Lecture 23: Support vector machines

Reading: Chapter 9

STATS 202: Data mining and analysis

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Review of support vector classifier

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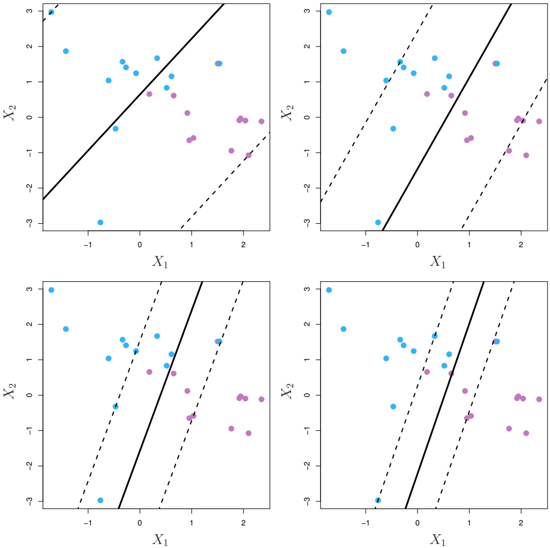
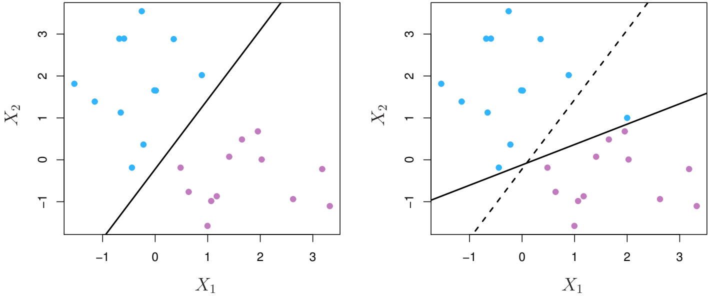
- Low budget C (high D) $\iff$ Few samples used $\iff$ High variance $\iff$ Tendency to overfit.
- Choose D (equiv. C) by cross-validation.

Tuning the budget, C (high to low)



If the budget is too low, we tend to overfit



Maximal margin classifier, $C = 0 (D = \infty)$. Adding one observation dramatically changes the classifier.

Finding the support vector classifier

The problem can be reduced to the optimization:

$$\hat{\alpha} \; = \; \arg\max_{\alpha} \;\; \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{i'=1}^{n} \alpha_i \alpha_{i'} y_i y_{i'} (x_i \cdot x_{i'})$$

$$\text{subject to } \; 0 \leq \alpha_i \leq D \; \text{ for all } i = 1, \ldots, n,$$

$$\sum_{i=1}^{n} \alpha_i y_i = 0.$$

$$\hat{w} = \sum_{i=1}^{n} \alpha_i y_i x_i, \qquad \hat{w} \cdot x_0 = \sum_{i=1}^{n} \alpha_i y_i (x_i \cdot x_0)$$

Key fact about the support vector classifier

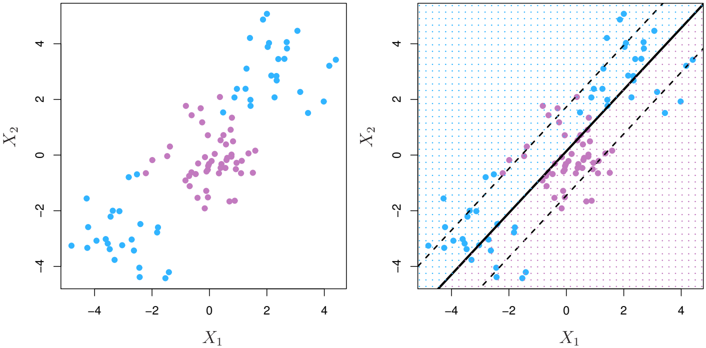
To **find the hyperplane** and **make predictions** all we need to know is the dot product between any pair of input vectors:

$$K(x_i, x_k) = (x_i \cdot x_k) = \langle x_i, x_k \rangle = \sum_{j=1}^{p} x_{ij} x_{kj}$$

We call this the **kernel matrix**.

How to deal with non-linear boundaries?

The support vector classifier can only produce a linear boundary.



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- With a quadratic predictor, we get a quadratic boundary:

$$\log\left[\frac{P(Y=1|X)}{P(Y=0|X)}\right] = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1^2 = 0.$$

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- This is in fact a linear boundary in the 3D space. However, we can classify a point knowing just (X_1, X_2). The boundary in this projection is quadratic in X_1.

How do we expand the space of predictors?

- **Idea:** Add polynomial terms up to degree d:

  $$Z = (X_1, X_1^2, \ldots, X_1^d, X_2, X_2^2, \ldots, X_2^d, \ldots, X_p, X_p^2, \ldots, X_p^d).$$

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- With the expanded set of predictors, we need:

  $$z_i \cdot z_k = \langle z_i, z_k \rangle = \sum_{j=1}^{p} \sum_{\ell=1}^{d} x_{ij}^{\ell} x_{kj}^{\ell}.$$

Kernels

The **kernel matrix** defined by $K(x_i, x_k) = \langle z_i, z_k \rangle$ for a set of linearly independent vectors $z_1, \ldots, z_n$ is always **positive semi-definite**, i.e. it is symmetric and has no negative eigenvalues.

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Theorem:

If K is a positive definite $n \times n$ matrix, there exist vectors $(z_1, \ldots, z_n)$ in some space $\mathbf{Z}$, such that $K(x_i, x_k) = \langle z_i, z_k \rangle$.

Finding the support vector classifier

With a kernel, the problem can be reduced to the optimization:

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$$\text{subject to} \ \ 0 \leq \alpha_i \leq D \ \ \text{for all } i = 1, \ldots, n,$$

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- This is the dual problem of a *different* optimization problem than we start with.
- Predictions can be computed similarly to original kernel $K(x, y) = x \cdot y$. Details omitted.

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- Often much easier!

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Example. The polynomial kernel with $d = 2$:

$$K(x_i, x_k) = f(x_i, x_k) = (1 + \langle x_i, x_k \rangle)^2$$

This is equivalent to the expansion:

$$\begin{aligned}\Phi(X) =& (\sqrt{2}X_1, \ldots, \sqrt{2}X_p, \\ & X_1^2, \ldots, X_p^2, \\ & \sqrt{2}X_1X_2, \sqrt{2}X_1X_3, \ldots, \sqrt{2}X_{p-1}X_p)\end{aligned}$$

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- Computing $K(x_i, x_k)$ directly is $O(p)$.
- Computing the kernel using the expansion is $O(p^2)$.

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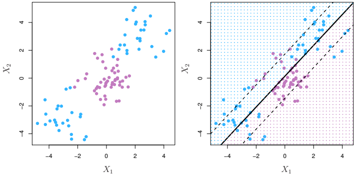
- However, we can easily define PD kernels by combining those we are familiar with:
  - Sums and products of PD kernels are PD.
- Intuitively, a kernel $K(x_i, x_k)$ defines a *similarity* between the samples x_i and x_k. This intuition can guide our choice in different problems.



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