Nonlinear SVM and kernel methods

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Changing the dot product

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Still have

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But explicit mapping too expensive to compute: $\phi(\mathbf{x}) \in \mathbb{R}^{p+p(p+1)/2}$.

Reproducing kernel Hilbert space

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Define the *reproducing kernel* as the function

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A space with these properties is called a *reproducing kernel Hilbert space* (RKHS).

Positive definite function

Definition (Positive definite function)

A symmetric positive definite function is a function $K : (x, y) \mapsto K(x, y)$ such that for all $x_1, \dots, x_n \in \mathcal{X}$ and $\alpha_1, \dots, \alpha_n \in \mathbb{R}$,

$$\sum_{1 \le i,j \le n} \alpha_i \alpha_j K(x_i, x_j) \ge 0.$$

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with equality if and only if $\alpha_i = 0$ for all i.

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Yes, any symmetric positive definite function is the reproducing kernel of a RKHS (Aronszajn, 1950).

Moore-Aronszajn theorem

Theorem

A symmetric function K on $\mathcal{X}$ is positive definite if and only if there exists a Hilbert space $\mathcal{H}$ and a mapping

$$\begin{aligned} \phi : \mathcal{X} &\to \mathcal{H} \\ x &\mapsto \phi(x) \end{aligned}$$

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When we work with kernels, we therefore always use a **feature map** but very often *implicitly*. We will not show this theorem in this course.

Common RKHSes for $\mathcal{X} = \mathbb{R}^p$

Linear kernel

- $K(x, y) = x^\top y$
- $\mathcal{H} = \{f_w : x \mapsto w^\top x \mid w \in \mathbb{R}^p\}$
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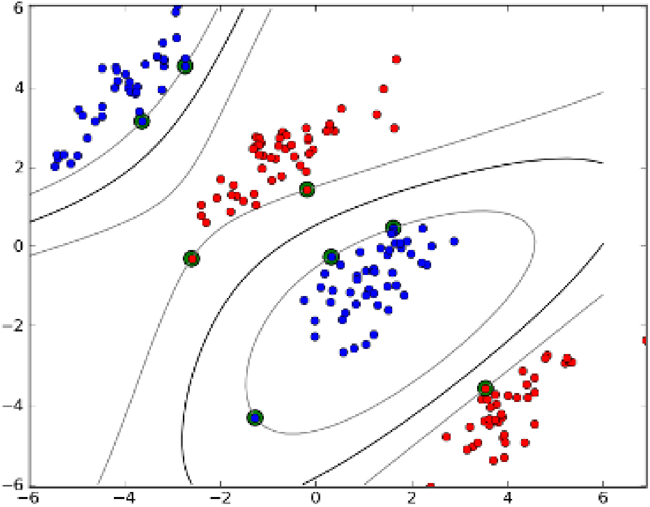
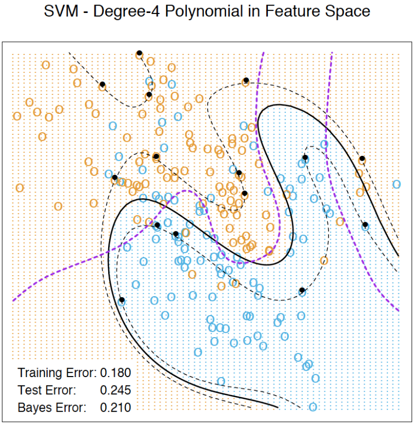
Radial Basis Function kernel (RBF)

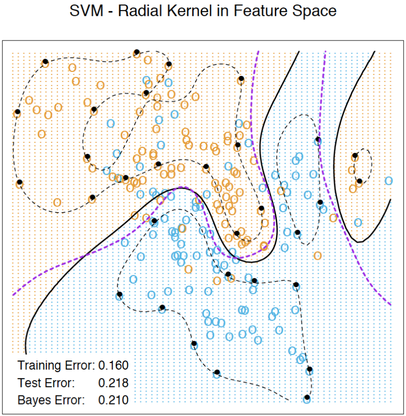
- $K_h(x, y) = \exp\left(-\frac{\|x-y\|_2^2}{2h}\right)$
- $\mathcal{H} =$ Gaussian RKHS

Nonlinear SVM : Hard margin



Nonlinear SVM: Soft margin





$\|f\|_{\mathcal{H}}$ measures the smoothness of the function f

Indeed:

$$|f(x) - f(x')| = |\left\langle f, K(x,\cdot) - K(x',\cdot)\right\rangle_{\mathcal{H}}| \leq \|f\|_{\mathcal{H}} \|K(x,\cdot) - K(x',\cdot)\|_{\mathcal{H}}$$

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- f is Lipschitz with respect to the ℓ_2 distance induced by the RKHS

  $$d(x,x') = \|K(x,\cdot) - K(x',\cdot)\|_{\mathcal{H}} = \sqrt{K(x,x) + K(x',x') - 2K(x,x')}$$

- $\|f\|_{\mathcal{H}}$ is the Lipschitz constant

Some data do not live in a vector space...

- Sequence of human hemoglobin subunit gamma-1 (HGB1)

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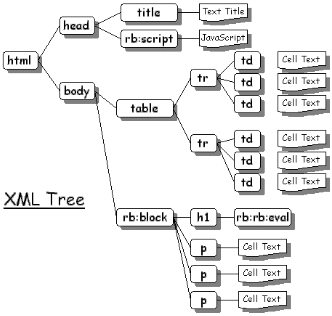

Graph structure of a molecule

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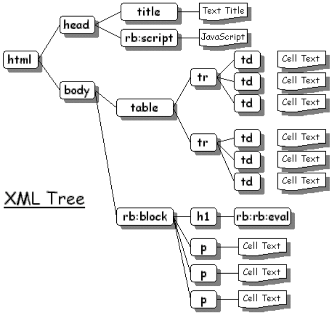

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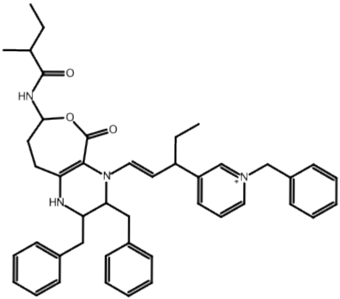

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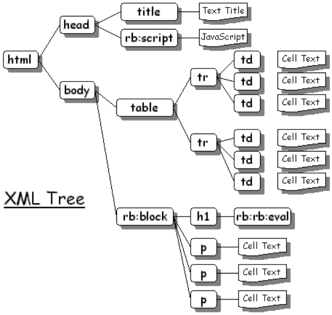

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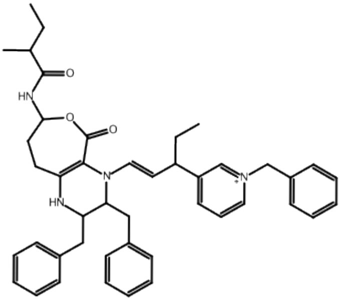


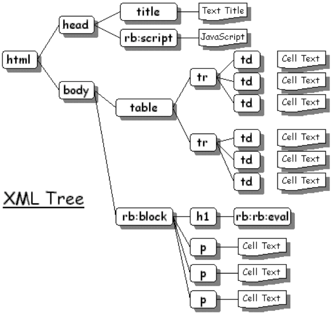
Can we learn functions of these?

Some data do not live in a vector space...

- Sequence of human hemoglobin subunit gamma-1 (HGB1)

`MGHFTEEDKATITSLWGKVNVEDAGGETLGRLLVVYPWTQRFFDSFGNLSSAS...`

Xml tree of a webpage



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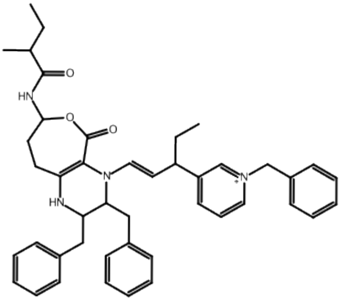

Can we learn functions of these? $\rightarrow$ Kernels for combinatorial objects

Working with strings

- Let Σ be an alphabet of symbols or letters (e.g. $\{\texttt{A},\texttt{C},\texttt{G},\texttt{T}\}$)

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- ε is the empty string and so $u = \varepsilon u = u\varepsilon$

Kernel for strings: p-spectrum kernel

Idea: a word is represented by the list of substrings of length p. For example the representation of `GAGA` for the 2-spectrum kernel on $\{$`A`,`C`,`G`$\}$ is

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The **feature map** for a string s is

$$\phi(s) = \left(\phi_u(s)\right)_{u \in \Sigma^p} \qquad \text{with} \qquad \phi_u(s) = \#\{i \mid s_{i:(i+p-1)} = u\}$$

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String kernels: other spectrum kernels

Blended spectrum kernel

$\tilde{K}_p(s,t) = \sum_{j=1}^{p} a_j K_i(s,t)$ with K_j the usual j-spectrum kernel.

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Like the spectrum kernel but allowing mistakes...

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with $d_H(u,v) = \sum_{k=1}^{n} 1_{\{u_i \neq v_i\}}$ the Hamming distance between u and v

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Kernel:

$$\begin{aligned} K(s,t) &= \sum_{u \in \Sigma^*} \phi_u(s)\, \phi_u(t) \\ &= \sum_{(I,J)} 1_{\{s_I = t_J\}} \\ &= \#\big\{ (I,J) \mid s_I = t_J \big\} \end{aligned}$$

- The empty substring ε is counted only once in each string.

Subsequence kernels: dynamic programming

$$K(sa, t) = K(s, t) + \sum_{k:t_k=a} K(s, t_{1:k-1})$$

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	ε	t_1	$\dots$	t_j	$\dots$
ε	1	1	$\dots$	1	$\dots$
s_1	1	$\kappa_{1,1}$	$\dots$	$\kappa_{1,j}$	$\dots$
s_2					
$\vdots$					
s_{i-1}	1	$\kappa_{i-1,1}$	$\dots$	$\kappa_{i-1,j}$	
s_i	1	$\kappa_{i,1}$	$\dots$	$\kappa_{i,j}$ $\vdots$	
$\vdots$					

Other types of kernels

- Fisher kernels
- Tree kernels
- Graph kernels
- Dedicated kernels for genomics/proteomics
- Set kernels

and more

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Representer theorem

Theorem (Kimmeldorf and Wahba, 1971)

Consider the optimization problem

$$\min_{f \in \mathcal{H}} L(f(x_1), \ldots, f(x_n)) + \lambda \|f\|_{\mathcal{H}}^2$$

Then any local minimum is of the form

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

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Proof Indeed, let f be a local optimum and consider the subspace

$$\mathcal{S} = \{g \mid g = \sum_{i=1}^{n} \alpha_i K(x_i, \cdot), \quad \boldsymbol{\alpha} \in \mathbb{R}^n\}.$$

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So that we must have $f_{\perp} = 0$.

Learning with functions from a RKHS

$$\min_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i) \; + \; \lambda \, \|f\|_{\mathcal{H}}^2 \qquad \text{(P)}$$

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The solution of (P) is therefore of the form (R) with $\alpha \in \mathbb{R}^n$ the solution of

$$\min_{\alpha \in \mathbb{R}^n} \frac{1}{n} \sum_{i=1}^{n} \ell\Big(\sum_{j=1}^{n} \alpha_j K(x_j, x_i), y_i\Big) + \lambda \sum_{1 \le i,j \le n} \alpha_i \alpha_j K(x_i, x_j).$$

Kernel ridge regression

$$\min \frac{1}{2}\sum_{i=1}^{n}(f(x_i) - y_i)_2^2 + \frac{\lambda}{2}\|f\|_{\mathcal{H}}^2$$

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- We could use the representer theorem and solve the optimization problem w.r.t. $\boldsymbol{\alpha}$
- We will show directly that the predictor can be expresses solely with the Gram matrix.

We know that the solution to ridge regression is

$$\widehat{\mathbf{w}} = (\mathbf{X}^\top\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^\top\mathbf{y}$$

A matrix identity and the matrix inversion lemma

Let $\mathbf{X} \in \mathbb{R}^{n \times p}$,

$$\mathbf{X}^\top + \mathbf{X}^\top \mathbf{X}\mathbf{X}^\top = (\mathbf{I}_p + \mathbf{X}^\top \mathbf{X})\mathbf{X}^\top = \mathbf{X}^\top(\mathbf{I}_n + \mathbf{X}\mathbf{X}^\top)$$

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$$\mathbf{X}^\top + \mathbf{X}^\top \mathbf{X} \mathbf{X}^\top = (\mathbf{I}_p + \mathbf{X}^\top \mathbf{X})\mathbf{X}^\top = \mathbf{X}^\top (\mathbf{I}_n + \mathbf{X}\mathbf{X}^\top)$$

$$\boxed{\mathbf{X}^\top (\mathbf{I}_n + \mathbf{X}\mathbf{X}^\top)^{-1} = (\mathbf{I}_p + \mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top}$$

$$\begin{aligned} \mathbf{I}_p - \mathbf{X}^\top (\mathbf{I}_n + \mathbf{X}\mathbf{X}^\top)^{-1} \mathbf{X} &= \mathbf{I}_p - (\mathbf{I}_p + \mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{X} \\ &= (\mathbf{I}_p + \mathbf{X}^\top \mathbf{X})^{-1} \left[(\mathbf{I}_p + \mathbf{X}^\top \mathbf{X}) - \mathbf{X}^\top \mathbf{X} \right] \end{aligned}$$

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Matrix inversion lemma

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Computational cost reduced from $\mathcal{O}(p^3)$ to $\mathcal{O}(n^2 p)$.

Kernel ridge regression

Denoting $\mathbf{k}(\mathbf{z})$ the vector with entries $[\mathbf{k}(\mathbf{z})]_i = K(\mathbf{x}_i, \mathbf{z})$, we have

$$\mathbf{z}^\top \widehat{\mathbf{w}} = \mathbf{z}^\top (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I}_p)^{-1} \mathbf{X}^\top \mathbf{y}$$

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&= \mathbf{k}(\mathbf{z})^\top (\lambda \mathbf{I}_n + \mathbf{K})^{-1} \mathbf{y}
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&= \mathbf{k}(\mathbf{z})^\top (\lambda \mathbf{I}_n + \mathbf{K})^{-1} \mathbf{y}
\end{aligned}$$

So we have $f(\mathbf{x}) = \sum_{i=1}^n \alpha_i K(\mathbf{x}_i, \mathbf{x})$ with

$$\boxed{\boldsymbol{\alpha} = (\lambda \mathbf{I}_n + \mathbf{K})^{-1} y}.$$

Ressources

http://www.kernel-machines.org/

References I

Aronszajn, N. (1950). Theory of reproducing kernels. *Transactions of the American mathematical society*, 68(3):337–404.