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

Dominique Guillot

Departments of Mathematical Sciences
University of Delaware

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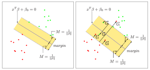
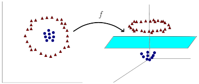
Separating sets: mapping the features

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



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:

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

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

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

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

Lagrange dual function: $g : \mathbb{R}^m \times \mathbb{R}^p \to \mathbb{R}$

$$g(\lambda, \nu) := \inf_{x \in \mathcal{D}} L(x, \lambda, \nu).$$

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

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

A brief intro to duality in optimization

Dual problem:

$$\begin{aligned} \max_{\lambda \in \mathbb{R}^m,\ \nu \in \mathbb{R}^p} \quad & g(\lambda, \nu) \\ \text{subject to } \quad & \lambda \geq 0. \end{aligned}$$

Denote by $d^\star$ the optimal value of the dual problem. Clearly

$$d^\star \leq p^\star \qquad \text{(weak duality)}.$$

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:

$$\min_{\beta_0,\beta,\xi} \frac{1}{2}\|\beta\|^2 + C\sum_{i=1}^n \xi_i$$
$$\text{subject to } y_i(x_i^T\beta+\beta_0) \geq 1-\xi_i$$
$$\xi_i \geq 0.$$

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. Setting the respective derivatives to 0, we obtain:

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

The kernel trick (cont.)

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

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

The function L_D provides a lower bound on the original objective function at any feasible point (weak duality).

The solution of the original SVM problem can be obtained by maximizing L_D under the previous constraints (strong duality).

Now suppose $h : \mathbb{R}^p \to \mathbb{R}^m$, transforming our features to

$$h(x_i) = (h_1(x_i), \dots, h_m(x_i)) \in \mathbb{R}^m.$$

The Lagrange dual function becomes:

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

Important observation: L_D only depends on $\langle h(x_i), h(x_j)\rangle$.

Positive definite kernels

Important observation: L_D only depends on $\langle h(x_i), h(x_j)\rangle$.

In fact, we don't even need to specify h, we only need:

$$K(x,x') = \langle h(x), h(x')\rangle.$$

Question: Given $K : \mathbb{R}^p \times \mathbb{R}^p \to \mathbb{R}$, when can we guarantee that

$$K(x,x') = \langle h(x), h(x')\rangle$$

for some function h?

Observation: Suppose K has the desired form. Then, for $x_1, \dots, x_N \in \mathbb{R}^p$, and $v_i := h(x_i)$,

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

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

Positive definite kernels (cont.)

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

$$(K(x_i,x_j))_{i,j=1}^N \text{ is psd}$$

for any $x_1, \dots, x_N$, and any $N \geq 1$.
- Note also that $K(x,x') = K(x',x)$ if $K(x,x') = \langle h(x), h(x')\rangle$.

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

$$(K(x_i,x_j))_{i,j=1}^N \text{ is positive (semi)definite}$$

for all $x_1, \dots, x_N \in \mathcal{X}$ and all $N \geq 1$.

- A *reproducing kernel Hilbert space* (RKHS) over a set $\mathcal{X}$ is a Hilbert space $\mathcal{H}$ of functions on $\mathcal{X}$ such that for each $x \in \mathcal{X}$, there is a function $k_x \in \mathcal{H}$ such that

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

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 $\Lambda_x : \mathcal{H} \to \mathbb{C}$

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

are continuous on $\mathcal{H}$ (use Riesz's representation theorem).

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

1. $k(\cdot, x) \in \mathcal{H}_k$ for all $x \in \mathcal{X}$.
2. $\mathrm{span}(k(\cdot, x) : x \in \mathcal{X})$ is dense in $\mathcal{H}_k$.
3. k is a reproducing kernel on $\mathcal{H}_k$.

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

$$h(x) := k(\cdot, x).$$

Then

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

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:

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

Three popular choice in the SVM literature:

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

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.

Definition: A function $h : \mathbb{R}^p \to \mathbb{R}$ is said to be *positive definite* if

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

is a positive definite kernel.

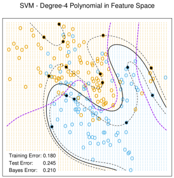
P.d. functions thus provide a way of constructing pd kernels.

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).