# PQHS 471
# Lecture 10: Support Vector Machines

# Support Vector Machines

- Dr. Vladimir Vapnik (1936 - present).
- Moved from USSR to USA in 1990, and worked at AT&T Bell Lab.
- Inventor of the Support Vector Machines.

# Support Vector Machines

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  - We try and find a plane that separates the classes in feature space.

# Support Vector Machines

- Here we approach the two-class classification problem in a direct way:
    - We try and find a plane that separates the classes in feature space.
- If we cannot, we get creative in two ways:
    1. We soften what we mean by "separates", and
    2. We enrich and enlarge the feature space so that separation is possible.

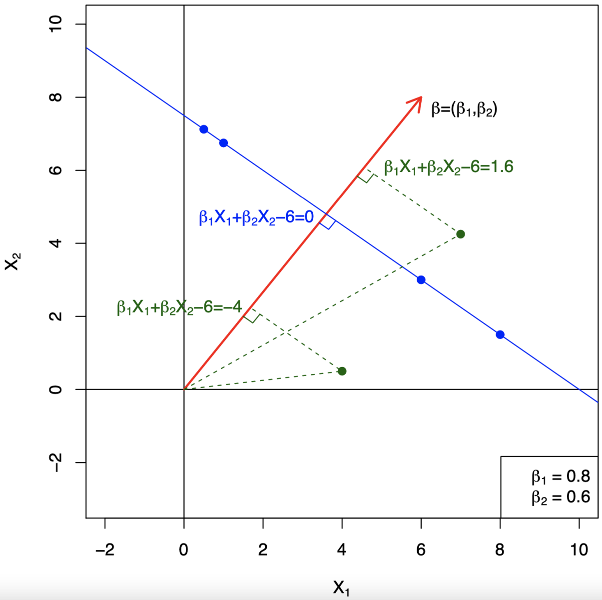
# Hyperplane

- A hyperplane in $p$ dimensions is a flat affine subspace of dimension $p-1$.
- In general the equation for a hyperplane has the form

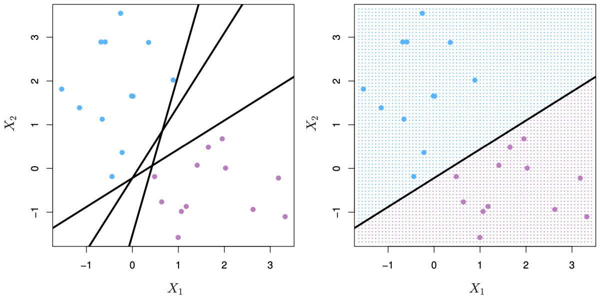
$$\beta_0 + \beta_1 X_1 + \beta_2 X_2 + ... + \beta_p X_p = 0$$

- In $p = 2$ dimensions a hyperplane is a line.
- If $\beta_0 = 0$, the hyperplane goes through the origin, otherwise not.
- The vector $\beta = (\beta_1, \beta_2, ..., \beta_p)$ is called the normal vector — it points in a direction orthogonal to the surface of a hyperplane.

# Hyperplane example in 2D



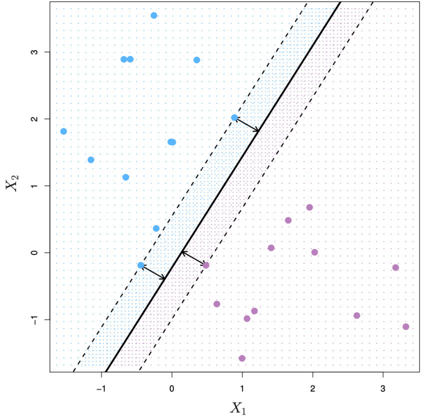
# Separating Hyperplanes




- If $f(X) = \beta_0 + \beta_1 X_1 + \ldots + \beta_p X_p$,then $f(X) > 0$ for points on one side of the hyperplane, and $f(X) < 0$ for points on the other.
- If we code the colored points as $Y_i = +1$ for blue, say, and $Y_i = -1$ for mauve, then if $Y_i \cdot f(X_i) > 0$ for all $i$, $f(X) = 0$ defines a separating hyperplane.

# Maximal Margin Classifier

Among all separating hyperplanes, find the one that makes the biggest gap or margin between the two classes.




Constrained optimization problem

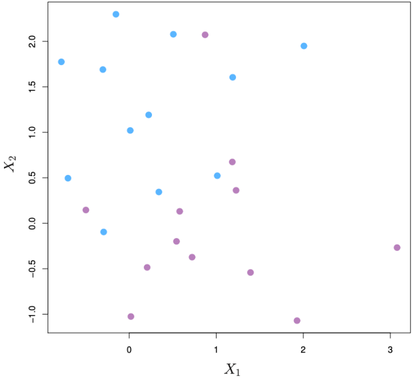
$$\underset{\beta_0,\beta_1,\ldots,\beta_p}{\text{maximize}}\; M$$

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

$$y_i(\beta_0 + \beta_1 x_{i1} + \ldots + \beta_p x_{ip}) \geq M$$

$$\text{for all } \; i = 1, \ldots, N.$$

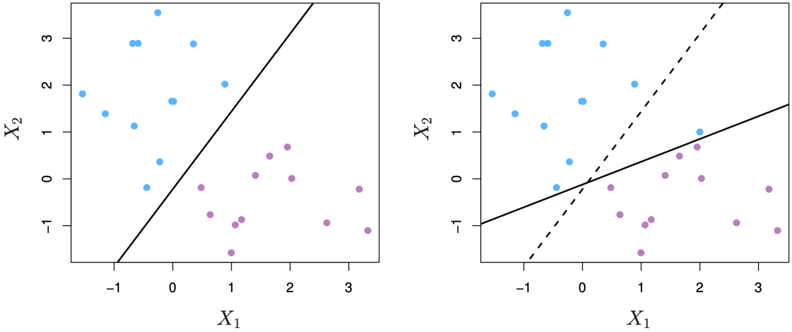
# Non-separable data




The data on the left are not separable by a linear boundary.

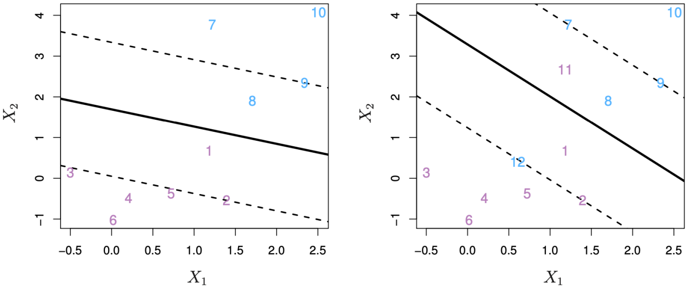
This is often the case, unless $N < p$.

# Noisy data




- Sometimes the data are separable, but noisy. This can lead to a poor solution for the maximal-margin classifier.
- The support vector classifier maximizes a soft margin.

# Support Vector Classifier




$$\underset{\beta_0,\beta_1,\ldots,\beta_p,\epsilon_1,\ldots,\epsilon_n}{\text{maximize}} \quad M \quad \text{subject to} \quad \sum_{j=1}^{p} \beta_j^2 = 1,$$

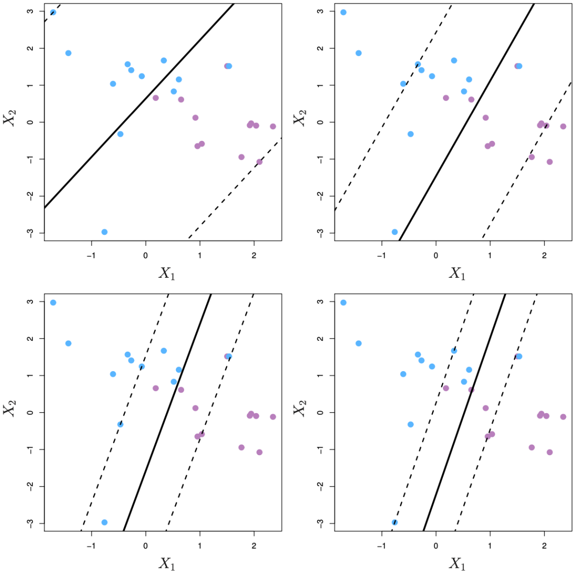
$$y_i(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \ldots + \beta_p x_{ip}) \geq M(1 - \epsilon_i),$$

$$\epsilon_i \geq 0, \quad \sum_{i=1}^{n} \epsilon_i \leq C,$$

- $C$: a budget

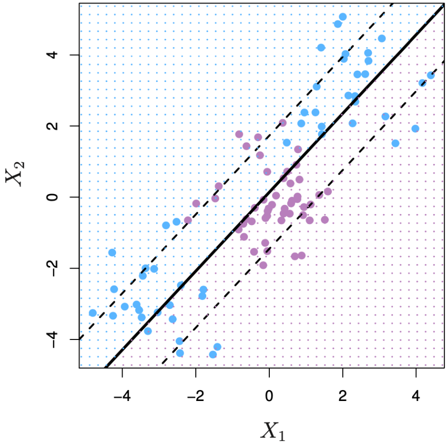
- When the data are not perfectly separable in the feature space, we may allow some observations to be on the "wrong" side of the margin.
- We give "allowances" to the observations but control the total "budget".
- A large $C$: the margin is large and many observations can be support vectors.

# Budget $C$: regularization parameter



## Feature Expansion and Kernels

# Linear boundary can fail




Sometime a linear boundary simply won't work, no matter what value of $C$.

The example on the left is such a case.

What to do?

# Feature Expansion

- Enlarge the space of features by including transformations; e.g. $X_1^2, X_1^3, X_1X_2, X_1X_2^2, \ldots$Hence go from a $p$-dimensional space to a $M > p$ dimensional space.
- Fit a support-vector classifier in the enlarged space.
- This results in non-linear decision boundaries in the original space.

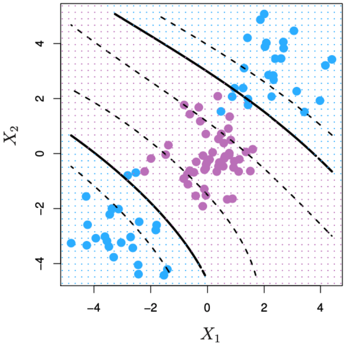
Example: Suppose we use $(X_1, X_2, X_1^2, X_2^2, X_1X_2)$ instead of just $(X_1, X_2)$. Then the decision boundary would be of the form

$$\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1^2 + \beta_4 X_2^2 + \beta_5 X_1 X_2 = 0$$

This leads to nonlinear decision boundaries in the original space (quadratic sections).

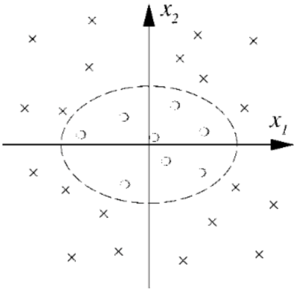
# Cubic polynomials example

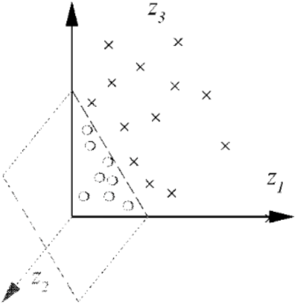
- Here we use a basis expansion of cubic polynomials
- From 2 variables to 9 variables
- The support-vector classifier in the enlarged space solves the problem in the lower-dimensional space




$$\beta_0+\beta_1 X_1+\beta_2 X_2+\beta_3 X_1^2+\beta_4 X_2^2+\beta_5 X_1 X_2+\beta_6 X_1^3+\beta_7 X_2^3+\beta_8 X_1 X_2^2+\beta_9 X_1^2 X_2 = 0$$

When domain knowledge is available, sometimes we could use explicit transformations. But often we cannot.




- 2D classification.
- Separable (and linear!) in features spaces of $x_1^2, x_2^2, x_1 x_2$
- The **linear** hyperplane $\rightarrow$ **nonlinear** ellipsoidal decision boundary in the original space.

# Nonlinearities and Kernels

- Polynomials (especially high-dimensional ones) get wild rather fast.
- There is a more elegant and controlled way to introduce nonlinearities in support-vector classifiers — through the use of kernels.
- Before we discuss these, we must understand the role of inner products in support-vector classifiers.

# Inner products and support vectors

- Inner product between two vectors:

$$\langle \mathbf{x}_i, \mathbf{x}_j \rangle = \sum_{k=1}^{p} x_{ik} x_{jk}$$

- The linear support vector classifier can be represented as (n parameters):

$$f(x) = \beta_0 + \sum_{i=1}^{n} \alpha_i \langle \mathbf{x}, \mathbf{x}_i \rangle$$

- To estimate the parameters $\alpha_1, ..., \alpha_n$ and $\beta_0$, all we need are the $\binom{n}{2}$ inner products $\langle \mathbf{x}, \mathbf{x}_i \rangle$ between all pairs of training observations.

It turns out that most of the $\hat{\alpha}_i$ can be zero:

$$f(x) = \beta_0 + \sum_{i \in \mathcal{S}} \hat{\alpha}_i \langle \mathbf{x}, \mathbf{x}_i \rangle$$

$\mathcal{S}$ is the support set of indices $i$ such that $\hat{\alpha}_i > 0$. See slides 10.

# Kernels and Support Vector Machines

- If we can compute inner-products between observations, we can fit a SV classifier. Can be quite abstract!
- Some special kernel functions can do this for us. E.g.

$$K(\mathbf{x}_i, \mathbf{x}_j) = (1 + \sum_{k=1}^{p} x_{ik} x_{jk})^d$$

  can computes the inner-products needed for $d$ dimensional polynomials — $\binom{p+d}{d}$ basis functions!
- The solution has the form:

$$f(x) = \beta_0 + \sum_{i \in \mathcal{S}} \hat{\alpha}_i K(\mathbf{x}, \mathbf{x}_i)$$

# the Kernels trick

- $h(x)$ is involved ONLY in the form of inner product! So, as long as we define the kernel function

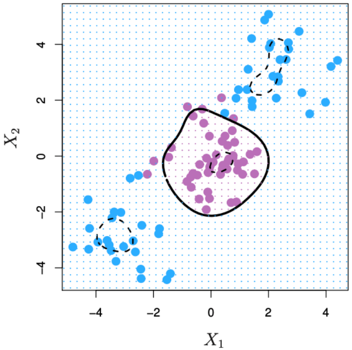
$$K(\mathbf{x}_i, \mathbf{x}_j) = \langle h(\mathbf{x}_i), h(\mathbf{x}_j) \rangle$$

which computes the inner product in the transformed space, we don't need to know what $h(x)$ itself is! (**Kernel trick**)

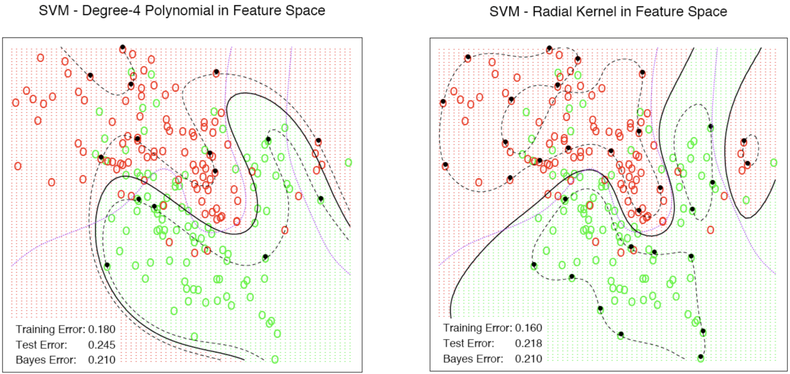
- Some commonly used Kernels:

$$\begin{aligned} d\text{th-Degree polynomial: } & K(x, x') = (1 + \langle x, x' \rangle)^d, \\ \text{Radial basis: } & K(x, x') = \exp(-\gamma \|x - x'\|^2), \\ \text{Neural network: } & K(x, x') = \tanh(\kappa_1 \langle x, x' \rangle + \kappa_2) \end{aligned}$$

$$K(x_i, x_{i'}) = \exp(-\gamma \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2)$$




- Implicit feature space; very high dimensional.
- Controls variance by squashing down most dimensions severely.

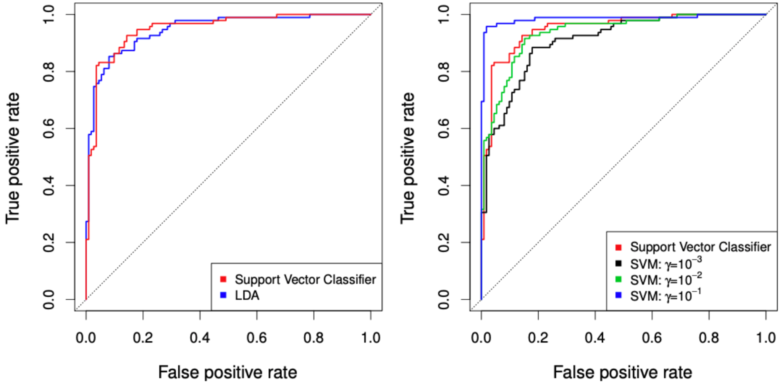



- Radial basis kernel with $\gamma = 1$
- $C$ was tuned and picked $= 1$
- Radial kernel performs the best here (close to Bayes optimal), as might be expected give the data arise from mixtures of Gaussians.

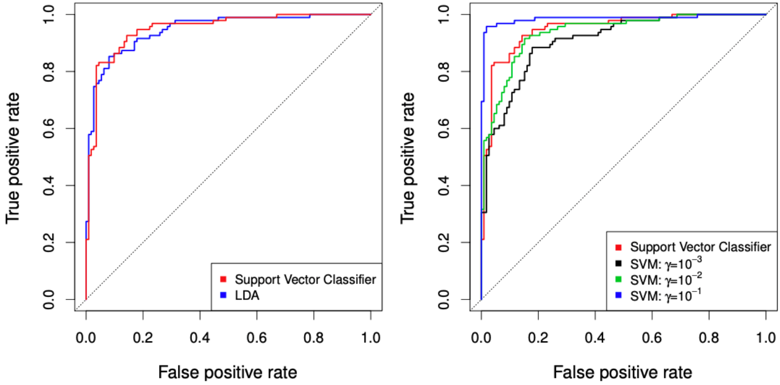
# SVM in R

- The function svm() in package e1071 provides svm solutions efficiently.

# Example: Heart Data

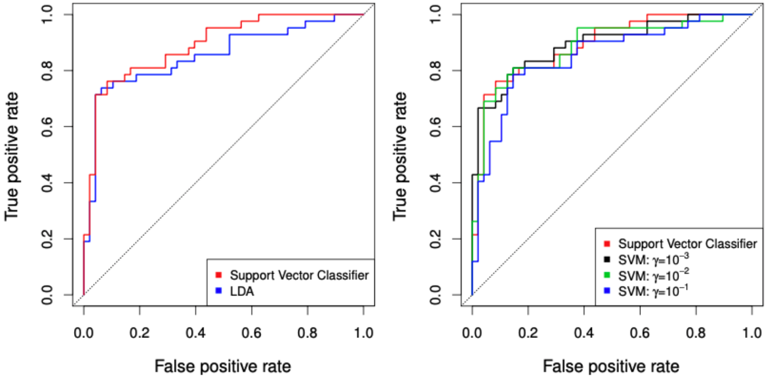


# Example: Heart Data

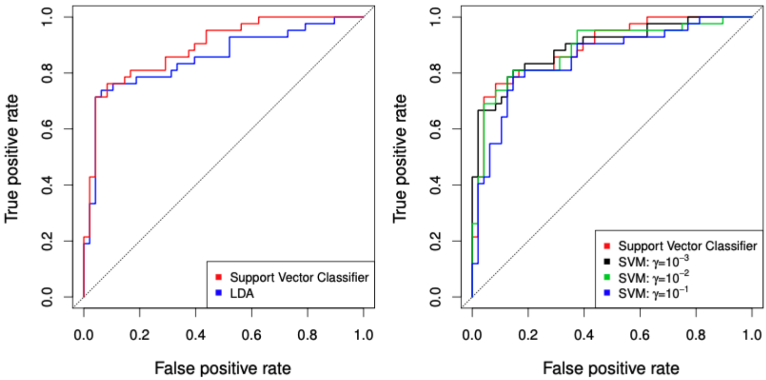



can we make conclusion using this ROC? NO.

# Example: Heart Testing Data



# Example: Heart Testing Data




can we make conclusions? Yes we are ready now.

# SVM for more than 2 classes

The SVM as defined works for $K = 2$ classes. What do we do if we have $K > 2$ classes?

- **OVA**:
  One versus All. Fit $K$ different 2-class SVM classifiers $\hat{f}_k(x), k = 1, ..., K$; each class versus the rest. Classify $x^*$ to the class for which $\hat{f}_k(x^*)$ is largest.
- **OVO**:
  One versus One. Fit all $\binom{K}{2}$ pairwise classifiers. Classify $x^*$ to the class that wins the most pairwise competitions.

Which to choose? If $K$ is not too large, use OVO.

# SVM usage

How to select kernel and parameters?

- Domain knowledge:
  - How complex should the space partition be?
  - Should the surface be smooth?
- Compare the models by their approximate testing error rate cross-validation:
  - Fit data using multiple kernels/parameters
  - Estimate error rate for each setting
  - Select the best-performing one

# SVM summary

Strengths of SVM:

- flexibility
- scales well for high-dimensional data
- can control complexity and error trade-off explicitly
- as long as a kernel can be defined, non-traditional(vector) data, like strings, trees can be input

Weakness:

- how to choose a good kernel?
  (a low degree polynomial or radial basis function can be a good start)

# Textbook chapters

- ISLR: chapter 9: 9.1 - 9.4