Statistical Methods for Data Mining

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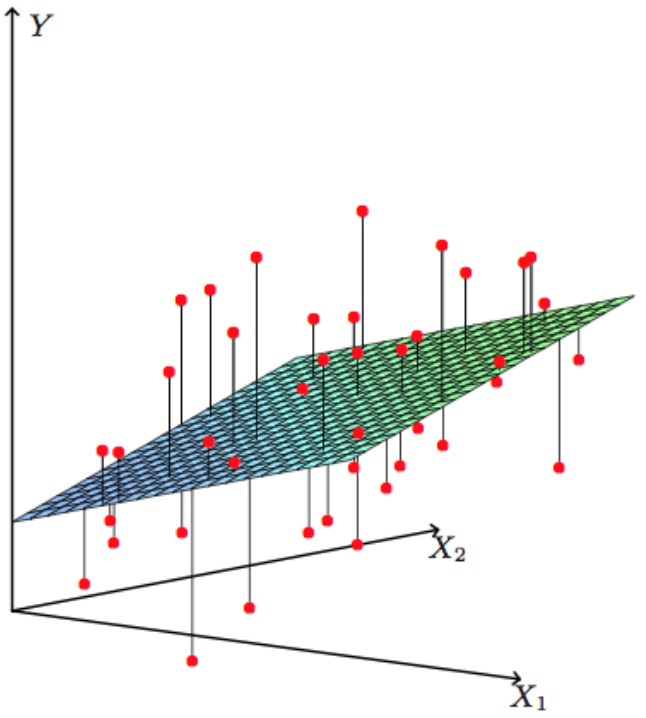


Support Vector Machines

support vector machine developed in CS community in the 1990s and that has grown in popularity since then.

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.*

maximal margin classifer

If we cannot, we get creative in two ways:

- We soften what we mean by "separates", and

support vector classifier

- We enrich and enlarge the feature space so that separation is possible.

support vector machine

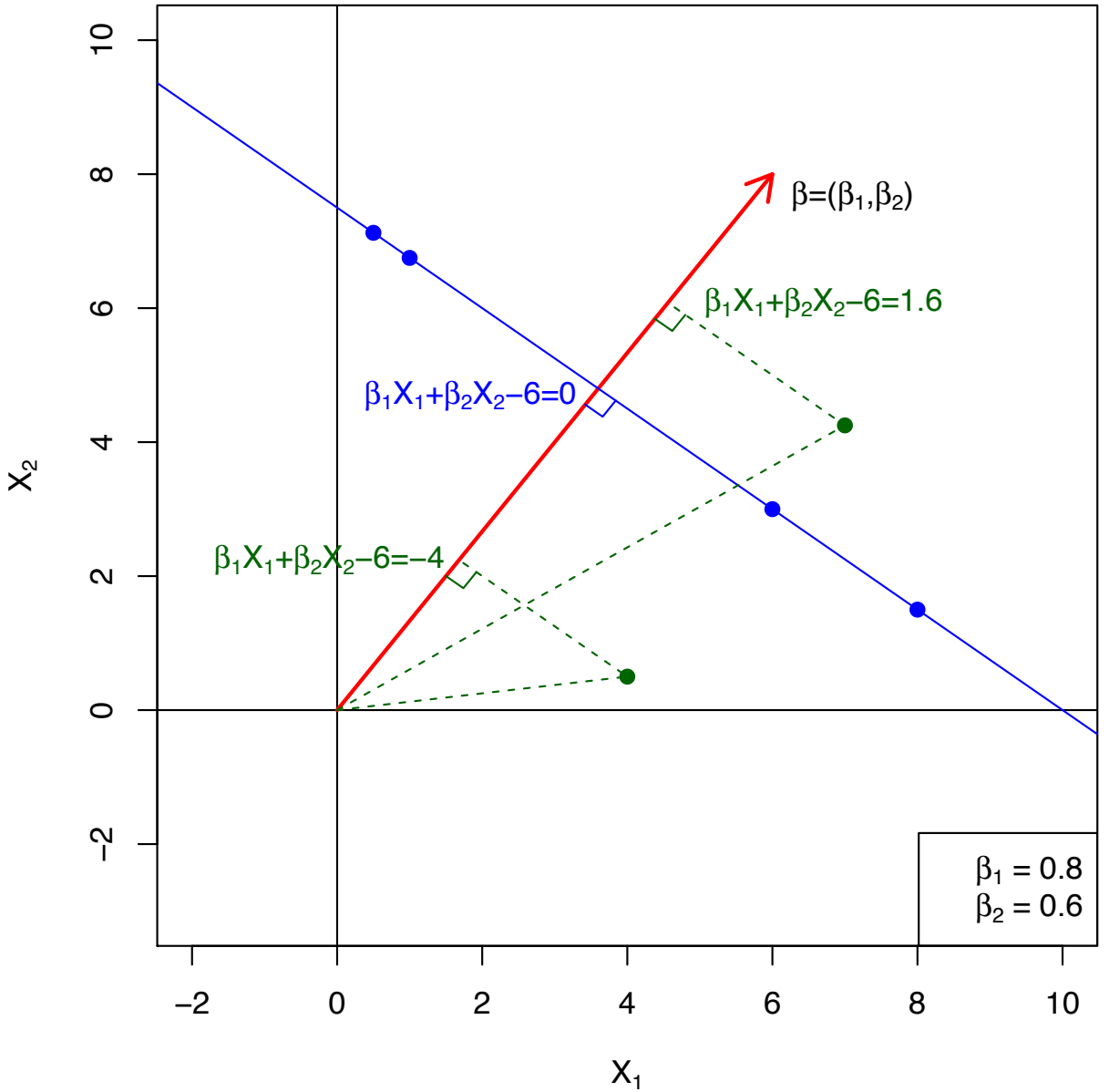
What is a Hyperplane?

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

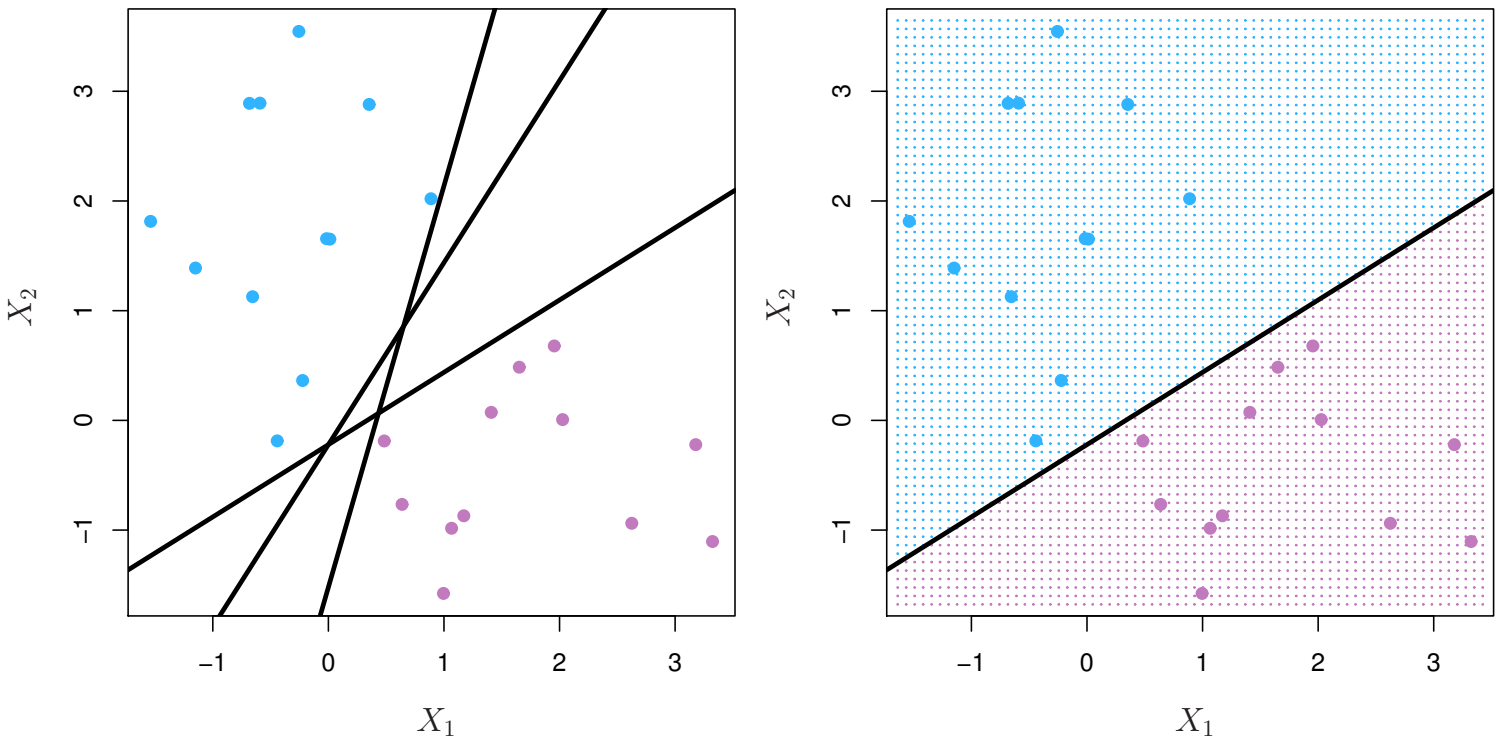
$$\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \ldots + \beta_p X_p = 0$$

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

Hyperplane in 2 Dimensions



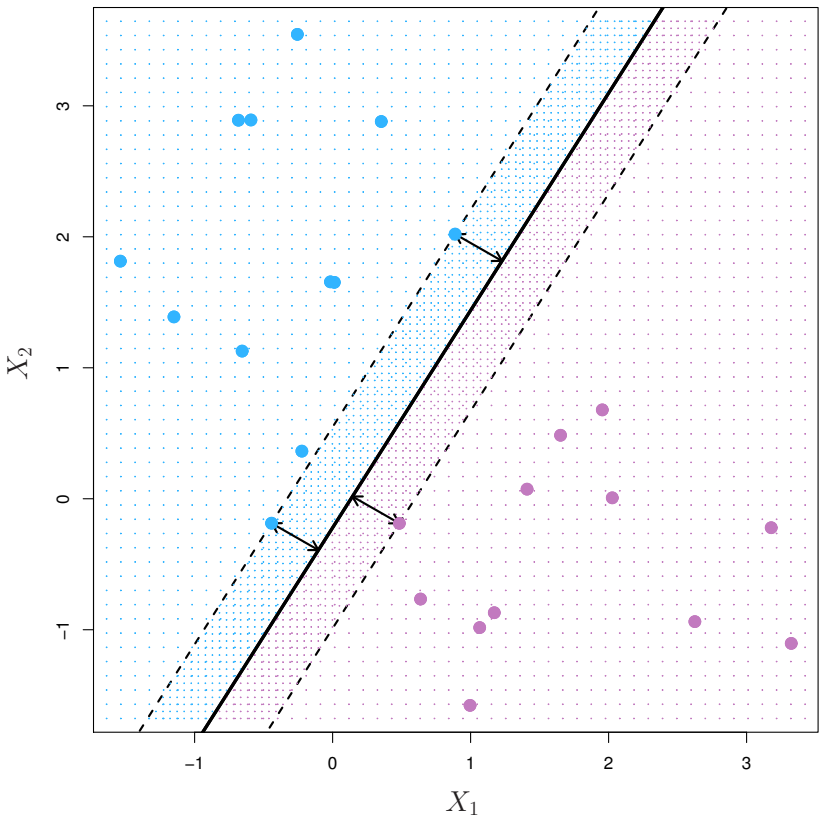
Separating Hyperplanes



- If $f(X) = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p$, 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

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

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

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

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

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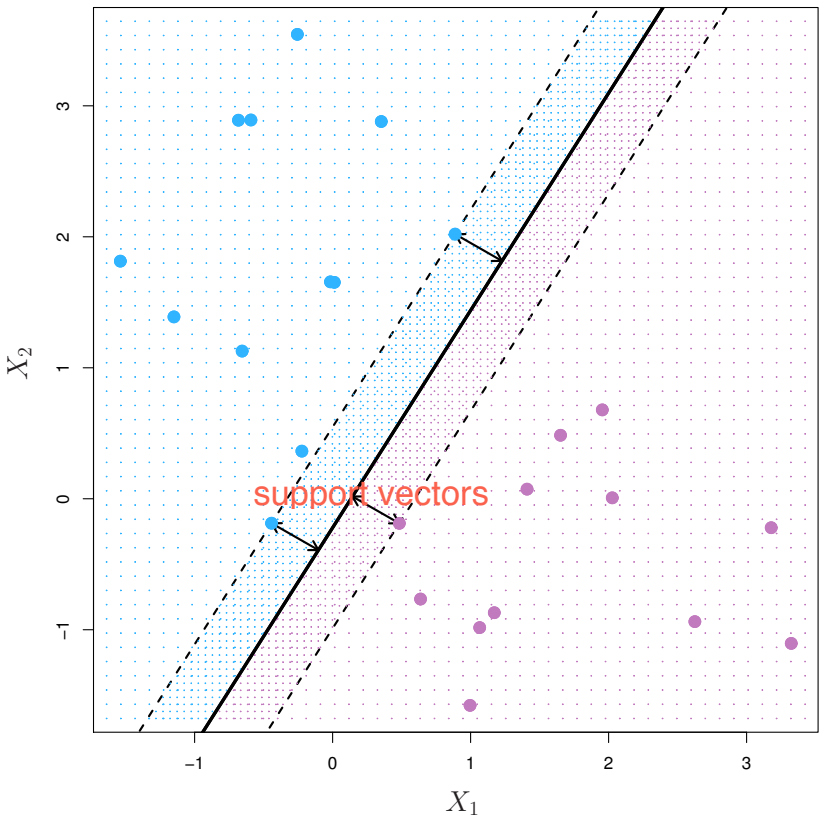

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This can be rephrased as a convex quadratic program, and solved efficiently. The function `svm()` in package `e1071` solves this problem efficiently

Maximal margin classifier

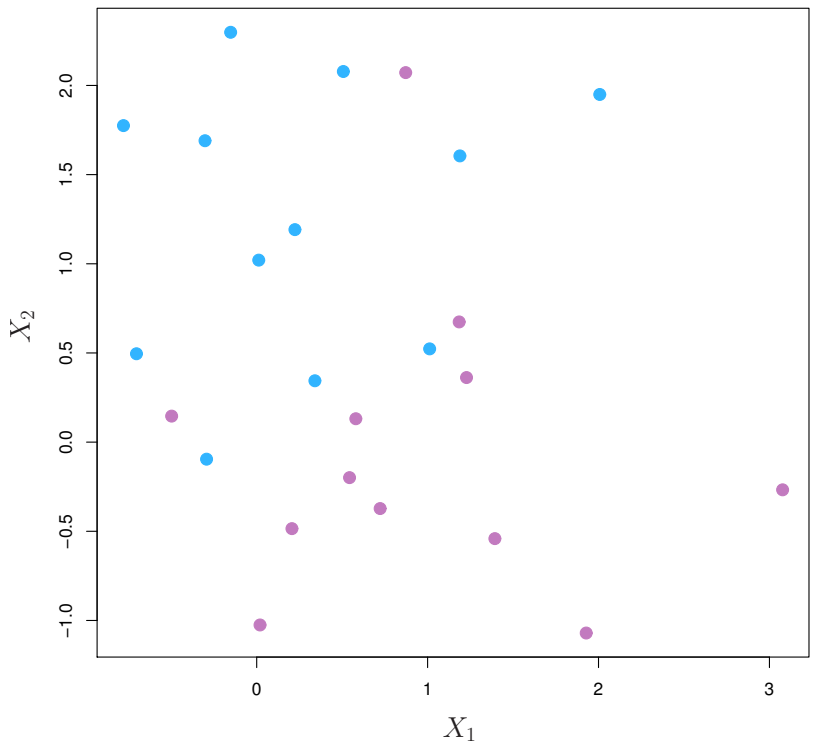
- We showed that this problem can be more conveniently rephrased as

$$min_{\beta,\beta_0}||\beta||$$

$$s.t.y_i(x_i^T\beta + \beta_0) \geq 1, i = 1, \cdots, N$$

- This is a convex optimization problem (quadratic criterion, linear inequality constraints)

Non-separable Data

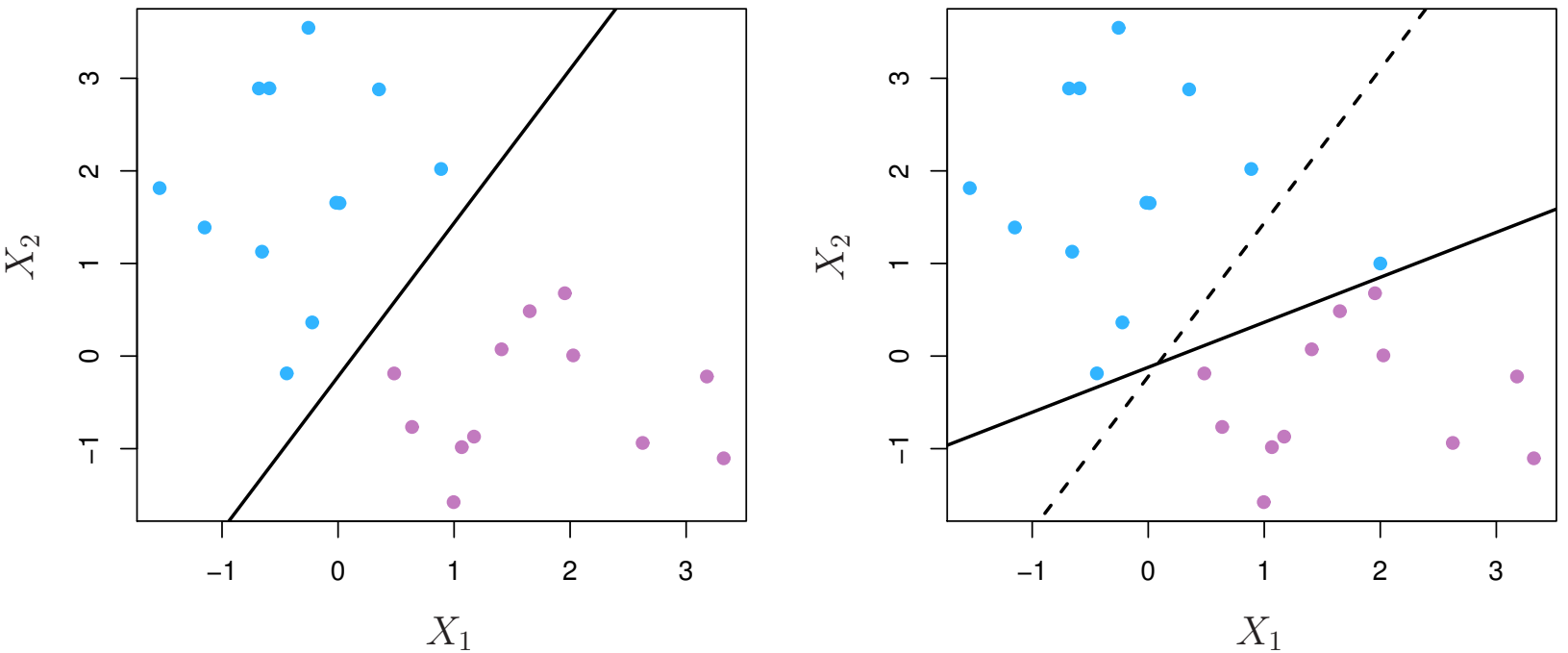


The data on the left are not separable by a linear boundary.

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

overlap

Noisy Data



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

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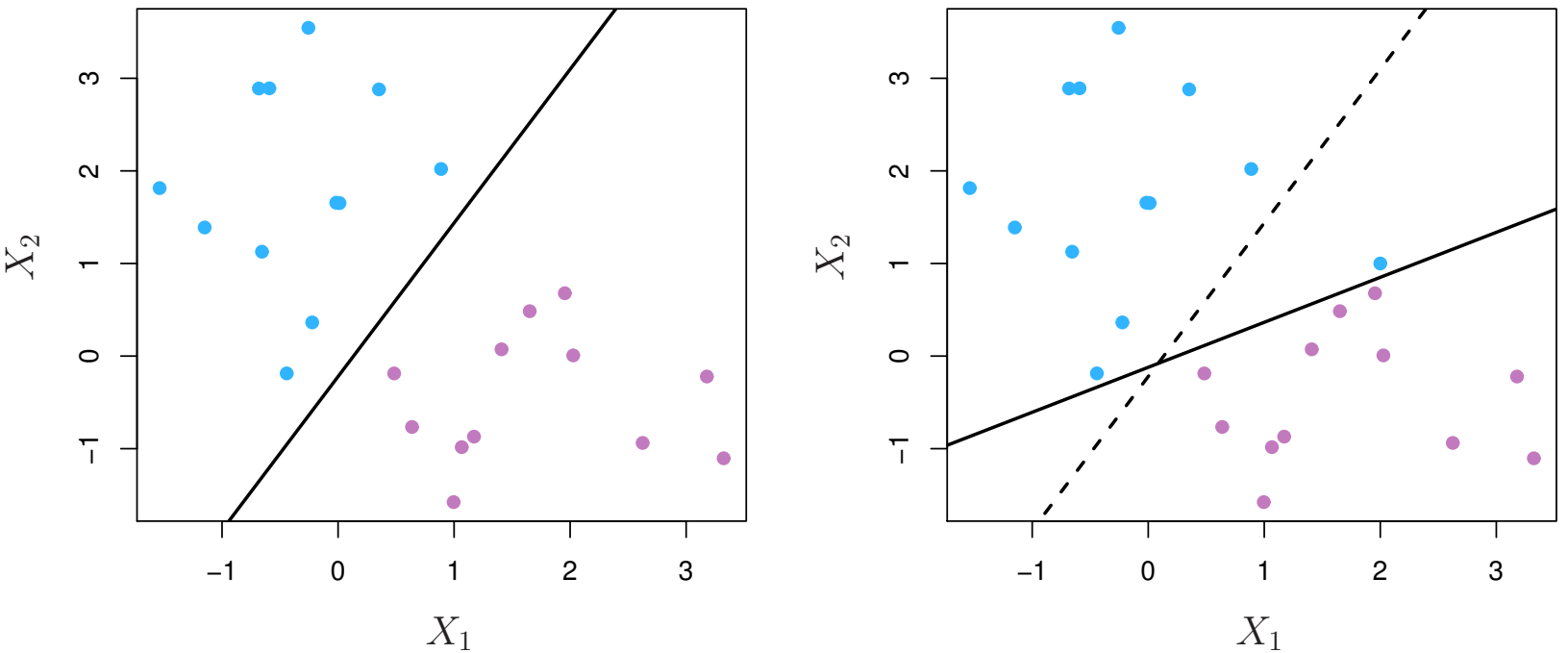

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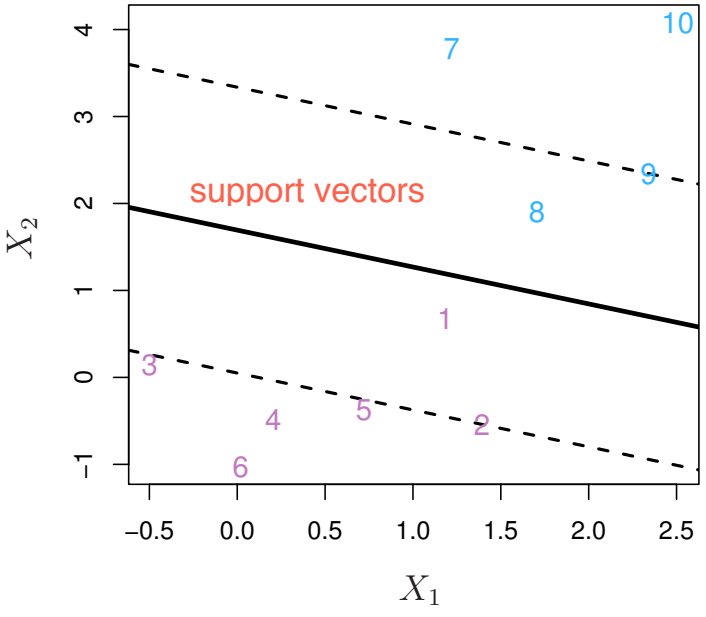
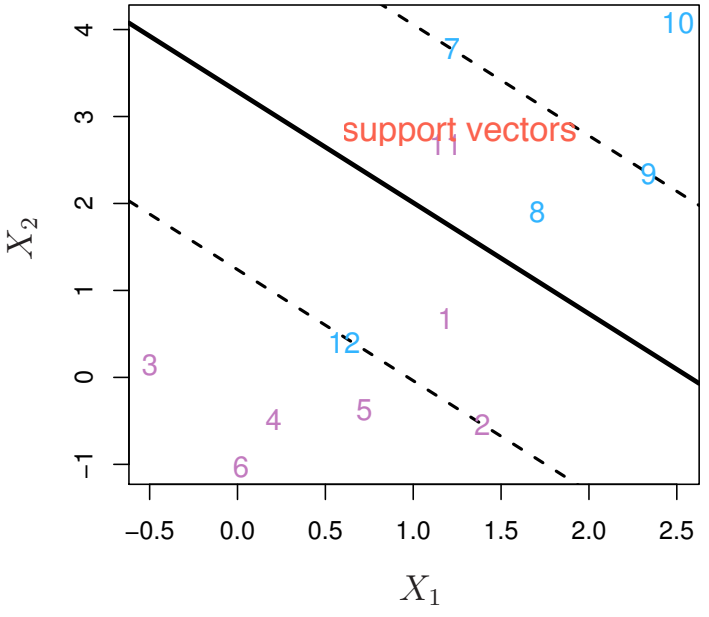
The *support vector classifier* maximizes a *soft* margin.

Support Vector Classifier





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

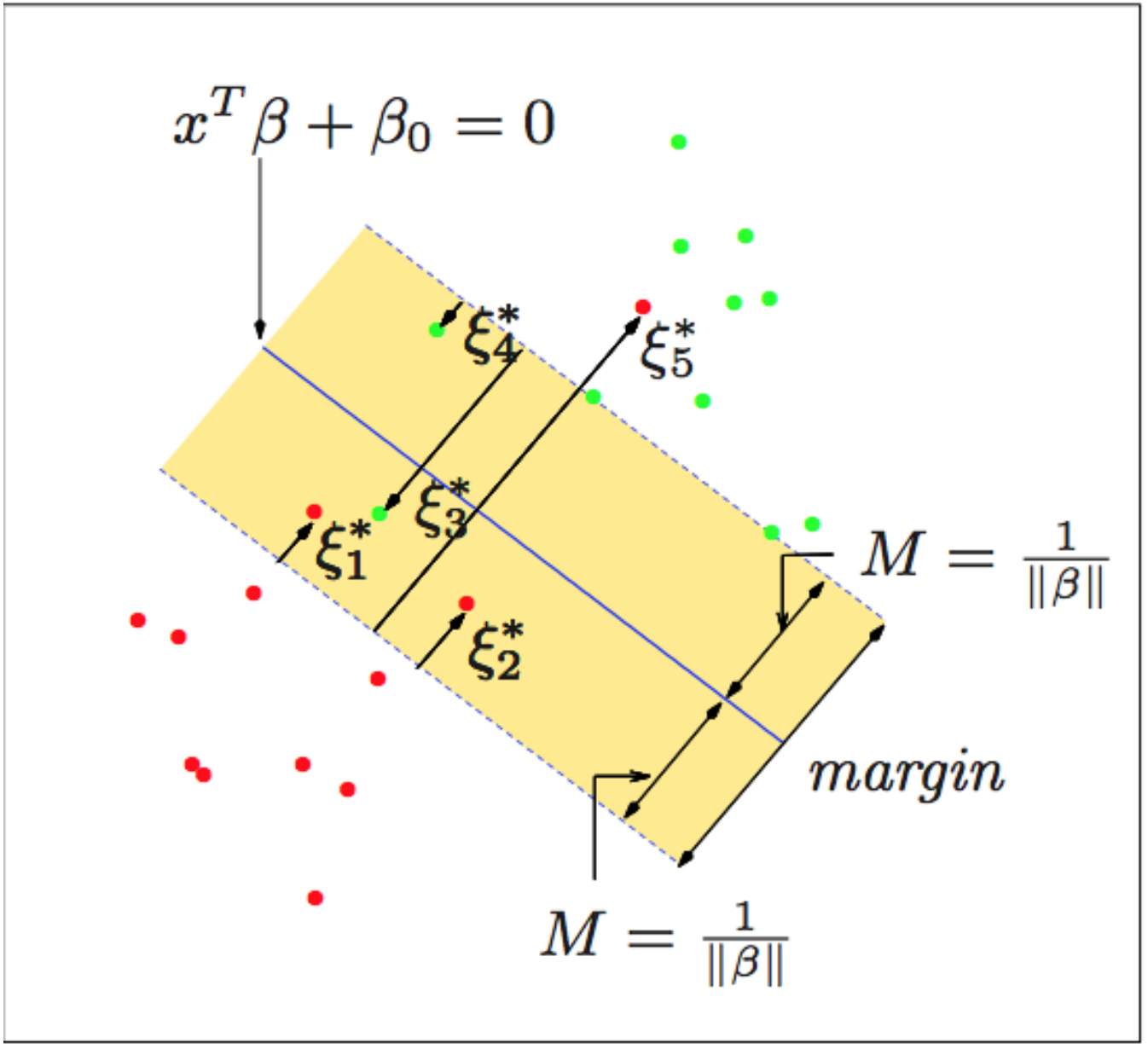
$$y_i(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \ldots + \beta_p x_{ip}) \geq M(1 - \epsilon_i),$$

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

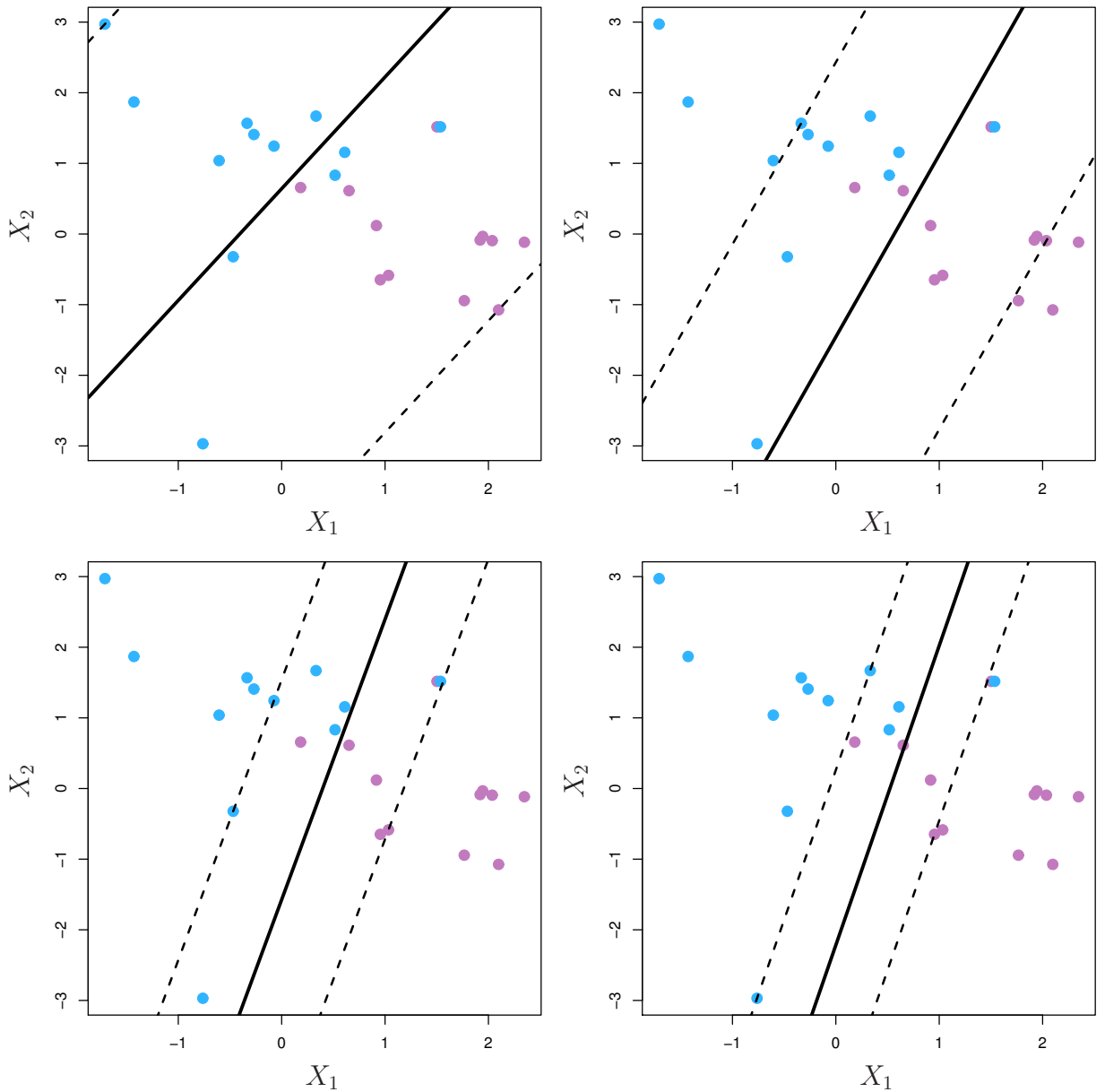
slack variables

budge
tunning parameter choosing by CV approach
C=0, \epsilon =0, maximal margin hyperplane
\epsilon >0, on the wrong margin
\epsilon >1, on the wrong hyperplane

Maximal margin classifier



C is a regularization parameter



Support vector classifier

- we can drop the norm constraint on β, define $M = \frac{1}{||\beta||}$ the equivalent form

$$\min \|\beta\| \quad \text{subject to} \begin{cases} y_i(x_i^T\beta + \beta_0) \geq 1 - \xi_i \ \forall i, \\ \xi_i \geq 0, \ \sum \xi_i \leq \text{constant}. \end{cases}$$

- This is the usual way the support vector classifier is defined for the non- separable case.
- points well inside their class boundary do not play a big role in shaping the boundary.

Computing the Support Vector Classifier

$$\min_{\beta,\beta_0} \frac{1}{2}\|\beta\|^2 + C\sum_{i=1}^{N}\xi_i \tag{12.8}$$
$$\text{subject to} \quad \xi_i \geq 0,\ y_i(x_i^T\beta + \beta_0) \geq 1 - \xi_i\ \forall i,$$

where the "cost" parameter C replaces the constant in (12.7); the separable case corresponds to $C = \infty$.

The Lagrange (primal) function is

$$L_P = \frac{1}{2}\|\beta\|^2 + C\sum_{i=1}^{N}\xi_i - \sum_{i=1}^{N}\alpha_i[y_i(x_i^T\beta + \beta_0) - (1 - \xi_i)] - \sum_{i=1}^{N}\mu_i\xi_i, \tag{12.9}$$

Computing the Support Vector Classifier

which we minimize w.r.t β, β_0 and ξ_i. Setting the respective derivatives to zero, we get

$$\beta = \sum_{i=1}^{N} \alpha_i y_i x_i, \tag{12.10}$$

$$0 = \sum_{i=1}^{N} \alpha_i y_i, \tag{12.11}$$

$$\alpha_i = C - \mu_i, \ \forall i, \tag{12.12}$$

as well as the positivity constraints α_i, μ_i, $\xi_i \geq 0$ $\forall i$. By substituting (12.10)–(12.12) into (12.9), we obtain the Lagrangian (Wolfe) dual objective function

$$L_D = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{i'=1}^{N} \alpha_i \alpha_{i'} y_i y_{i'} x_i^T x_{i'}, \tag{12.13}$$

Computing the Support Vector Classifier

which gives a lower bound on the objective function (12.8) for any feasible point. We maximize L_D subject to $0 \leq \alpha_i \leq C$ and $\sum_{i=1}^{N} \alpha_i y_i = 0$. In addition to (12.10)–(12.12), the Karush–Kuhn–Tucker conditions include the constraints

$$\begin{aligned} \alpha_i[y_i(x_i^T\beta + \beta_0) - (1 - \xi_i)] &= 0, && (12.14) \\ \mu_i \xi_i &= 0, && (12.15) \\ y_i(x_i^T\beta + \beta_0) - (1 - \xi_i) &\geq 0, && (12.16) \end{aligned}$$

for $i = 1, \ldots, N$. Together these equations (12.10)–(12.16) uniquely characterize the solution to the primal and dual problem.

Computing the Support Vector Classifier

From (12.10) we see that the solution for β has the form

$$\hat{\beta} = \sum_{i=1}^{N} \hat{\alpha}_i y_i x_i, \tag{12.17}$$

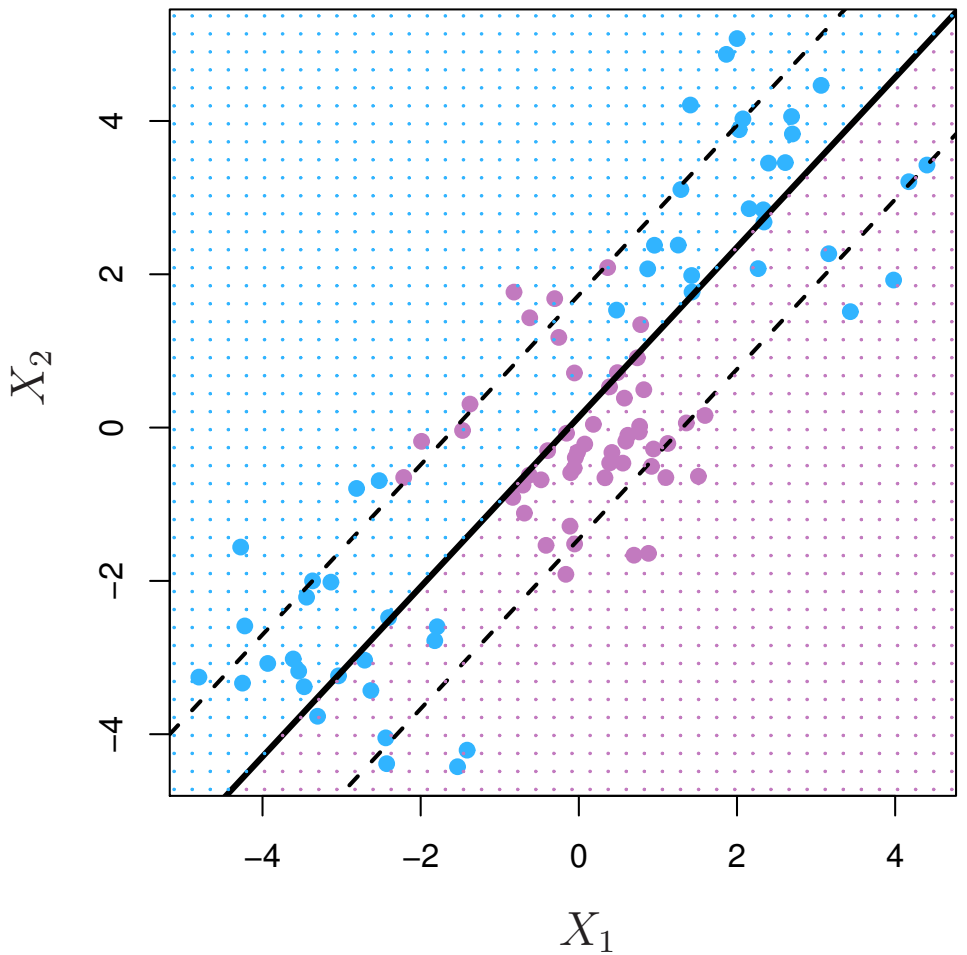
with nonzero coefficients $\hat{\alpha}_i$ only for those observations i for which the constraints in (12.16) are exactly met (due to (12.14)). These observations are called the *support vectors*, since $\hat{\beta}$ is represented in terms of them alone. Among these support points, some will lie on the edge of the margin ($\hat{\xi}_i = 0$), and hence from (12.15) and (12.12) will be characterized by $0 < \hat{\alpha}_i < C$; the remainder ($\hat{\xi}_i > 0$) have $\hat{\alpha}_i = C$. From (12.14) we can see that any of these margin points ($0 < \hat{\alpha}_i$, $\hat{\xi}_i = 0$) can be used to solve for β_0, and we typically use an average of all the solutions for numerical stability.

Maximizing the dual (12.13) is a simpler convex quadratic programming problem than the primal (12.9), and can be solved with standard techniques (Murray et al., 1981, for example).

Given the solutions $\hat{\beta}_0$ and $\hat{\beta}$, the decision function can be written as

$$\begin{aligned} \hat{G}(x) &= \text{sign}[\hat{f}(x)] \\ &= \text{sign}[x^T \hat{\beta} + \hat{\beta}_0]. \end{aligned} \tag{12.18}$$

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, $X_1X_2^2$,.... 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.

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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

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

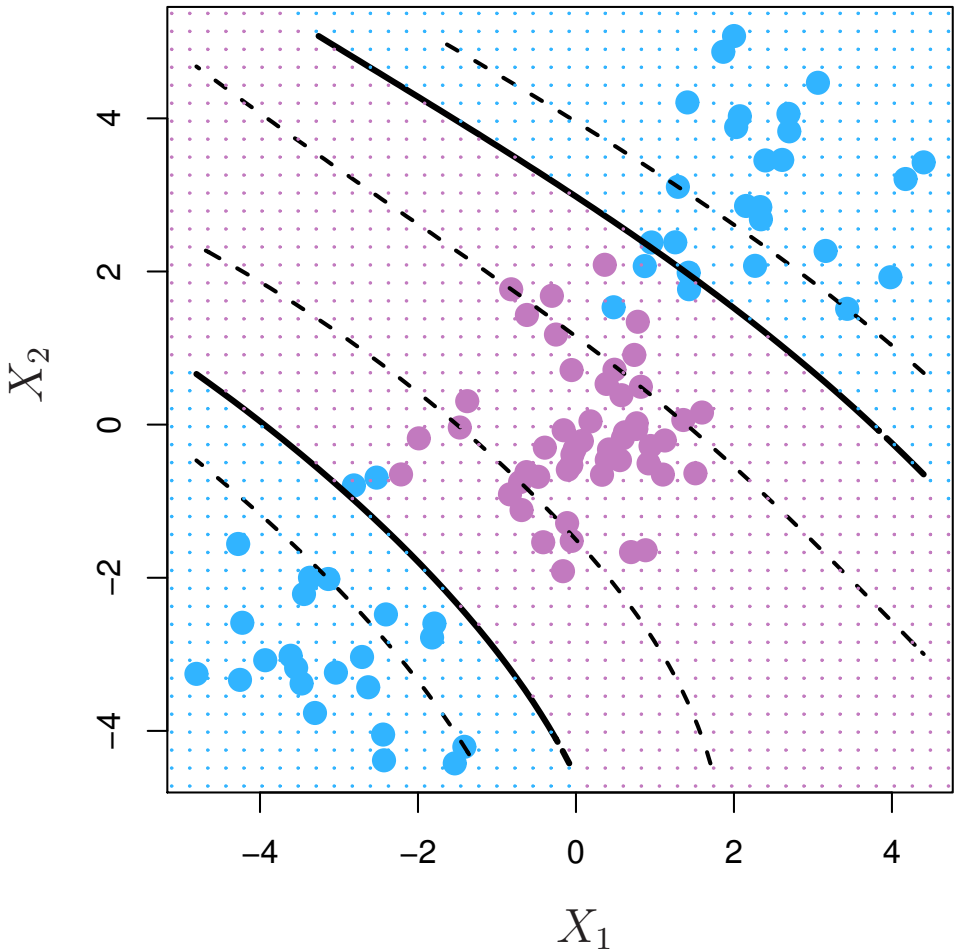
This leads to nonlinear decision boundaries in the original space (quadratic conic sections).

Cubic Polynomials

Here we use a basis expansion of cubic polynomials

From 2 variables to 9

The support-vector classifier in the enlarged space solves the problem in the lower-dimensional space



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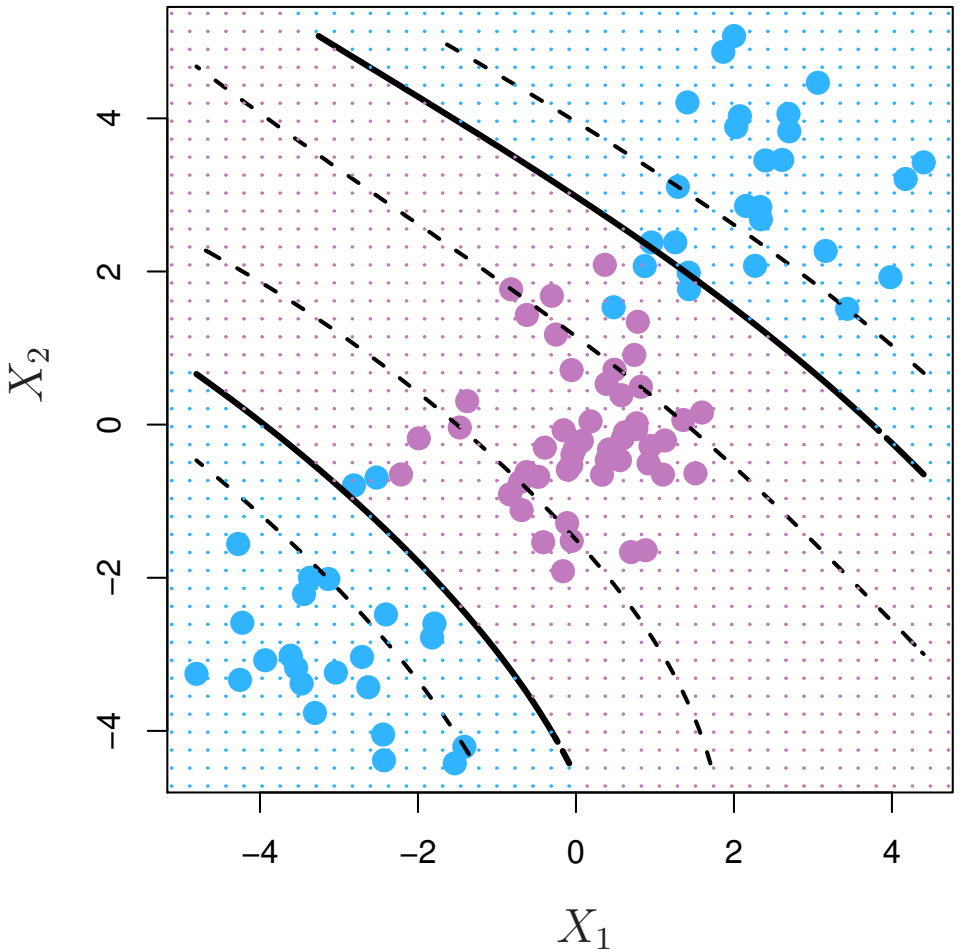

$$\beta_0+\beta_1X_1+\beta_2X_2+\beta_3X_1^2+\beta_4X_2^2+\beta_5X_1X_2+\beta_6X_1^3+\beta_7X_2^3+\beta_8X_1X_2^2+\beta_9X_1^2X_2=0$$

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

$$\langle x_i, x_{i'} \rangle = \sum_{j=1}^{p} x_{ij} x_{i'j} \quad \text{— } \textit{inner product between vectors}$$

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- The linear support vector classifier can be represented as

$$f(x) = \beta_0 + \sum_{i=1}^{n} \alpha_i \langle x, x_i \rangle \quad \text{— } \textit{n parameters}$$

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- To estimate the parameters $\alpha_1, \ldots, \alpha_n$ and β_0, all we need are the $\binom{n}{2}$ inner products $\langle x_i, x_{i'} \rangle$ between all pairs of training observations.

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

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

$\mathcal{S}$ is the *support set* of indices i such that $\hat{\alpha}_i > 0$. [see slide 8]

Kernels and Support Vector Machines

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- Some special *kernel functions* can do this for us. E.g.

$$K(x_i, x_{i'}) = \left(1 + \sum_{j=1}^{p} x_{ij} x_{i'j}\right)^d$$

computes the inner-products needed for d dimensional polynomials — $\binom{p+d}{d}$ basis functions!

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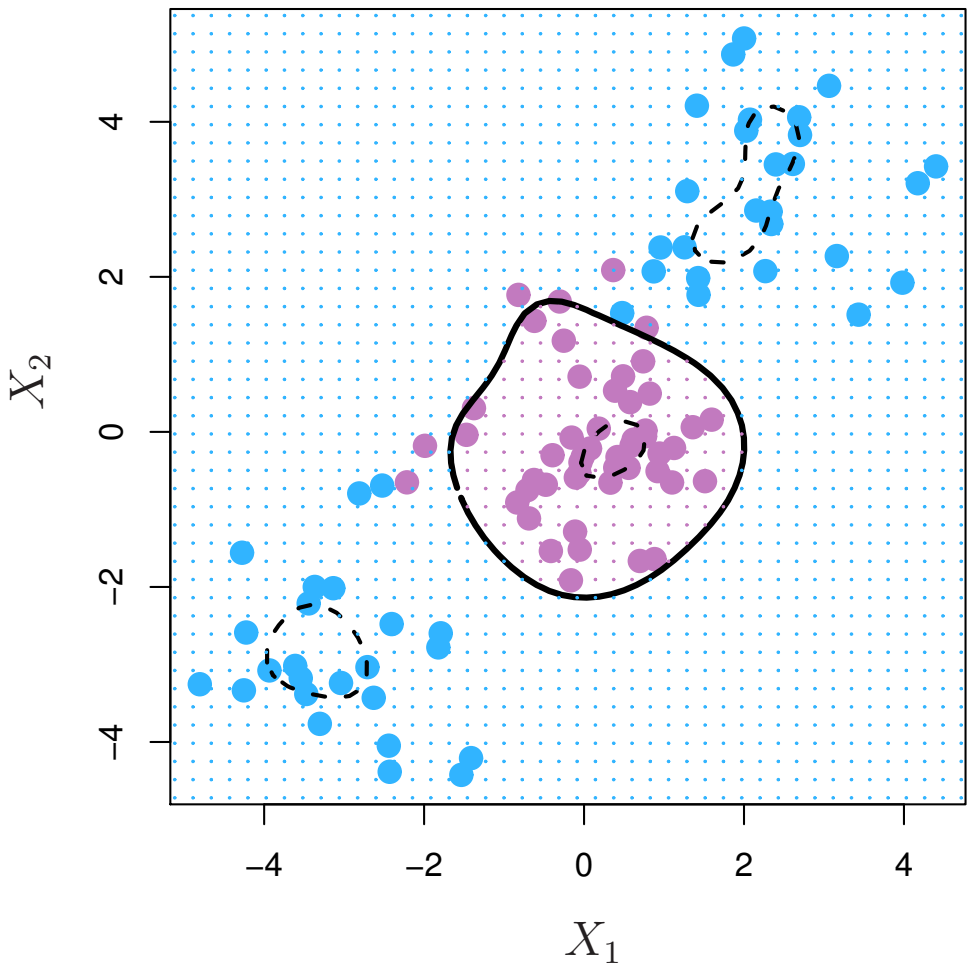
- The solution has the form

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

Radial Kernel

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

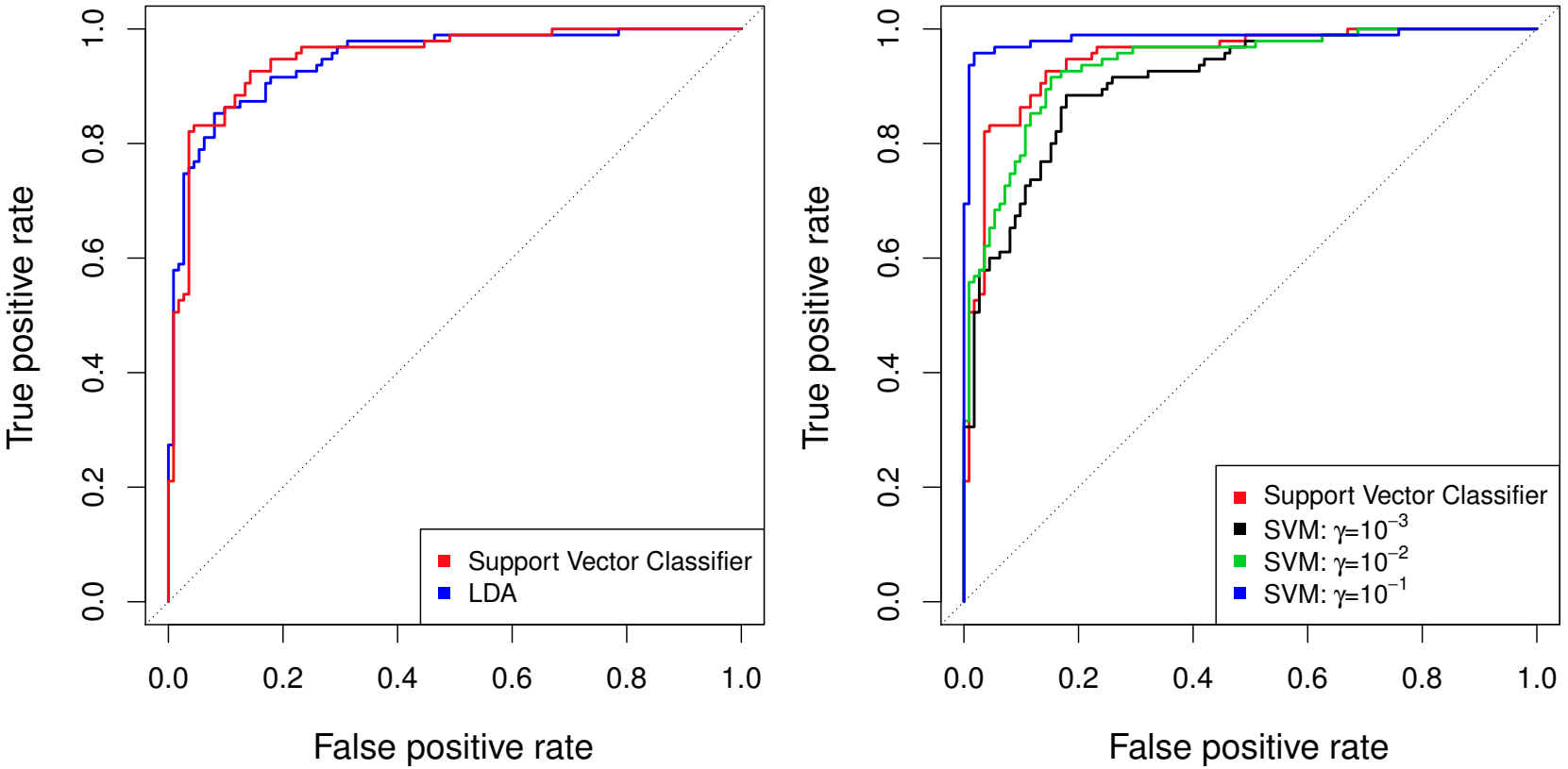


$$f(x) = \beta_0 + \sum_{i \in \mathcal{S}} \hat{\alpha}_i K(x, x_i)$$

Implicit feature space; very high dimensional.

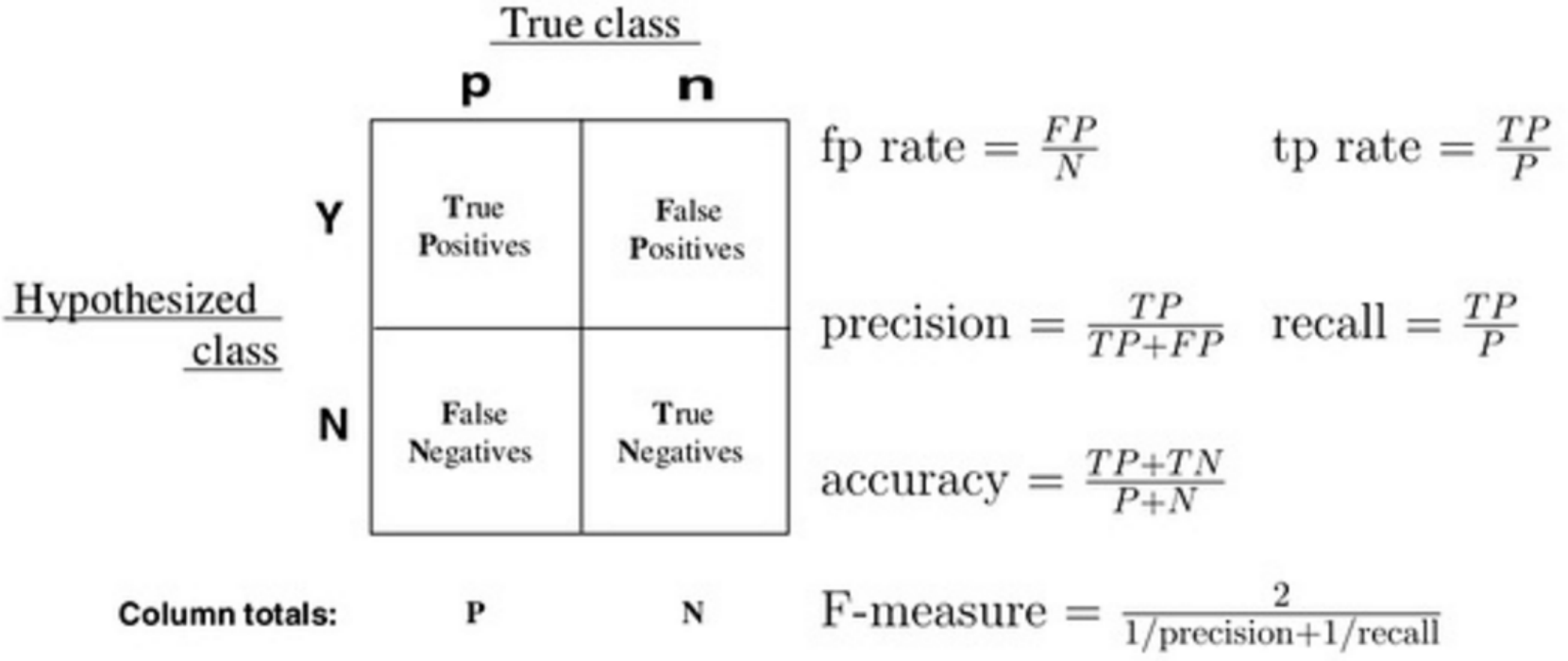
Controls variance by squashing down most dimensions severely

Example: Heart Data

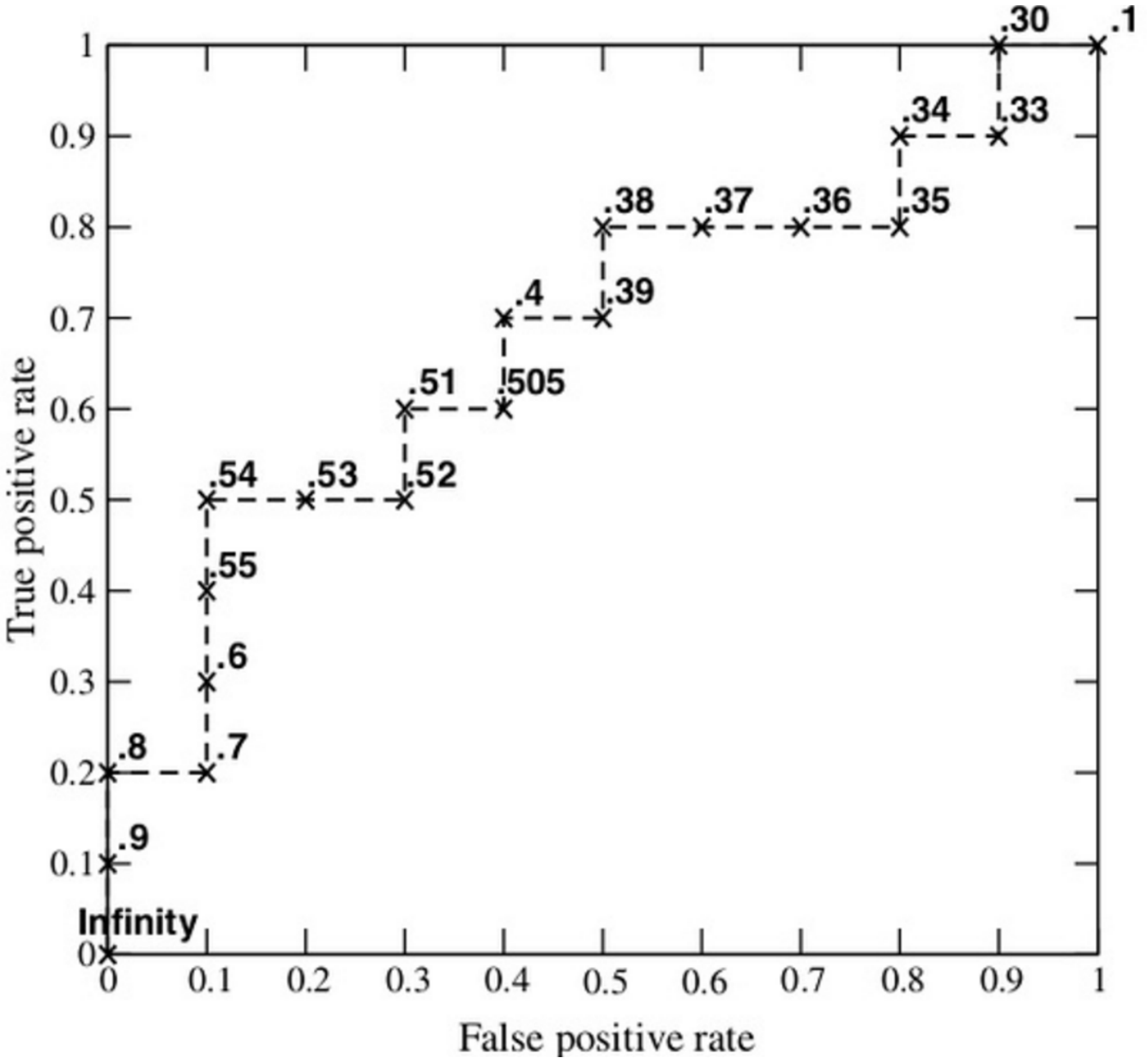


ROC curve is obtained by changing the threshold 0 to threshold t in $\hat{f}(X) > t$, and recording *false positive* and *true positive* rates as t varies. Here we see ROC curves on training data.

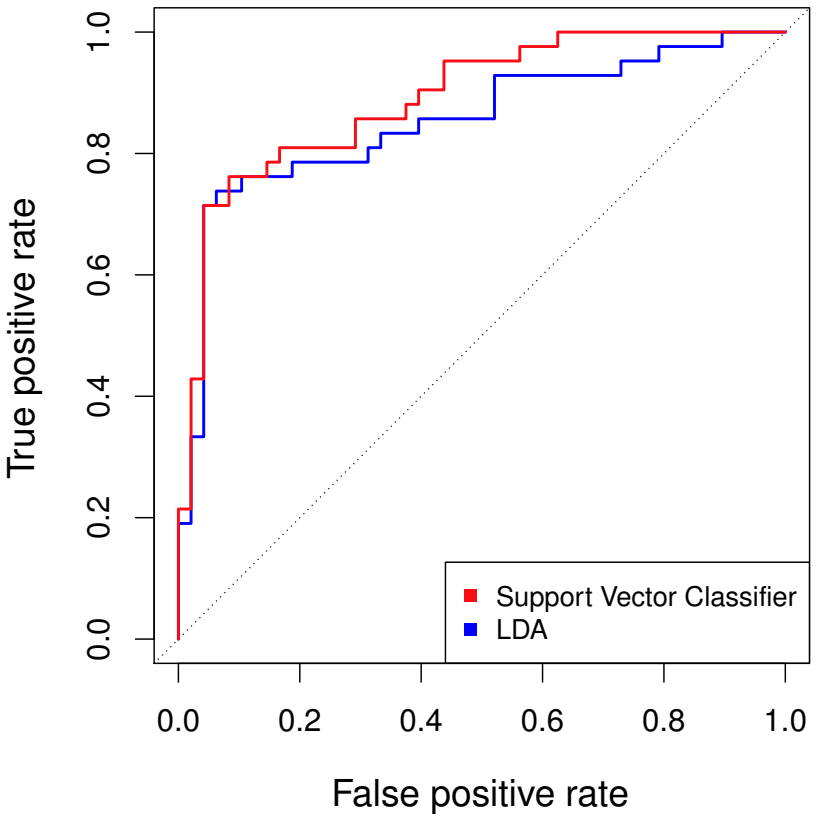
ROC curve

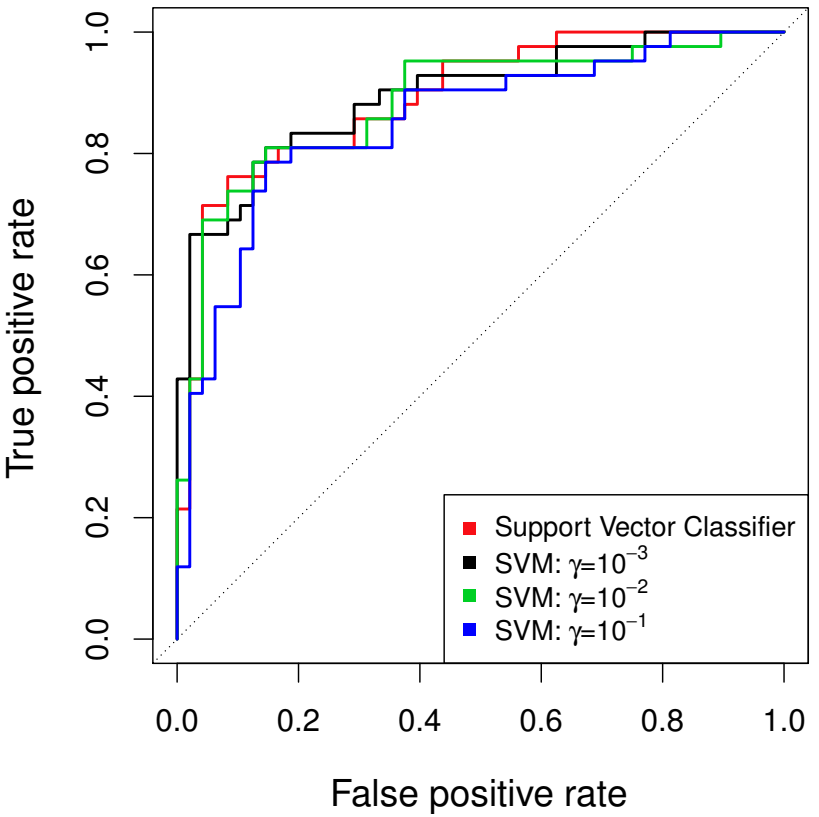

True class
p
n
Hypothesized class
Y
N
True Positives
False Positives
False Negatives
True Negatives
Column totals:
P
N
fp rate = FP/N
tp rate = TP/P
precision = TP/(TP+FP)
recall = TP/P
accuracy = (TP+TN)/(P+N)
F-measure = 2/(1/precision+1/recall)

ROC curve


True positive rate
False positive rate
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
.30
.1
.34
.33
.38
.37
.36
.35
.4
.39
.51
.505
.54
.53
.52
.55
.6
.8
.7
.9
Infinity

Example continued: Heart Test Data





SVMs: more than 2 classes?

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

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OVA One versus All. Fit K different 2-class SVM classifiers $\hat{f}_k(x)$, $k = 1, \ldots, K$; each class versus the rest. Classify x^* to the class for which $\hat{f}_k(x^*)$ is largest.

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OVO One versus One. Fit all $\binom{K}{2}$ pairwise classifiers $\hat{f}_{k\ell}(x)$. Classify x^* to the class that wins the most pairwise competitions.

SVMs: 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 $\hat{f}_k(x)$, $k = 1, \ldots, K$; each class versus the rest. Classify x^* to the class for which $\hat{f}_k(x^*)$ is largest.

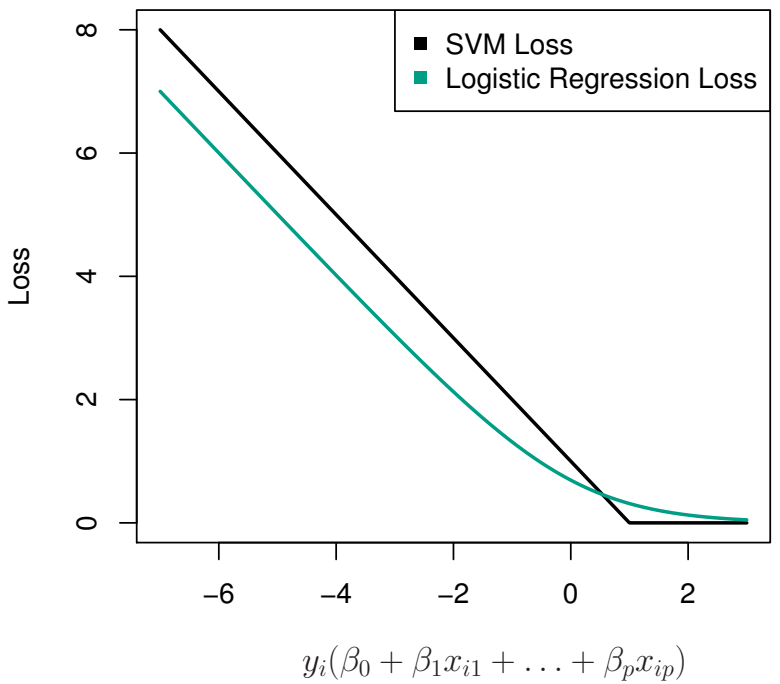
OVO One versus One. Fit all $\binom{K}{2}$ pairwise classifiers $\hat{f}_{k\ell}(x)$. Classify x^* to the class that wins the most pairwise competitions.

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

Support Vector versus Logistic Regression?

With $f(X) = \beta_0 + \beta_1 X_1 + \ldots + \beta_p X_p$ can rephrase support-vector classifier optimization as

$$\underset{\beta_0,\beta_1,\ldots,\beta_p}{\text{minimize}} \left\{ \sum_{i=1}^{n} \max\left[0, 1 - y_i f(x_i)\right] + \lambda \sum_{j=1}^{p} \beta_j^2 \right\}$$



This has the form *loss plus penalty*.

The loss is known as the *hinge loss*.

Very similar to "loss" in logistic regression (negative log-likelihood).

Which to use: SVM or Logistic Regression

- When classes are (nearly) separable, SVM does better than LR. So does LDA.
- When not, LR (with ridge penalty) and SVM very similar.
- If you wish to estimate probabilities, LR is the choice.
- For nonlinear boundaries, kernel SVMs are popular. Can use kernels with LR and LDA as well, but computations are more expensive.

Support vector regression

In this section we show how SVMs can be adapted for regression with a quantitative response, in ways that inherit some of the properties of the SVM classifier. We first discuss the linear regression model

$$f(x) = x^T\beta + \beta_0, \tag{12.35}$$

and then handle nonlinear generalizations. To estimate β, we consider minimization of

$$H(\beta, \beta_0) = \sum_{i=1}^{N} V(y_i - f(x_i)) + \frac{\lambda}{2}\|\beta\|^2, \tag{12.36}$$

Support vector regression

$$V_\epsilon(r) = \begin{cases} 0 & \text{if } |r| < \epsilon, \\ |r| - \epsilon, & \text{otherwise.} \end{cases} \tag{12.37}$$

This is an "ϵ-insensitive" error measure, ignoring errors of size less than ϵ (left panel of Figure 12.8). There is a rough analogy with the support vector classification setup, where points on the correct side of the decision boundary and far away from it, are ignored in the optimization. In regression, these "low error" points are the ones with small residuals.

It is interesting to contrast this with error measures used in robust regression in statistics. The most popular, due to Huber (1964), has the form

$$V_H(r) = \begin{cases} r^2/2 & \text{if } |r| \le c, \\ c|r| - c^2/2, & |r| > c, \end{cases} \tag{12.38}$$

shown in the right panel of Figure 12.8. This function reduces from quadratic to linear the contributions of observations with absolute residual greater than a prechosen constant c. This makes the fitting less sensitive to outliers. The support vector error measure (12.37) also has linear tails (beyond ϵ), but in addition it flattens the contributions of those cases with small residuals.

Support vector regression

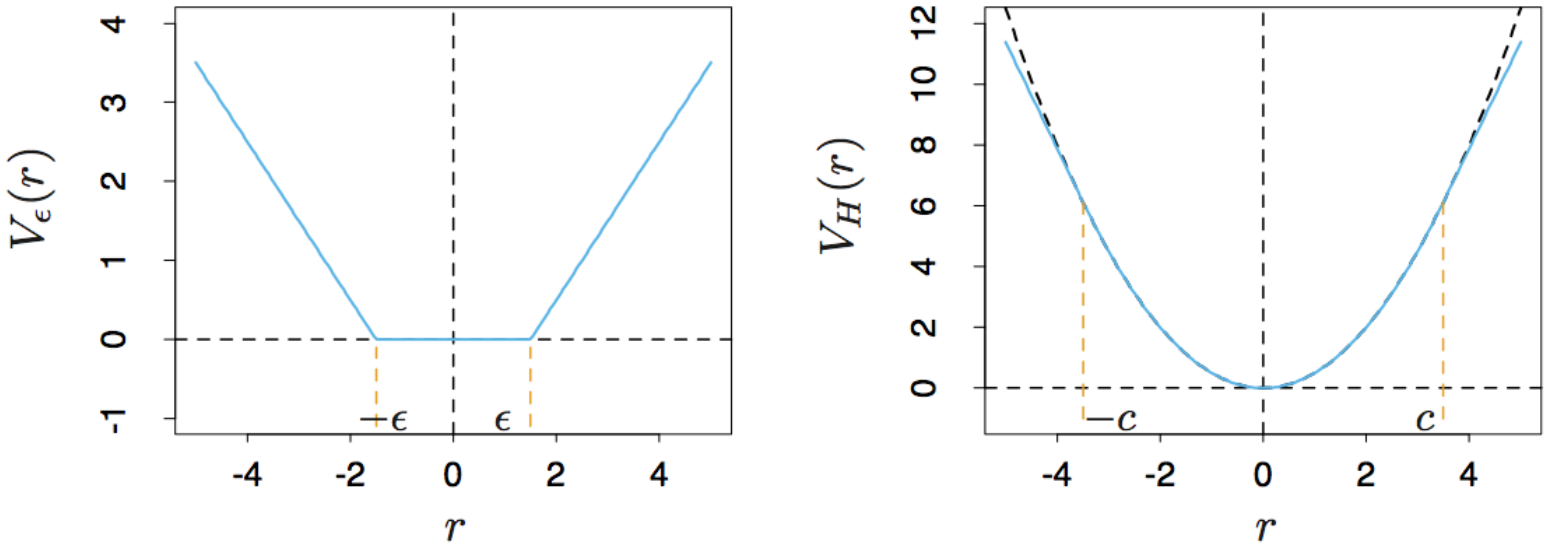


FIGURE 12.8. *The left panel shows the ϵ-insensitive error function used by the support vector regression machine. The right panel shows the error function used in Huber's robust regression (blue curve). Beyond $|c|$, the function changes from quadratic to linear.*

Support vector regression

As discussed in Section 12.3.3, this kernel property is not unique to support vector machines. Suppose we consider approximation of the regression function in terms of a set of basis functions $\{h_m(x)\}, m = 1, 2, \ldots, M$:

$$f(x) = \sum_{m=1}^{M} \beta_m h_m(x) + \beta_0. \tag{12.42}$$

To estimate β and β_0 we minimize

$$H(\beta, \beta_0) = \sum_{i=1}^{N} V(y_i - f(x_i)) + \frac{\lambda}{2} \sum \beta_m^2 \tag{12.43}$$

for some general error measure $V(r)$. For any choice of $V(r)$, the solution $\hat{f}(x) = \sum \hat{\beta}_m h_m(x) + \hat{\beta}_0$ has the form

$$\hat{f}(x) = \sum_{i=1}^{N} \hat{a}_i K(x, x_i) \tag{12.44}$$

Support vector regression

with $K(x,y) = \sum_{m=1}^{M} h_m(x)h_m(y)$. Notice that this has the same form as both the radial basis function expansion and a regularization estimate, discussed in Chapters 5 and 6.

For concreteness, let's work out the case $V(r) = r^2$. Let $\mathbf{H}$ be the $N \times M$ basis matrix with imth element $h_m(x_i)$, and suppose that $M > N$ is large. For simplicity we assume that $\beta_0 = 0$, or that the constant is absorbed in h; see Exercise 12.3 for an alternative.

We estimate β by minimizing the penalized least squares criterion

$$H(\beta) = (\mathbf{y} - \mathbf{H}\beta)^T(\mathbf{y} - \mathbf{H}\beta) + \lambda\|\beta\|^2. \tag{12.45}$$

The solution is

$$\hat{\mathbf{y}} = \mathbf{H}\hat{\beta} \tag{12.46}$$

with $\hat{\beta}$ determined by

$$-\mathbf{H}^T(\mathbf{y} - \mathbf{H}\hat{\beta}) + \lambda\hat{\beta} = 0. \tag{12.47}$$

Support vector regression

From this it appears that we need to evaluate the $M \times M$ matrix of inner products in the transformed space. However, we can premultiply by $\mathbf{H}$ to give

$$\mathbf{H}\hat{\beta} = (\mathbf{H}\mathbf{H}^T + \lambda\mathbf{I})^{-1}\mathbf{H}\mathbf{H}^T\mathbf{y}. \tag{12.48}$$

The $N \times N$ matrix $\mathbf{H}\mathbf{H}^T$ consists of inner products between pairs of observations i, i'; that is, the evaluation of an inner product kernel $\{\mathbf{H}\mathbf{H}^T\}_{i,i'} = K(x_i, x_{i'})$. It is easy to show (12.44) directly in this case, that the predicted values at an arbitrary x satisfy

$$\begin{aligned} \hat{f}(x) &= h(x)^T\hat{\beta} \\ &= \sum_{i=1}^{N} \hat{\alpha}_i K(x, x_i), \end{aligned} \tag{12.49}$$

where $\hat{\alpha} = (\mathbf{H}\mathbf{H}^T + \lambda\mathbf{I})^{-1}\mathbf{y}$. As in the support vector machine, we need not specify or evaluate the large set of functions $h_1(x), h_2(x), \ldots, h_M(x)$. Only the inner product kernel $K(x_i, x_{i'})$ need be evaluated, at the N training points for each i, i' and at points x for predictions there. Careful choice of h_m (such as the eigenfunctions of particular, easy-to-evaluate kernels K) means, for example, that $\mathbf{H}\mathbf{H}^T$ can be computed at a cost of $N^2/2$ evaluations of K, rather than the direct cost N^2M.