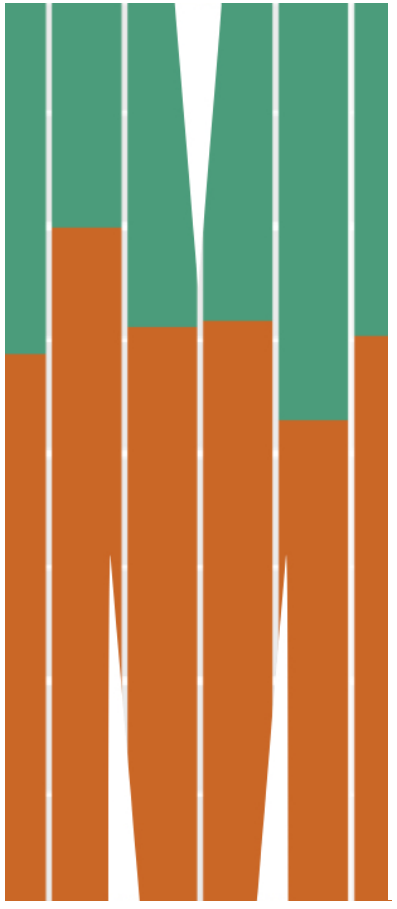


# ETC3250: Support Vector Machines

## Semester 1, 2020

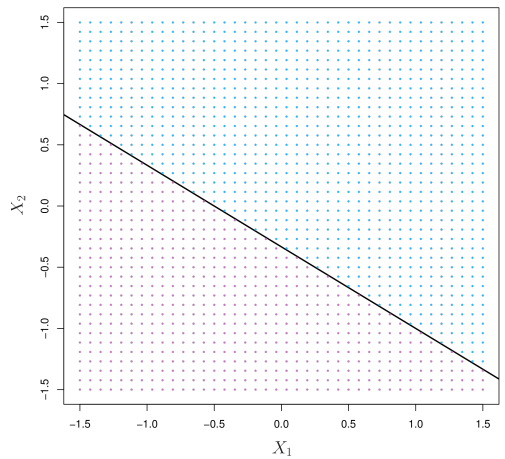
Professor Di Cook

Econometrics and Business Statistics
Monash University

Week 7 (b)

# Separating hyperplanes

In a $p$-dimensional space, a hyperplane is a flat affine subspace of dimension $p - 1$.




(ISLR: Fig 9.1)

## Separating hyperplanes

The equation of $p$-dimensional hyperplane is given by

$$\beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p = 0$$

If $x_i \in \Re^p$ and $y_i \in \{-1, 1\}$ for $i = 1, \ldots, n$, then

$$\beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip} > 0 \text{ if } y_i = 1,$$

$$\beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip} < 0 \text{ if } y_i = -1$$

Equivalently,

$$y_i(\beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip}) > 0$$

# Separating hyperplanes

- A new observation is assigned a class depending on which side of the hyperplane it is located
- Classify the test observation $x^*$ based on the sign of

$$s(x^*) = \beta_0 + \beta_1 x_1^* + \cdots + \beta_p x_p^*$$

- If $s(x^*) > 0$, class $1$, and if $s(x^*) < 0$, class $-1$, i.e. $h(x^*) = \text{sign}(s(x^*))$.

# Separating hyperplanes

What about the magnitude of $s(x^*)$?

- $s(x^*)$ far from zero $\rightarrow x^*$ lies far from the hyperplane + **more confident** about our classification
- $s(x^*)$ close to zero $\rightarrow x^*$ near the hyperplane + **less confident** about our classification

# Separating hyperplane classifiers

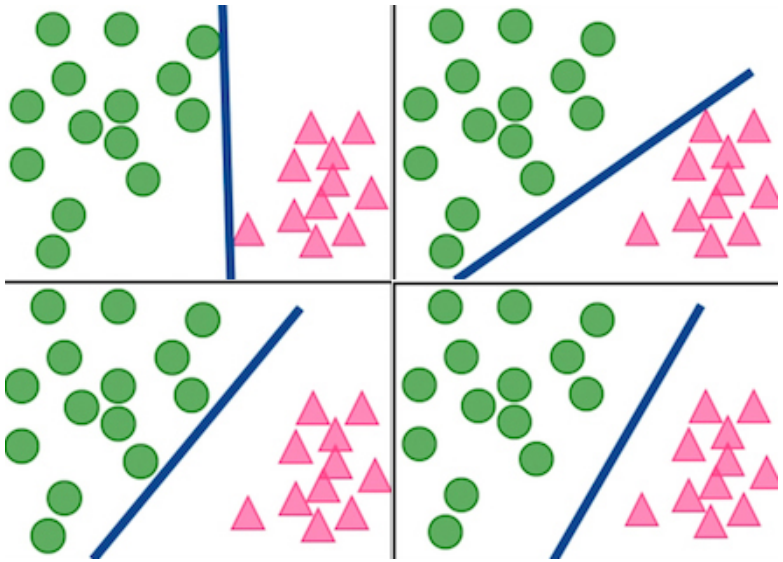
We will explore *three* different types of hyperplane classifiers, with each method generalising the one before it.

- Maximal marginal classifier for when the data is perfectly separated by a hyperplane
- Support vector classifier/ soft margin classifier for when data is NOT perfectly separated by a hyperplane but still has a linear decision boundary, and
- Support vector machines used for when the data has non-linear decision boundaries.

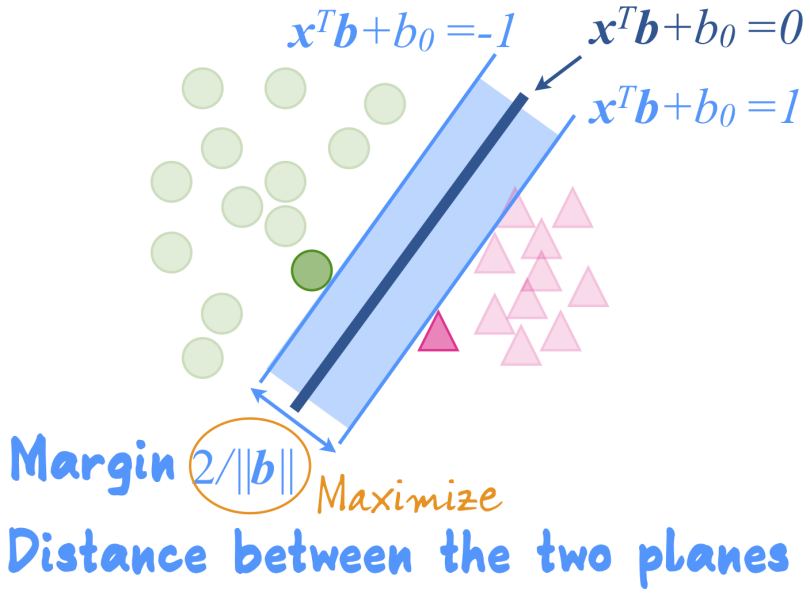
In practice, SVMs are used to refer to all three methods, however we will distinguish between the three notions in this lecture.

# Maximal margin classifier

All are separating hyperplanes. Which is best?



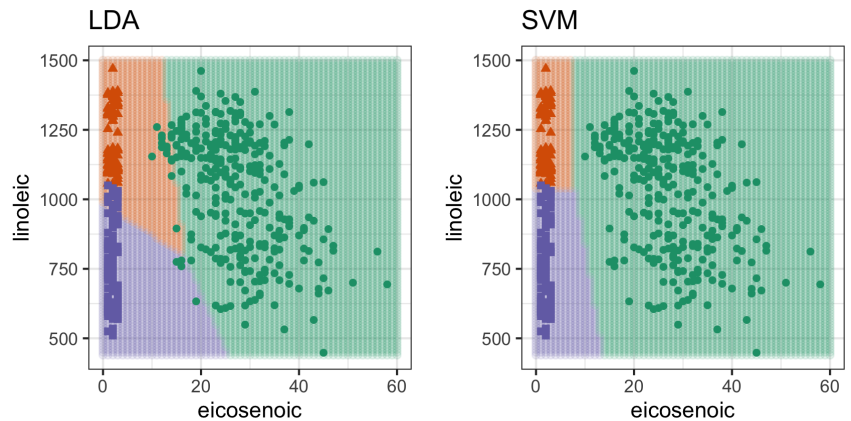
# Maximal margin classifier




Source: Machine Learning Memes for Convolutional Teens

# From LDA to SVM

- Linear discriminant analysis uses the difference between means to set the separating hyperplane.
- Support vector machines uses gaps between points on the outer edge of clusters to set the separating hyperplane.

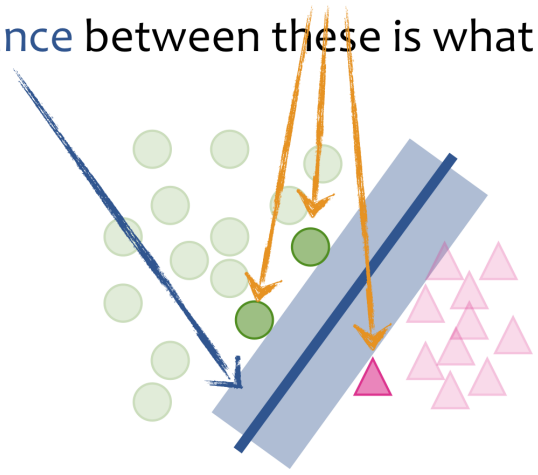


# SVM vs Logistic Regression

- If our data can be perfectly separated using a hyperplane, then there will in fact exist an **infinite number of such hyperplanes**.
- We compute the (perpendicular) distance from each training observation to a given separating hyperplane. The smallest such distance is known as the margin.
- The optimal separating hyperplane (or maximal margin hyperplane) is the separating hyperplane for which the margin is largest.
- We can then classify a test observation based on which side of the maximal margin hyperplane it lies. This is known as the maximal margin classifier.

# Support vectors

- Hyperplane is defined by a subset of the point, the support vectors
- Distance between these is what is maximized



# Support vectors

- The support vectors are equidistant from the maximal margin hyperplane and lie along the dashed lines indicating the width of the margin.
- They support the maximal margin hyperplane in the sense that if these points were moved slightly then the maximal margin hyperplane would move as well

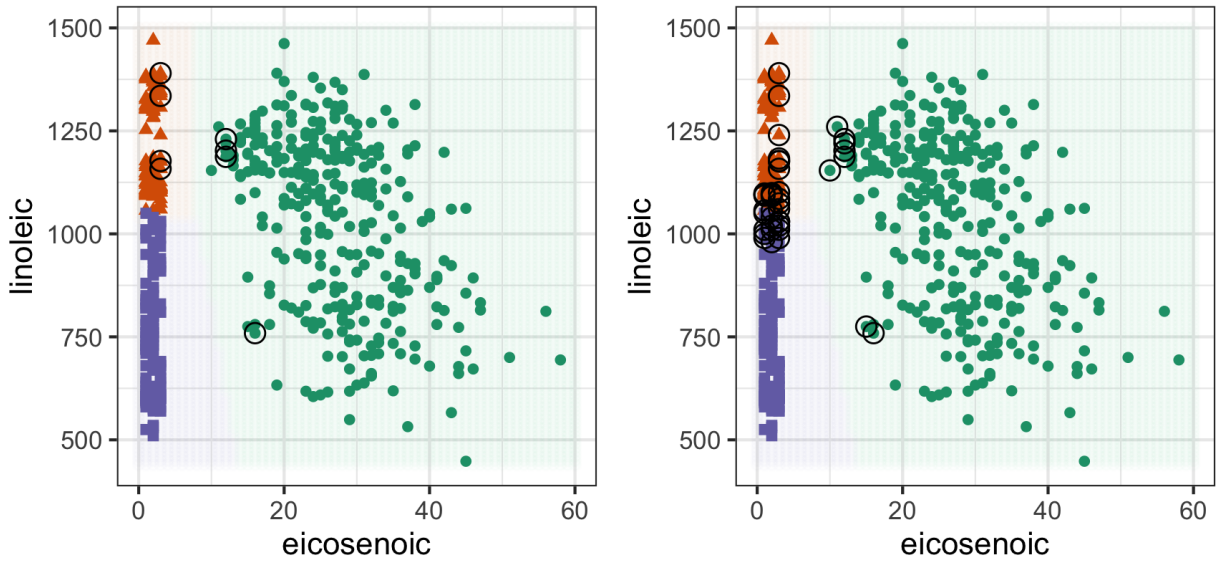
**The maximal margin hyperplane depends directly on the support vectors, but not on the other observations**

# Support vectors

**Training Example:**
***not a support vector***

**SVM:**

## Example: Support vectors (and slack vectors)



# Maximal margin classifier

If $x_i \in \mathbb{R}^p$ and $y_i \in \{-1, 1\}$ for $i = 1, \ldots, n$, the separating hyperplane is defined as

$$\{x : \beta_0 + x^T \beta = 0\}$$

where $\beta = \sum_{i=1}^{s} (\alpha_i y_i) x_i$ and $s$ is the number of support vectors. Then the maximal margin hyperplane is found by

*maximising* $M$, subject to $\sum_{j=1}^{p} \beta_j^2 = 1$, and $y_i(x_i^T \beta + \beta_0) \geq M, i = 1, \ldots, n$.

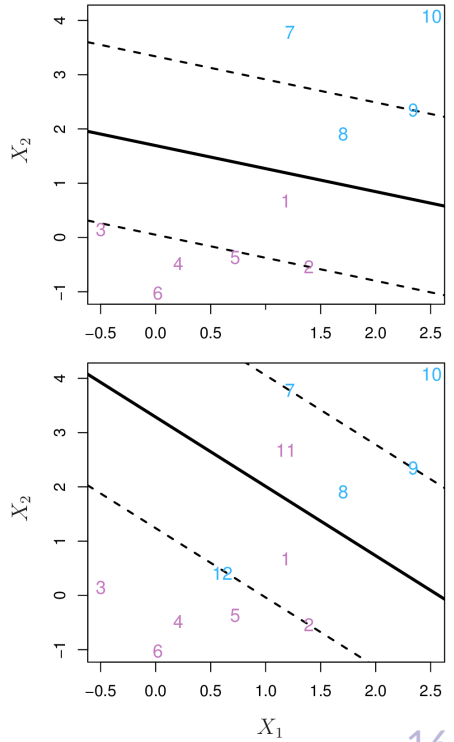
# Non-separable case

The maximal margin classifier only works when we have perfect separability in our data.

What do we do if data is not perfectly separable by a hyperplane?

**The support vector classifier** allows points to either lie on the wrong side of the margin, or on the wrong side of the hyperplane altogether.

Right: ISLR Fig 9.6



# Support vector classifier - optimisation

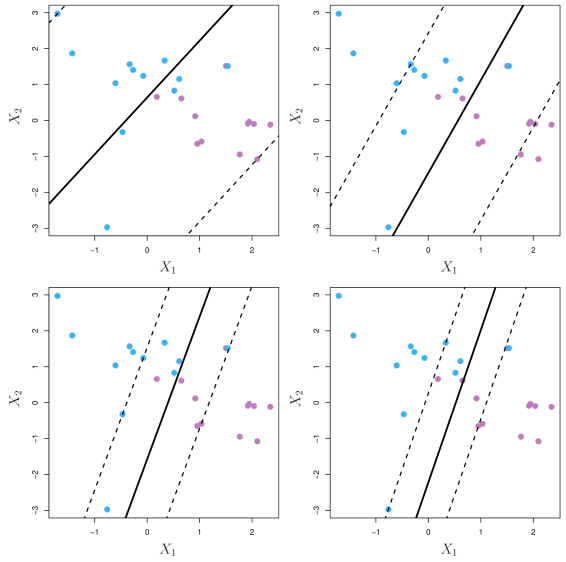
*Maximise* $M$, subject to $\sum_{i=1}^{p} \beta_i^2 = 1$, and
$y_i(x_i'\beta + \beta_0) \geq M(1 - \epsilon_i), i = 1, \ldots, n$, AND $\epsilon_i \geq 0, \sum_{i=1}^{n} \epsilon_i \leq C$.

$\varepsilon_i$ tells us where the $i$th observation is located and $C$ is a nonnegative tuning parameter.

- $\varepsilon_i = 0$: correct side of the margin,
- $\varepsilon_i > 0$: wrong side of the margin (violation of the margin),
- $\varepsilon_i > 1$: wrong side of the hyperplane.

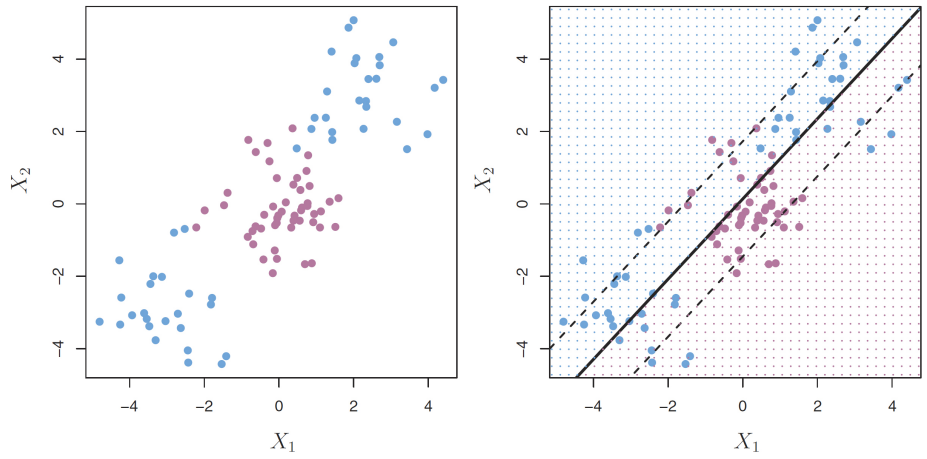
# Non-separable case

Tuning parameter: decreasing the value of $C$



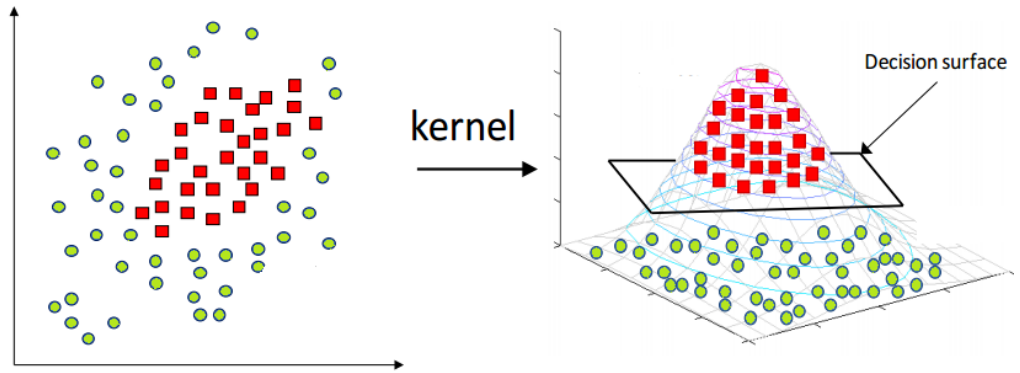
# Non-linear boundaries

The support vector classifier doesn't work well for non-linear boundaries. What solution do we have?



# Enlarging the feature space

Consider the following 2D non-linear classification problem. We can transform this to a linear problem separated by a maximal margin hyperplane by introducing an additional third dimension.




Source: Grace Zhang @zxr.nju

# The inner product

Consider two $p$-vectors

$$\begin{aligned} & \mathbf{x} = (x_1, x_2, \ldots, x_p) \in \mathbb{R}^p \\ \text{and} \quad & \mathbf{y} = (y_1, y_2, \ldots, y_p) \in \mathbb{R}^p. \end{aligned}$$

The inner product is defined as

$$\langle \mathbf{x}, \mathbf{y} \rangle = x_1 y_1 + x_2 y_2 + \cdots + x_p y_p = \sum_{j=1}^{p} x_j y_j$$

A linear measure of similarity, and allows geometric constrctions such as the maximal marginal hyperplane.

# Kernel functions

A kernel function is an inner product of vectors mapped to a (higher dimensional) feature space $\mathcal{H} = \mathbb{R}^d, d > p$.

$$\mathcal{K}(\mathbf{x}, \mathbf{y}) = \langle \psi(\mathbf{x}), \psi(\mathbf{y}) \rangle$$

$$\psi : \mathbb{R}^p \to \mathcal{H}$$

Non-linear measure of similarity, and allows geometric constructions in high dimensional space.

## Examples of kernels

Standard kernels include:

$$\begin{aligned} \text{Linear} \quad & \mathcal{K}(\mathbf{x}, \mathbf{y}) = \langle \mathbf{x}, \mathbf{y} \rangle \\ \text{Polynomial} \quad & \mathcal{K}(\mathbf{x}, \mathbf{y}) = (\langle \mathbf{x}, \mathbf{y} \rangle + 1)^d \\ \text{Radial} \quad & \mathcal{K}(\mathbf{x}, \mathbf{y}) = \exp(-\gamma ||\mathbf{x} - \mathbf{y}||^2) \end{aligned}$$

# Support Vector Machines

## The kernel trick

The linear support vector classifier can be represented as follows:

$$f(x) = \beta_0 + \sum_{i \in \mathcal{S}} \alpha_i \langle x, x_i \rangle.$$

We can generalise this by replacing the inner product with the kernel function as follows:

$$f(x) = \beta_0 + \sum_{i \in \mathcal{S}} \alpha_i \mathcal{K}(x, x_i).$$

$K(\mathbf{x}_i, \mathbf{x}_j)$

| Name | Function |
|---|---|
| Polynomial | $(\|\mathbf{x}_i{}^T \mathbf{x}_j\|+d)^p$ |
| Gaussian radial basis | $exp(-\|\mathbf{x}_i - \mathbf{x}_j\|^2/2\sigma^2)$ |
| Sigmoid | $tanh(a\|\mathbf{x}_i{}^T \mathbf{x}_j\|+d)$ |

## Your turn

Let $\mathbf{x}$ and $\mathbf{y}$ be vectors in $\mathbb{R}^2$. By expanding $\mathcal{K}(\mathbf{x}, \mathbf{y}) = (1 + \langle \mathbf{x}, \mathbf{y} \rangle)^2$ show that this is equilvalent to an inner product in $\mathcal{H} = \mathbb{R}^6$.

Remember: $\langle \mathbf{x}, \mathbf{y} \rangle = \sum_{j=1}^{p} x_j y_j$.

03:00

## Solution

$$
\begin{aligned}
\mathcal{K}(\mathbf{x}, \mathbf{y}) &= (1 + \langle \mathbf{x}, \mathbf{y} \rangle)^2 \\
&= \left(1 + \sum_{j=1}^{2} x_j y_j\right)^2 \\
&= (1 + x_1 y_1 + x_2 y_2)^2 \\
&= (1 + x_1^2 y_1^2 + x_2^2 y_2^2 + 2x_1 y_1 + 2x_2 y_2 + 2x_1 x_2 y_1 y_2) \\
&= \langle \psi(\mathbf{x}), \psi(\mathbf{y}) \rangle
\end{aligned}
$$

where $\psi(\mathbf{x}) = (1, x_1^2, x_2^2, \sqrt{2}x_1, \sqrt{2}x_2, \sqrt{2}x_1 x_2)$.

# The kernel trick - why is it a trick?

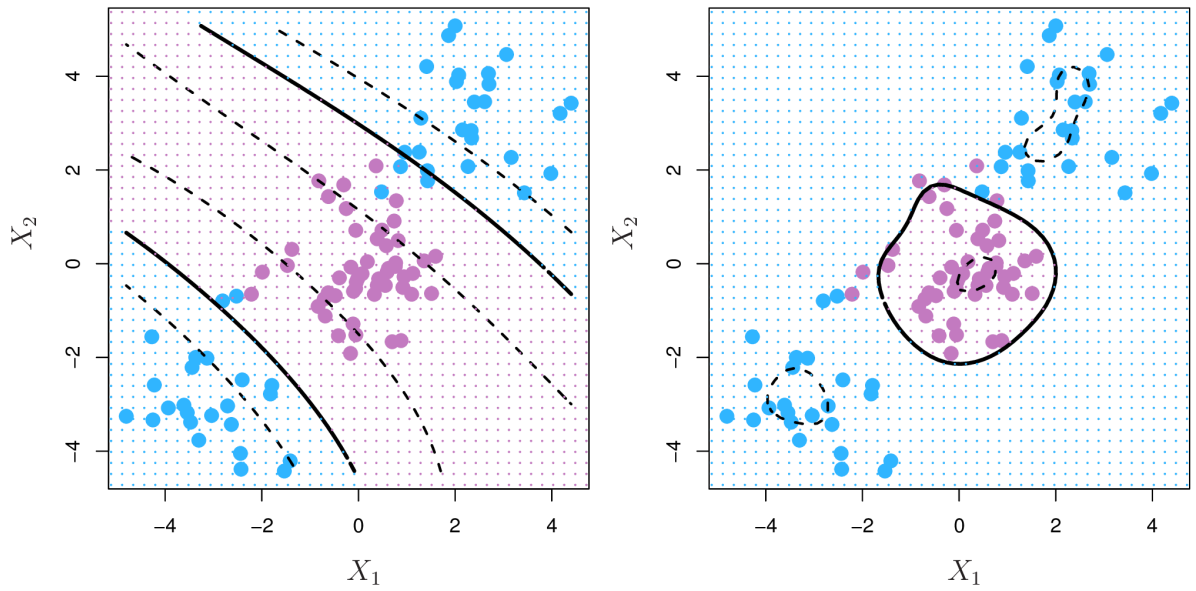
We do not need to know what the high dimensional enlarged feature space $\mathcal{H}$ really looks like.

We just need to know the which kernel function is most appropriate as a measure of similarity.

The Support Vector Machine (SVM) is a maximal margin hyperplane in $\mathcal{H}$ built by using a kernel function in the low dimensional feature space $\mathbb{R}^p$.

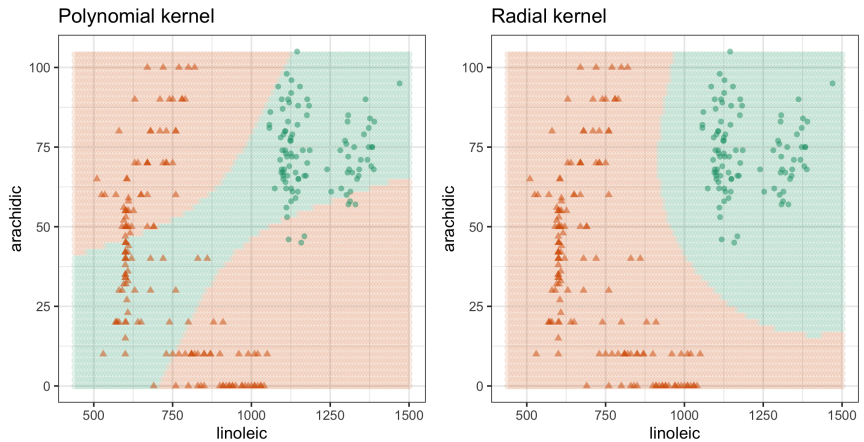
# Non-linear boundaries

## Polynomial and radial kernel SVMs



# Non-linear boundaries

## Italian olive oils: Regions 2, 3 (North and Sardinia)



# SVM in high dimensions

Examining misclassifications and which points are selected to be support vectors

# SVM in high dimensions

## Examining boundaries

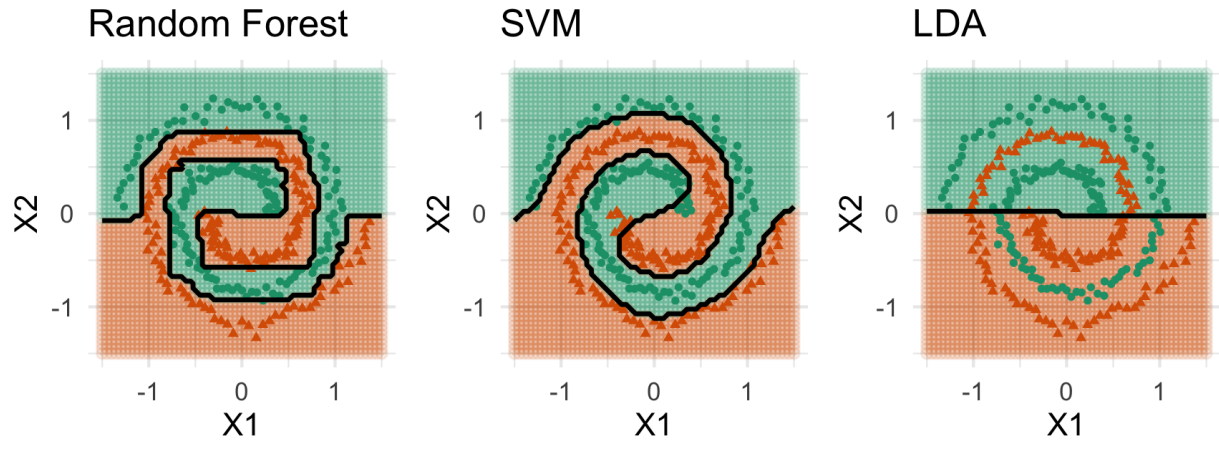
# SVM in high dimensions

## Boundaries of a radial kernel in 3D

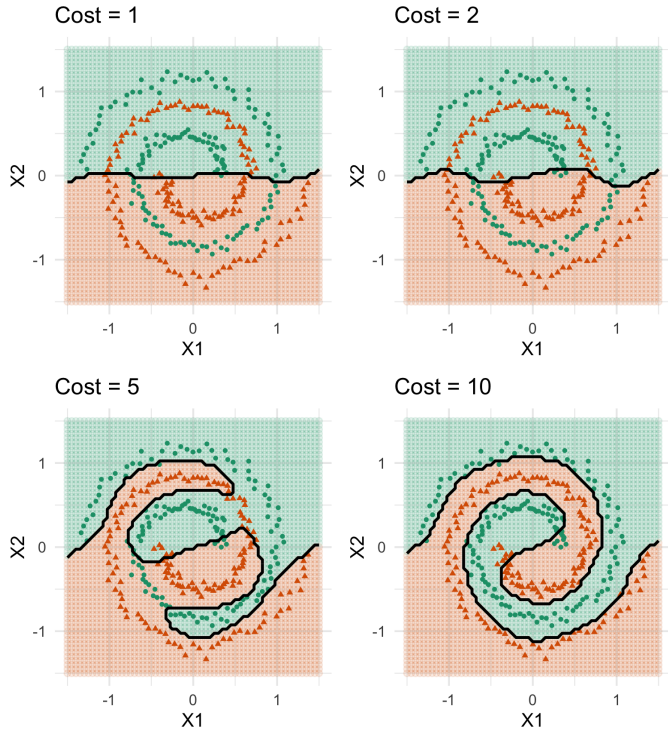
# SVM in high dimensions

## Boundaries of a polynomial kernel in 5D

# Comparing decision boundaries



# Increasing the value of `cost` in `svm`



# 👩‍💻 Made by a human with a computer

Slides at https://iml.numbat.space.

Code and data at https://github.com/numbats/iml.

Created using R Markdown with flair by **xaringan**, and **kunoichi** (female ninja) style.