $h(\vec{x}) = sign\left(\left[\sum_{i=1}^{n} \alpha_i y_i \Phi(\vec{x}_i)\right] \cdot \Phi(\vec{x}) + b\right)$

$= sign\left(\sum_{i=1}^{n} \alpha_i y_i K(\vec{x}_i, \vec{x}) + b\right)$

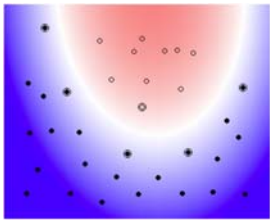
New hypotheses spaces through new Kernels:

- **Linear:** $K(\vec{a},\vec{b}) = \vec{a}\cdot\vec{b}$
- **Polynomial:** $K(\vec{a},\vec{b}) = [\vec{a}\cdot\vec{b}+1]^d$
- **Radial Basis Function:** $K(\vec{a},\vec{b}) = exp(-\gamma[\vec{a}-\vec{b}]^2)$
- **Sigmoid:** $K(\vec{a},\vec{b}) = tanh(\gamma[\vec{a}\cdot\vec{b}]+c)$

Examples of Kernels

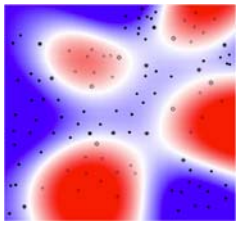
Polynomial

$K(\vec{a},\vec{b}) = [\vec{a}\cdot\vec{b}+1]^2$



Radial Basis Function

$K(\vec{a},\vec{b}) = exp(-\gamma[\vec{a}-\vec{b}]^2)$



What is a Valid Kernel?

Definition: Let *X* be a nonempty set. A function is a valid kernel in *X* if for all *n* and all $x_1, \ldots, x_n \in X$ it produces a Gram matrix

$$G_{ij} = K(x_i, x_j)$$

that is symmetric

$$G = G^T$$

and positive semi-definite

$$\forall \vec{\alpha} : \vec{\alpha}^T G \vec{\alpha} \ge 0$$

How to Construct Valid Kernels

Theorem: Let K_1 and K_2 be valid Kernels over $X \times X$, $X \subseteq \Re^N$, $\alpha \ge 0$, $0 \le \lambda \le 1$, f a real-valued function on X, $\phi: X \to \Re^m$ with a kernel K_3 over $\Re^m \times \Re^m$, and K a symmetric positive semi-definite matrix. Then the following functions are valid Kernels

$$K(x,z) = \lambda K_1(x,z) + (1-\lambda) K_2(x,z)$$

$$K(x,z) = \alpha K_1(x,z)$$

$$K(x,z) = K_1(x,z)\, K_2(x,z)$$

$$K(x,z) = f(x)\, f(z)$$

$$K(x,z) = K_3(\phi(x),\phi(z))$$

$$K(x,z) = x^T K z$$

Kernels for Discrete and Structured Data

Kernels for Sequences: Two sequences are similar, if the have many common and consecutive subsequences.

Example [Lodhi et al., 2000]: For $0 \le \lambda \le 1$ consider the following features space

	c-a	c-t	a-r	b-a	b-t	c-r	a-r	b-r
ϕ(cat)	λ^2	λ^3	λ^2	0	0	0	0	0
ϕ(car)	λ^2	0	0	0	0	λ^3	λ^2	0
ϕ(bat)	0	0	λ^2	λ^2	λ^3	0	0	0
ϕ(bar)	0	0	0	λ^2	0	0	λ^2	λ^3

=> $K(car,cat) = \lambda^4$, efficient computation via dynamic programming

Kernels for Non-Vectorial Data

- **Applications with Non-Vectorial Input Data**
  → classify non-vectorial objects
  - Protein classification (x is string of amino acids)
  - Drug activity prediction (x is molecule structure)
  - Information extraction (x is sentence of words)
  - Etc.
- **Applications with Non-Vectorial Output Data**
  → predict non-vectorial objects
  - Natural Language Parsing (y is parse tree)
  - Noun-Phrase Co-reference Resolution (y is clustering)
  - Search engines (y is ranking)

→ Kernels can compute inner products efficiently!

Properties of SVMs with Kernels

- **Expressiveness**
  - SVMs with Kernel can represent any boolean function (for appropriate choice of kernel)
  - SVMs with Kernel can represent any sufficiently "smooth" function to arbitrary accuracy (for appropriate choice of kernel)
- **Computational**
  - Objective function has no local optima (only one global)
  - Independent of dimensionality of feature space
- **Design decisions**
  - Kernel type and parameters
  - Value of C

SVMs for other Problems

- **Multi-class Classification**
  - [Schoelkopf/Smola Book, Section 7.6]
- **Regression**
  - [Schoelkopf/Smola Book, Section 1.6]
- **Outlier Detection**
  - D.M.J. Tax and R.P.W. Duin, "Support vector domain description", Pattern Recognition Letters, vol. 20, pp. 1191-1199, 1999b. 26
- **Structural Prediction**
  - B. Taskar, C. Guestrin, D. Koller - Advances in Neural Information Processing Systems, 2003.
  - I. Tsochantaridis, T. Hofmann, T. Joachims, and Y. Altun, Support Vector Machine Learning for Interdependent and Structured Output Spaces, Proceedings of the International Conference on Machine Learning (ICML), 2004.