Lecture 22: Support vector classifier

Reading: Sections 9.1-9.2

STATS 202: Data mining and analysis

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Hyperplanes and normal vectors

- Consider a p-dimensional space of predictors.

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- An **(affine) hyperplane** H is an affine space which separates the space into two regions.
- It is determined by a normal vector $\beta = (\beta_1, \ldots, \beta_p)$, is a unit vector $\sum_{j=1}^{p} \beta_j^2 = 1$ which is perpendicular to the hyperplane and an "intercept" β_0

$$H = \left\{ x : \sum_{j=1}^{p} x_j \beta_j + \beta_0 = 0 \right\}.$$

Hyperplanes and normal vectors

- If the hyperplane goes through the origin ($\beta_0 = 0$), the deviation between a point $(x_1, \ldots, x_p)$ and the hyperplane is the dot product:

$$x \cdot \beta = x_1\beta_1 + \cdots + x_p\beta_p.$$

- If the hyperplane goes through a point $-\beta_0\beta$, i.e. it is displaced from the origin by $-\beta_0$ along the normal vector $(\beta_1, \ldots, \beta_p)$, the deviation of a point $(x_1, \ldots, x_p)$ from the hyperplane is:

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Maximal margin classifier

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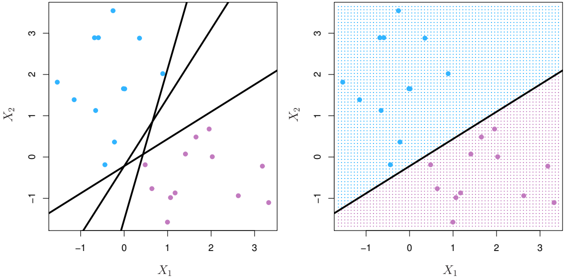
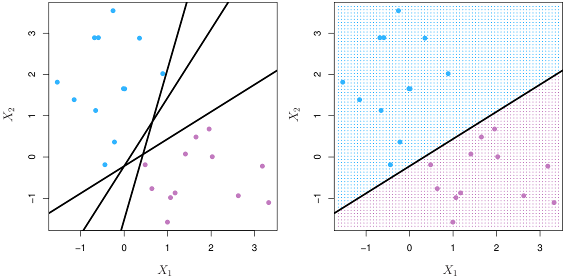


Maximal margin classifier

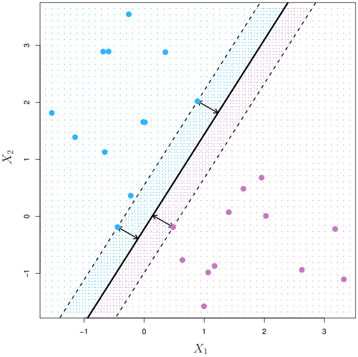
- Suppose we have a classification problem with response $Y = -1$ or $Y = 1$.
- If the classes can be separated, most likely, there will be an infinite number of hyperplanes separating the classes.



Maximal margin classifier

Idea:

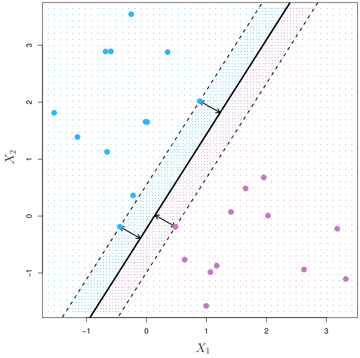
- Draw the largest possible empty margin around the hyperplane.



Maximal margin classifier

Idea:

- Draw the largest possible empty margin around the hyperplane.
- Out of all possible hyperplanes that separate the 2 classes, choose the one with the widest margin.



Maximal margin classifier

This can be written as an optimization problem:

$$\max_{\beta_0,\beta_1,\ldots,\beta_p} \quad M$$

$$\text{subject to } \sum_{j=1}^{p} \beta_j^2 = 1,$$

$$\underbrace{y_i(\beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip})}_{\text{How far is } x_i \text{ from the hyperplane}} \geq M \qquad \text{for all } i = 1, \ldots, n.$$

M is simply the width of the margin in either direction.

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This is a quadratic optimization problem. Having found $(\hat{\beta}_0, \hat{w})$ we can recover $\hat{\beta} = \hat{w}/\|\hat{w}\|_2, M = 1/\|\hat{w}\|_2$.

Finding the maximal margin classifier

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$$y_i(\beta_0 + w \cdot x_i) \geq 1 \qquad \text{for all } i = 1, \ldots, n.$$

Introducing Karush-Kuhn-Tucker multipliers, $\alpha_1, \ldots, \alpha_n$, this is equivalent to:

$$\max_{\alpha} \; \min_{\beta_0, w} \quad \frac{1}{2}\|w\|^2 - \sum_{i=1}^{n} \alpha_i [y_i(\beta_0 + w \cdot x_i) - 1]$$

subject to $\alpha_i \geq 0$.

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- Setting the partial derivatives with respect to w and β_0 to 0, we get:

$$\hat{w} = \sum_{i=1}^{n} \alpha_i y_i x_i, \quad \sum_{i=1}^{n} \alpha_i y_i = 0$$

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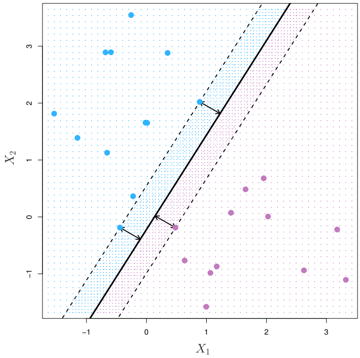
$$\hat{w} = \sum_{i=1}^{n} \alpha_i y_i x_i, \quad \sum_{i=1}^{n} \alpha_i y_i = 0$$

- Furthermore, one of the KKT conditions yields $\alpha_i > 0$ if and only if $y_i(\beta_0 + w \cdot x_i) = 1$, that is, if x_i falls on the margin.

Support vectors

The vectors that fall on the margin and determine the solution are called **support vectors**:



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subject to $\quad \alpha_i \geq 0.$

The solution is $\hat{w} = \sum_{i=1}^{n} \alpha_i y_i x_i$, and $\sum_{i=1}^{n} \alpha_i y_i = 0$ so we can plug this in above to obtain the dual problem:

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$$\text{subject to} \quad \alpha_i \geq 0, \quad \sum_{i} \alpha_i y_i = 0.$$

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$$\text{subject to} \quad \alpha_i \geq 0, \quad \sum_i \alpha_i y_i = 0.$$

This only depends on the training sample inputs through the inner products $x_i \cdot x_j$ for every pair i, j.

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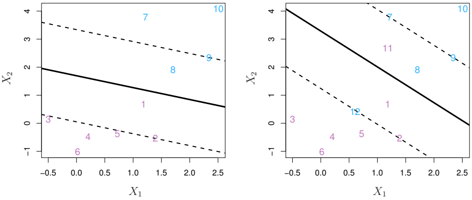

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This can be written as an optimization problem:

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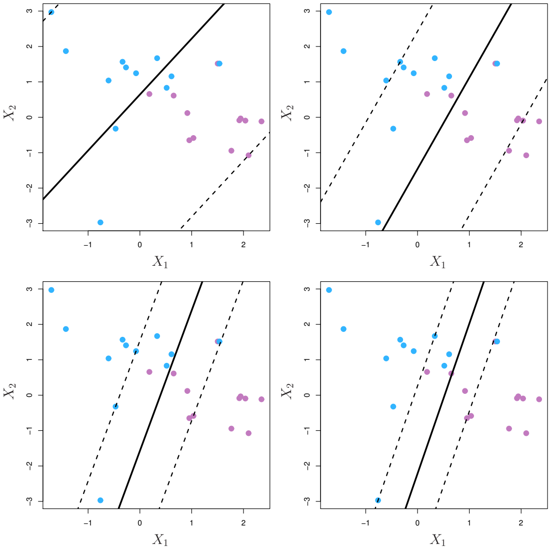
$$\underbrace{y_i(\beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip})}_{\text{How far is } x_i \text{ from the hyperplane}} \geq M(1 - \epsilon_i) \quad \text{for all } i = 1, \ldots, n$$

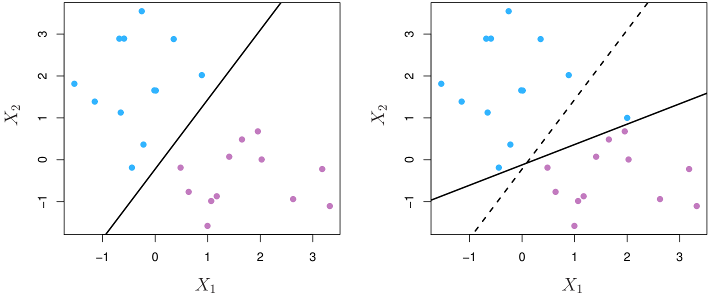
$$\epsilon_i \geq 0 \text{ for all } i = 1, \ldots, n, \quad \sum_{i=1}^{n} \epsilon_i \leq C.$$

M is the width of the margin in either direction.
$\epsilon = (\epsilon_1, \ldots, \epsilon_n)$ are called *slack* variables.
C is called the *budget*.

Tuning the budget, C (high to low)



If the budget is too low, we tend to overfit



Maximal margin classifier, $C = 0$. Adding one observation dramatically changes the classifier.

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We can reformulate the problem by defining a vector $w = (w_1, \ldots, w_p) = \beta/M$:

$$\min_{\beta_0, w, \epsilon} \quad \frac{1}{2}\|w\|^2 + D\sum_{i=1}^{n} \epsilon_i$$

subject to

$$y_i(\beta_0 + w \cdot x_i) \geq (1 - \epsilon_i) \quad \text{for all } i = 1, \ldots, n,$$

$$\epsilon_i \geq 0 \quad \text{for all } i = 1, \ldots, n.$$

The penalty $D \geq 0$ serves a function similar to the budget C, but is inversely related to it.

Finding the support vector classifier

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$$\max_{\alpha, \mu} \min_{\beta_0, w, \epsilon} \quad \frac{1}{2}\|w\|^2 - \sum_{i=1}^{n} \alpha_i [y_i(\beta_0 + w \cdot x_i) - 1 + \epsilon_i] + \sum_{i=1}^{n} (D - \mu_i)\epsilon_i$$

subject to $\alpha_i \geq 0, \mu_i \geq 0,$ for all $i = 1, \ldots, n$.

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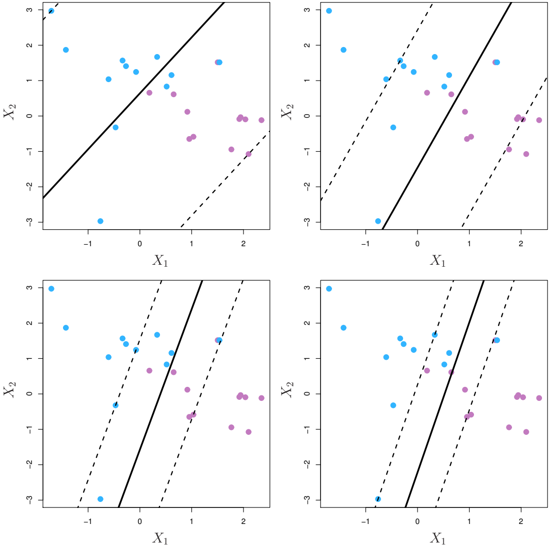

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