MATH 829: Introduction to Data Mining and Analysis
Support vector machines and kernels

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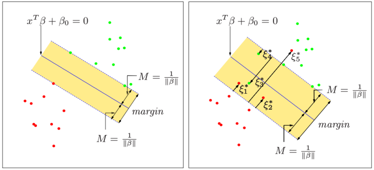
March 14, 2016

Separating sets: mapping the features

We saw in the previous lecture how support vector machines provide a robust way of finding a separating hyperplane:



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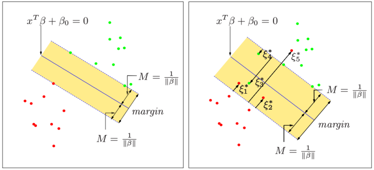
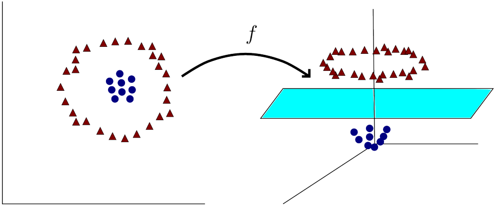


What if the data is not separable? Can map into a high-dimensional space.



$$f : \mathbb{R}^2 \to \mathbb{R}^3$$

A brief intro to duality in optimization

Consider the problem:

$$\begin{aligned} \min_{x \in \mathcal{D} \subset \mathbb{R}^n} \quad & f_0(x) \\ \text{subject to} \quad & f_i(x) \le 0, \qquad i = 1, \ldots, m \\ & h_i(x) = 0, \qquad i = 1, \ldots, p. \end{aligned}$$

Denote by $p^\star$ the optimal value of the problem.

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Lagrangian: $L : \mathcal{D} \times \mathbb{R}^m \times \mathbb{R}^p \to \mathbb{R}$

$$L(x, \lambda, \nu) := f_0(x) + \sum_{i=1}^{m} \lambda_i f_i(x) + \sum_{i=1}^{p} \nu_i h_i(x).$$

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Claim: for every $\lambda \ge 0$,

$$g(\lambda, \nu) \le p^\star.$$

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Dual problem:

$$\max_{\lambda \in \mathbb{R}^m,\ \nu \in \mathbb{R}^p} g(\lambda, \nu)$$
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Strong duality: $d^\star = p^\star$.

- Does not hold in general.
- Usually holds for convex problems.
- (See e.g. Slater's constraint qualification).

The kernel trick

Recall that SVM solves:

$$\min_{\beta_0,\beta,\xi} \frac{1}{2}\|\beta\|^2 + C\sum_{i=1}^{n}\xi_i$$

$$\text{subject to } y_i(x_i^T\beta + \beta_0) \geq 1 - \xi_i$$

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The associated Lagrangian is

$$L_P = \frac{1}{2}\|\beta\|^2 + C\sum_{i=1}^{n}\xi_i - \sum_{i=1}^{n}\alpha_i[y_i(x_i^T\beta + \beta_0) - (1-\xi_i)] - \sum_{i=1}^{n}\mu_i\xi_i,$$

which we minimize w.r.t. β, β_0, ξ.

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which we minimize w.r.t. β, β_0, ξ. Setting the respective derivatives to 0, we obtain:

$$\beta = \sum_{i=1}^{n}\alpha_i y_i x_i, \quad 0 = \sum_{i=1}^{n}\alpha_i y_i, \quad \alpha_i = C - \mu_i \quad (i = 1, \ldots, n).$$

The kernel trick (cont.)

Substituting into L_P, we obtain the Lagrange (dual) objective function:

$$L_D = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j x_i^T x_j.$$

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$$\begin{aligned}(K(x_i, x_j)) &= (\langle h(x_i), h(x_j)\rangle) \\ &= (\langle v_i, v_j\rangle) \\ &= V^T V, \qquad \text{where } V = (v_1^T, \dots, v_N^T).\end{aligned}$$

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Conclusion: the matrix $(K(x_i, x_j))$ is positive semidefinite.

Positive definite kernels (cont.)

- **Necessary condition to have $K(x, x') = \langle h(x), h(x') \rangle$:**

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for any $x_1, \ldots, x_N$, and any $N \geq 1$.

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Definition: Let $\mathcal{X}$ be a set. A symmetric kernel $K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is said to be a *positive (semi)definite kernel* if

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$$\langle f, k_x\rangle_{\mathcal{H}} = f(x) \qquad \forall f \in \mathcal{H}.$$

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Write $k(\cdot, x) := k_x(\cdot)$ (k = the reproducing kernel of $\mathcal{H}$).

Positive definite kernels (cont.)

One can show that $\mathcal{H}$ is a RKHS over $\mathcal{X}$ iff the evaluation functionals $\Lambda_x : \mathcal{H} \to \mathbb{C}$

$$f \mapsto \Lambda_x(f) = f(x)$$

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Theorem: Let $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ be a positive definite kernel. Then there exists a RKHS $\mathcal{H}_k$ over $\mathcal{X}$ such that

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Now, define $h : \mathcal{X} \to \mathcal{H}_k$ by

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Then

$$\langle h(x), h(x') \rangle_{\mathcal{H}_k} = \langle k(\cdot, x), k(\cdot, x') \rangle_{\mathcal{H}_k} = k(x, x').$$

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Moral: Positive definite kernels arise as $\langle h(x), h(x') \rangle_{\mathcal{H}}$.

Back to SVM

We can replace h by any positive definite kernel in the SVM problem:

$$\begin{aligned} L_D &= \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{h}(\mathbf{x_i})^{\mathbf{T}} \mathbf{h}(\mathbf{x_j}) \\ &= \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{K}(\mathbf{x_i}, \mathbf{x_j}). \end{aligned}$$

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Three popular choice in the SVM literature:

$$K(x, x') = e^{-\gamma \|x - x'\|_2^2} \qquad \text{(Gaussian kernel)}$$
$$K(x, x') = (1 + \langle x, x' \rangle)^d \qquad \text{(d-th degree polynomial)}$$
$$K(x, x') = \tanh(\kappa_1 \langle x, x' \rangle + \kappa_2) \qquad \text{(Neural networks).}$$

Constructing pd kernels

Properties of pd kernels:

1. If $k_1, \dots, k_n$ are pd, then $\sum_{i=1}^n \lambda_i k_i$ is pd for any $\lambda_1, \dots, \lambda_n \geq 0$.
2. If k_1, k_2 are pd, then $k_1 k_2$ is pd (Schur product theorem).
3. If $(k_i)_{i \geq 1}$ are kernels, then $\lim k_i$ is a kernel (if the limit exists).

Exercise: Use the above properties to show that $e^{-\gamma \|x - x'\|_2^2}$ and $(1 + \langle x, x' \rangle)^d$ are positive definite kernels.

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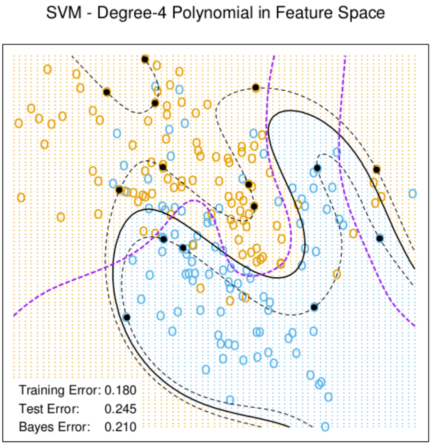
Theorem: (Bochner) A continuous function $h : \mathbb{R}^p \to \mathbb{C}$ is positive definite if and only if

$$h(x) = \int_{\mathbb{R}^p} e^{-i\langle x, \omega \rangle} \, d\mu(\omega),$$

for some finite nonnegative Borel measure on $\mathbb{R}^p$.

Example: decision function



ESL, Figure 12.3 (solid black line = decision boundary, dotted line = margin).