Support Vector Machines: Kernels

CS4780/5780 – Machine Learning Fall 2012

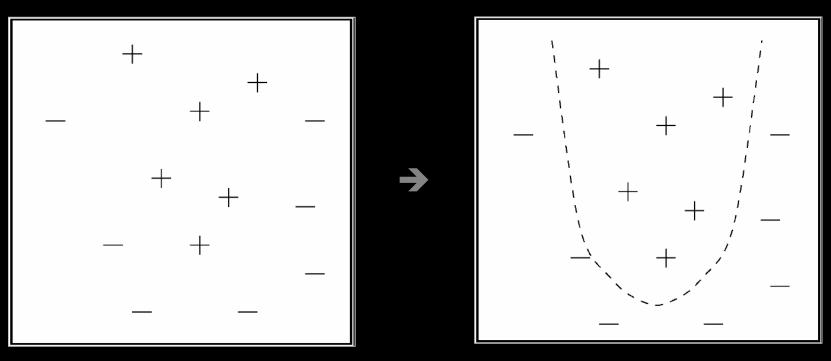
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Reading: Schoelkopf/Smola Chapter 7.4, 7.6, 7.8 Cristianini/Shawe-Taylor 3.1, 3.2, 3.3.2, 3.4

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

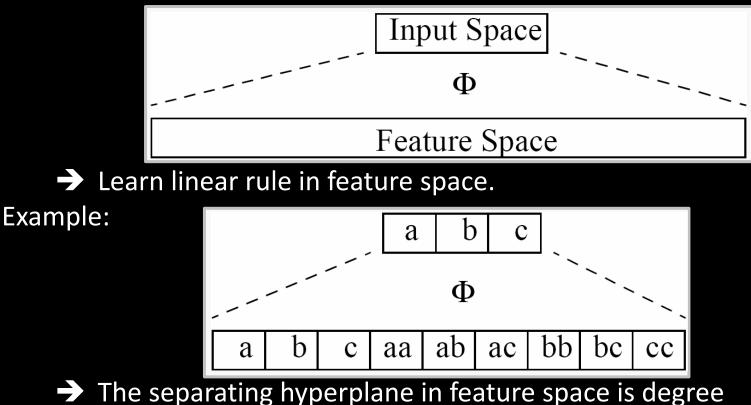


Problem:

- some tasks have non-linear structure
- no hyperplane is sufficiently accurate
 How can SVMs learn non-linear classification rules?

Extending the Hypothesis Space

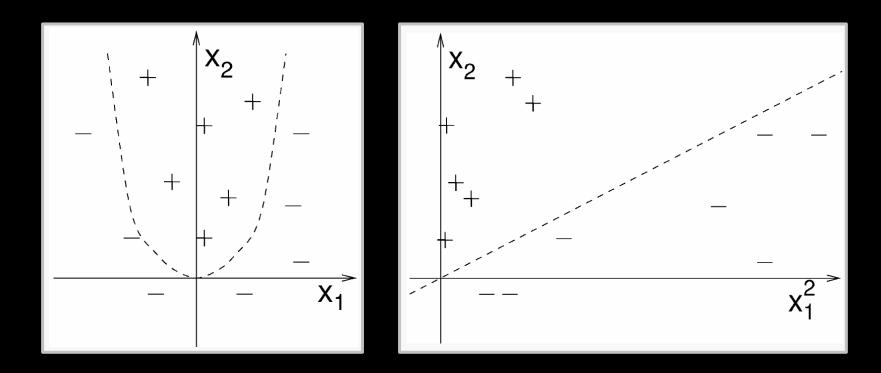
Idea: add more features



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: $\Phi(\vec{x}) = (x_1^2, x_2^2, x_1, x_2, x_1, x_2, 1)$ (6 attributes)



Dual SVM Optimization Problem

• Primal Optimization Problem

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

• Dual Optimization Problem

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

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

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

 $\Phi(\vec{x})$

• 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(Np) attributes in feature space!
- Solution:
 - 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

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

 $\cdot \cdot 0 < \alpha \leq C$

• Training:

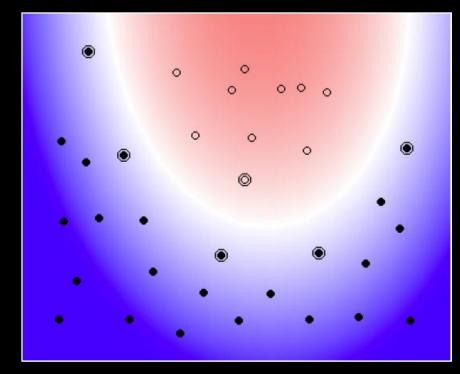
subject to: $\sum_{i=1}^{n} y_i \alpha_i = 0$

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

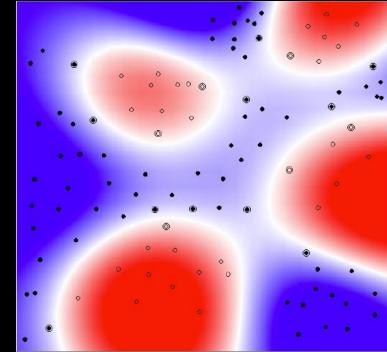
- New hypotheses spaces through new Kernels:
 - Linear: $K(\vec{a}, \vec{b}) = \vec{a} \cdot \vec{b}$
 - Polynomial: $K(\vec{a}, \vec{b}) = [\vec{a} \cdot \vec{b} + 1]^{a}$
 - $\left|-\right|$ Radial Basis Function: $K\left(ec{a},ec{b}
 ight)=\exp\left(-\gamma\left[ec{a}-ec{b}
 ight]^{2}
 ight)$
 - Sigmoid: $K(\vec{a}, \vec{b}) = \tanh(\gamma[\vec{a} \cdot \vec{b}] + c)$

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 $x_1, ..., x_n \in X$ 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 $X \times X$, $\alpha \ge 0$, $0 \le \lambda \le 1$, f a real-valued function on X, $\phi: X \rightarrow \Re^m$ 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

$$\begin{split} \mathsf{K}(\mathsf{x},\mathsf{z}) &= \lambda \; \mathsf{K}_{1}(\mathsf{x},\mathsf{z}) + (1-\lambda) \; \mathsf{K}_{2}(\mathsf{x},\mathsf{z}) \\ & \mathsf{K}(\mathsf{x},\mathsf{z}) = \alpha \; \mathsf{K}_{1}(\mathsf{x},\mathsf{z}) \\ & \mathsf{K}(\mathsf{x},\mathsf{z}) = \mathsf{K}_{1}(\mathsf{x},\mathsf{z}) \; \mathsf{K}_{2}(\mathsf{x},\mathsf{z}) \\ & \mathsf{K}(\mathsf{x},\mathsf{z}) = \mathsf{K}_{1}(\mathsf{x},\mathsf{z}) \; \mathsf{K}_{2}(\mathsf{x},\mathsf{z}) \\ & \mathsf{K}(\mathsf{x},\mathsf{z}) = \mathsf{K}(\mathsf{x},\mathsf{z}) = \mathsf{K}(\mathsf{x},\mathsf{z}) \\ & \mathsf{K}(\mathsf{x},\mathsf{z}) = \mathsf{K}(\mathsf{x},\mathsf{z}) = \mathsf{K}(\mathsf{x},\mathsf{z}) \\ & \mathsf{K}(\mathsf{x},\mathsf{z}) = \mathsf{K}(\mathsf{x},\mathsf{z}) = \mathsf{x}^{\mathsf{T}} \; \mathsf{K} \; \mathsf{z} \end{split}$$

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 ≤ λ ≤ 1 consider the following features space

	c-a	c-t	a-t	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	λ²	0
φ(bat)	0	0	λ²	λ²	λ ³	0	0	0
φ(bar)	0	0	0	λ²	0	0	λ²	λ ³

=> K(car,cat) = λ^4 , efficient computation via dynamic programming

Kernels for Non-Vectorial Data

- Applications with Non-Vectorial Input Data
 - \rightarrow 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
 - \rightarrow 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
- Structured Output 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.