Lecture 12

Support Vector Machines

ISLR 9

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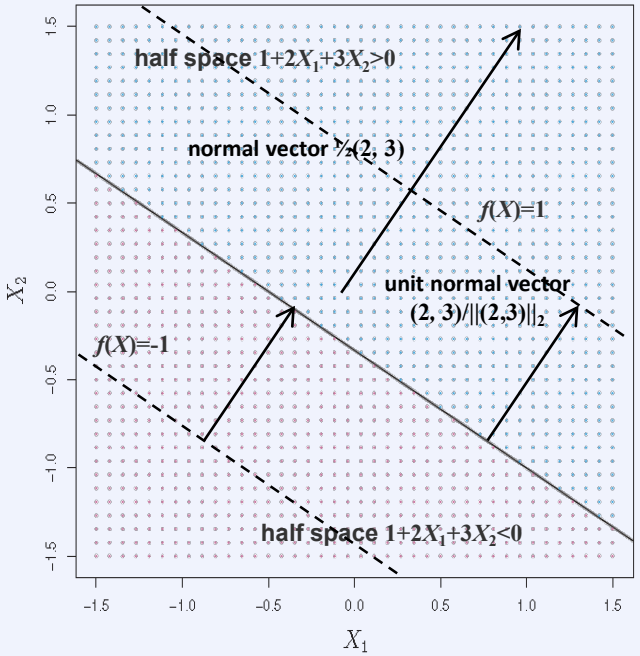
Hyperplanes

- in p-dimensional vector space, a linear hyperplane is a $(p-1)$-dimensional subspace
- equivalently, a linear hyperplane is the set of points that satisfy a linear equation of the form $\beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p = 0$
- an affine hyperplane is the set of points that fulfills $\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p = 0$ for some $\beta_0 \neq 0$
- a hyperplane divides the vector space into two half spaces
- the vector $(\beta_1, \ldots, \beta_p)$ is the normal vector of the hyperplane

Example hyperplane
$f(X) = 1 + 2X_1 + 3X_2 = 0$



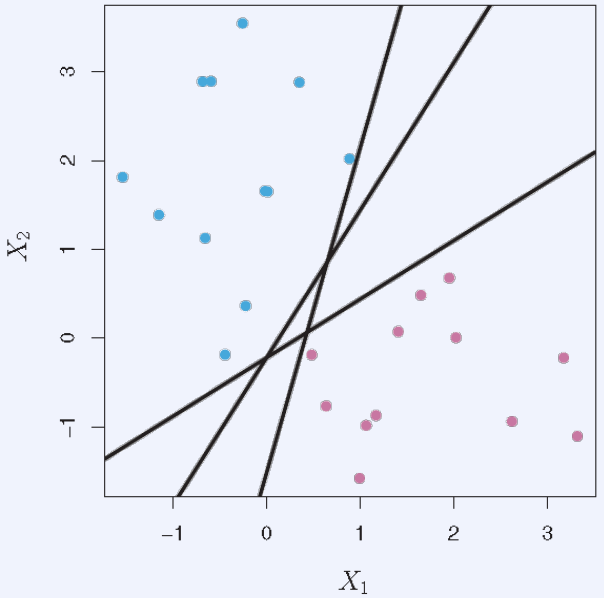
Classification using Separating Hyperplanes

- assume a data matrix $x_1 = \begin{pmatrix} x_{11} \\ \vdots \\ x_{1p} \end{pmatrix}, \dots, x_n = \begin{pmatrix} x_{n1} \\ \vdots \\ x_{np} \end{pmatrix}$
  for a binary classification problem with classes $\{1, -1\}$
- assume further a test vector $x^* = \left(x_1^*, \dots, x_p^*\right)^T$

We define a classifier based on a **separating hyperplane**

- the data points of the two classes locate in separate half spaces

different separating hyperplanes



(ISLR 9.1.2)

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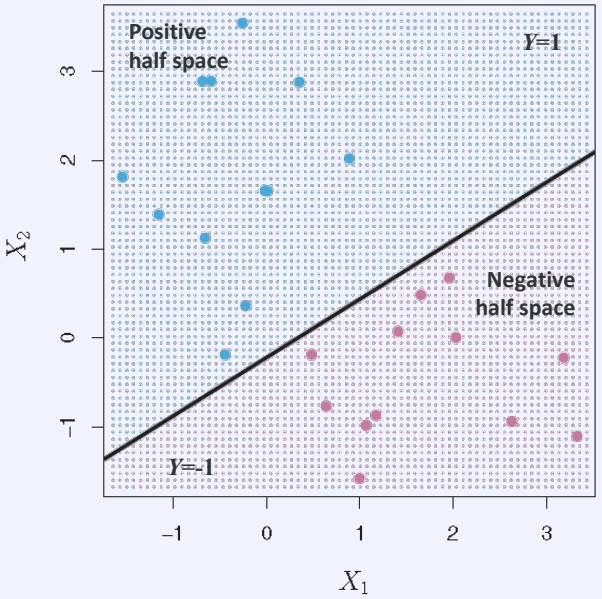
We define a classifier based on a **separating hyperplane**

- the data points of the two classes locate in separate half spaces
- the hyperplane is defined by $\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p = 0$
- the classification is $\mathbf{sign}\left(\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p\right)$

- the distance of a point from the hyperplane is informative about the confidence in the classification

separating hyperplane and resulting classifier



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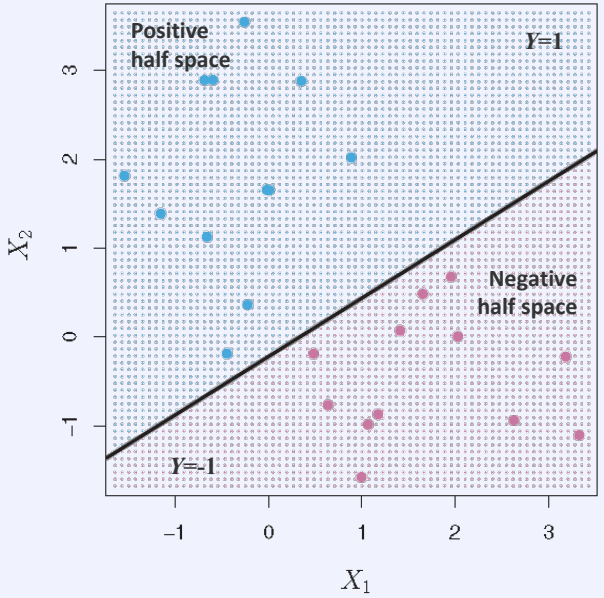
The Maximal Margin Classifier

- a hyperplane that maximizes the **distance of the closest point** in the training set to it can be considered optimal

separating hyperplane and resulting classifier



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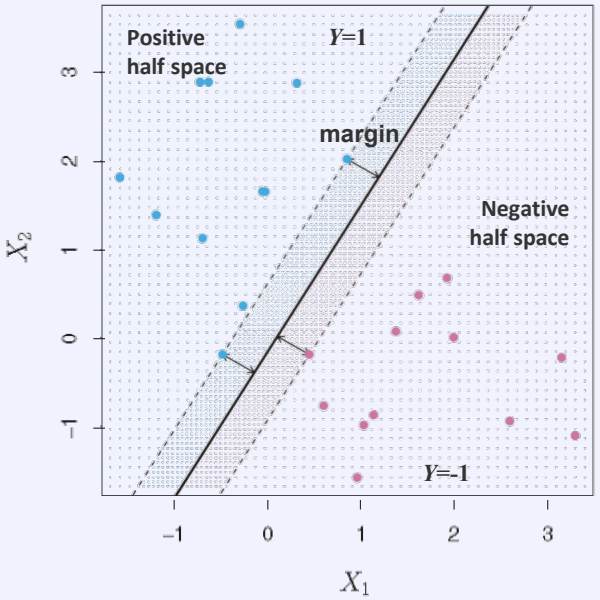
The Maximal Margin Classifier

- a hyperplane that maximizes the **distance of the closest point** in the training set to it can be considered optimal
- this distance is called the **margin**

The closest data points are called the **support vectors**

- only they determine the hyperplane
- can be a small subset of all points

separating hyperplane and resulting classifier



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Constructing the Maximal Margin Classifier

The optimization problem is

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

normal vector is unit vector

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

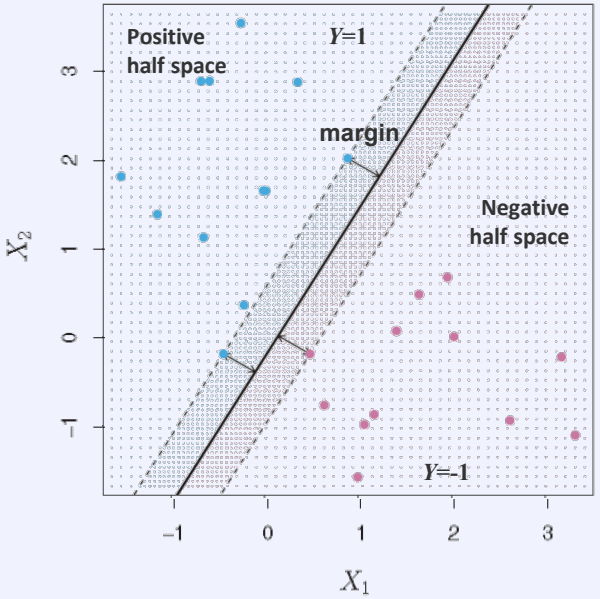
correct classification, if $M>0$

$$y_i(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip}) \geq M,\ i = 1, \ldots, n$$

- since the normal is a unit vector, the distance of point i from the hyperplane is given by $y_i(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip})$
- solve the problem with convex optimization techniques

- often, there is no separating hyperplane

separating hyperplane and resulting classifier



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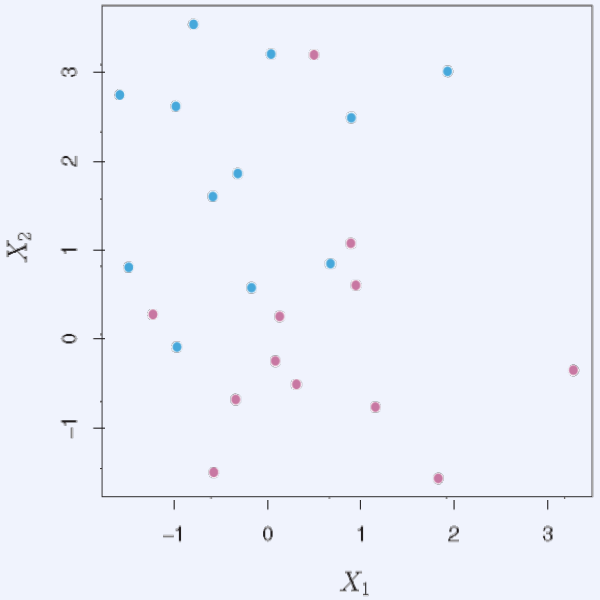
- solve the problem with convex optimization techniques

- often, there is no separating hyperplane
- then we have to generalize to allow for misclassifications

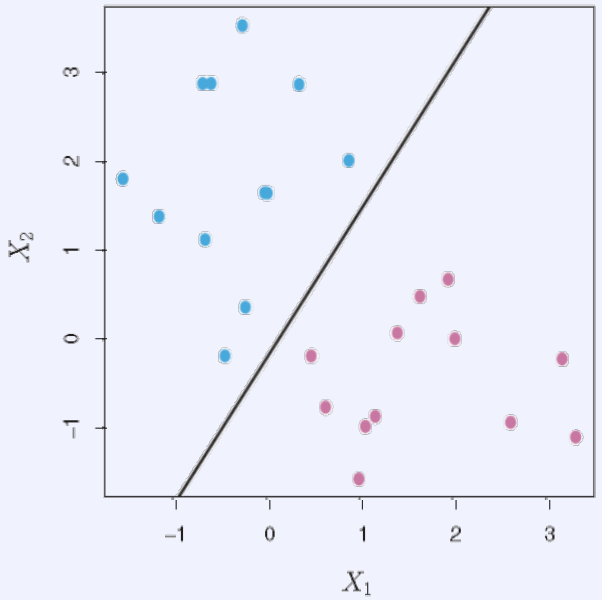
a non-separable dataset



The Support Vector Classifier

Even if the dataset is separable, a separating hyperplane may not be desirable

a nicely separable dataset



(ISLR 9.2.1)

The Support Vector Classifier

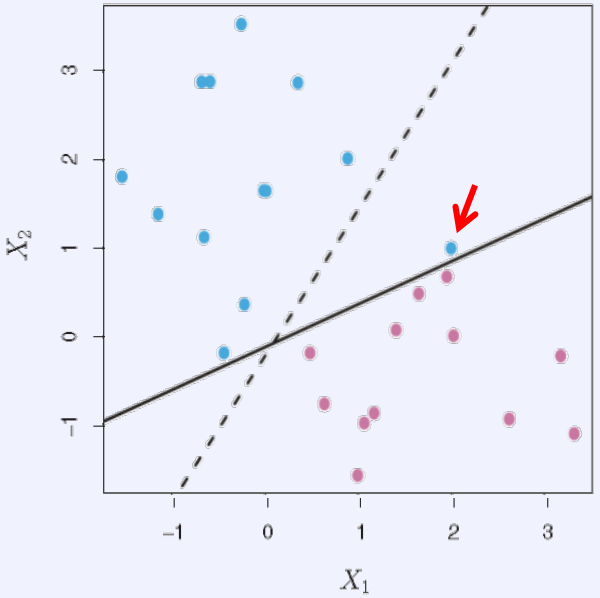
Even if the dataset is separable, a separating hyperplane may not be desirable

- adding a single data point leads to a hard-to-separate dataset
- the classifier is extremely sensitive to changes in the data

Sometimes it may be preferable to have a classifier that misplaces a few points in the training set but has a large margin to the other data points

- greater robustness w.r.t to small changes in the data
- better classification of most of the training points
- the soft-margin classifier does exactly this

a nicely separable dataset with an outlier



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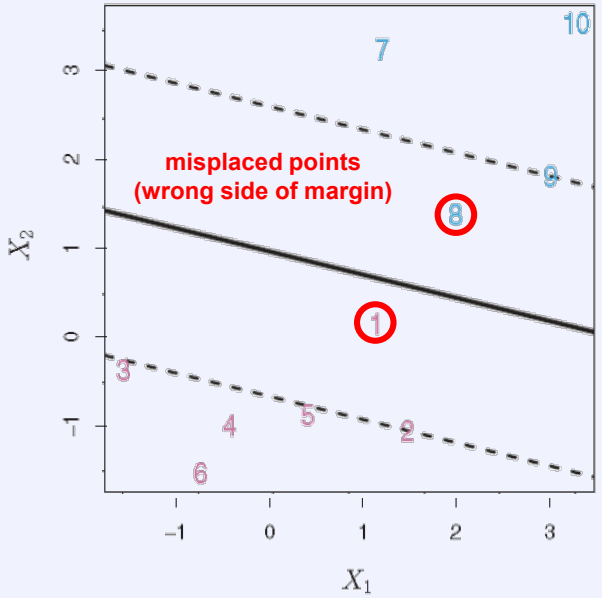
soft-margin classifier



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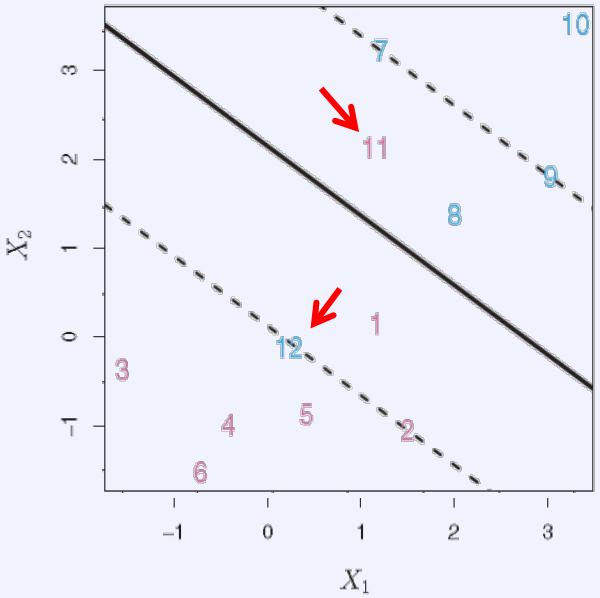

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The Support Vector Classifier

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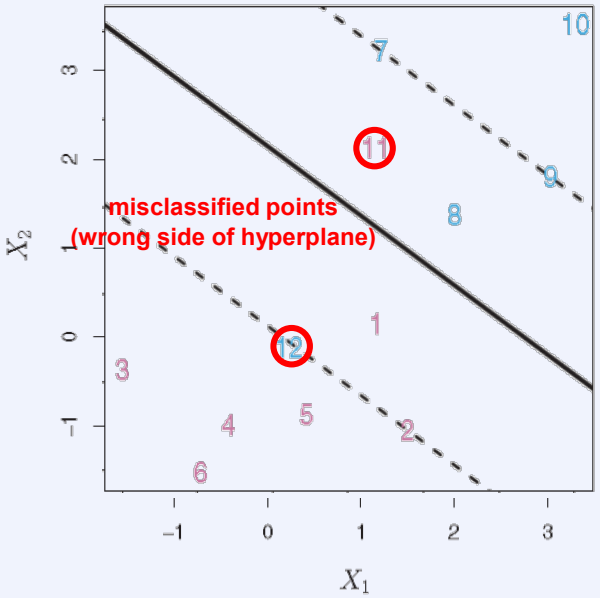
soft-margin classifier



- points can be on the wrong side of the margin (misplaced but correct) or the hyperplane (misclassified)

Details of Soft-Margin Support Vector Classifier

The optimization problem is now

$$\max_{\beta_0,\beta_1,\dots\beta_p,M} M$$

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

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

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

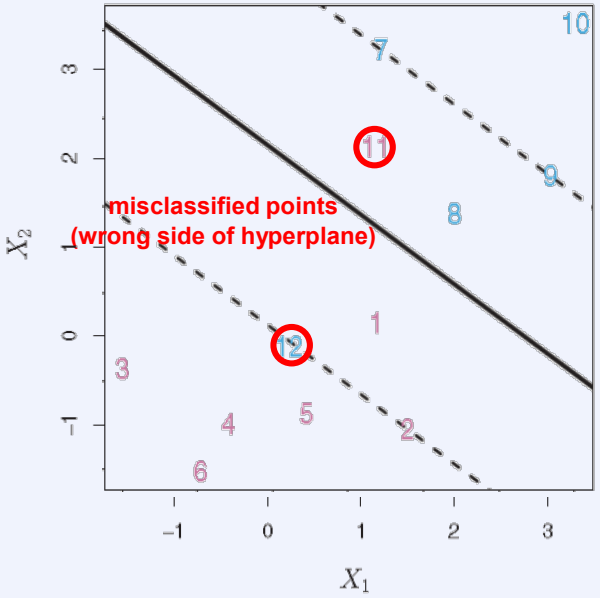
Slack variables allow for a fractional violation of the hard margin constraint

Budget for total admissible misclassification

The following holds if we also choose the smallest possible ϵ_i:

- $\epsilon_i = 0 \Rightarrow$ the observation is on the **correct** side of the **margin**
- $\epsilon_i > 0 \Rightarrow$ the observation is on the **wrong** side of the **margin**
- $\epsilon_i > 1 \Rightarrow$ the observation is on the **wrong** side of the **hyperplane**
- furthermore: no more than C observations can be on the wrong side of the hyperplane

soft-margin classifier



On the Effect of the Budget C

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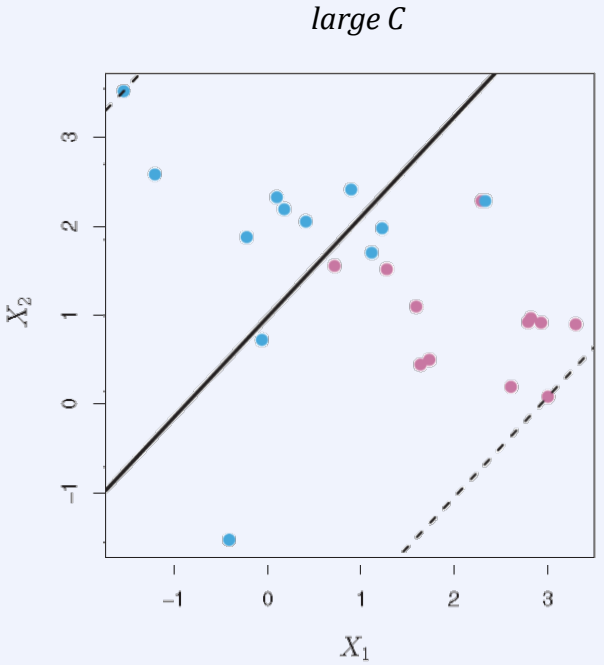
As C increases, we become more tolerant to violations



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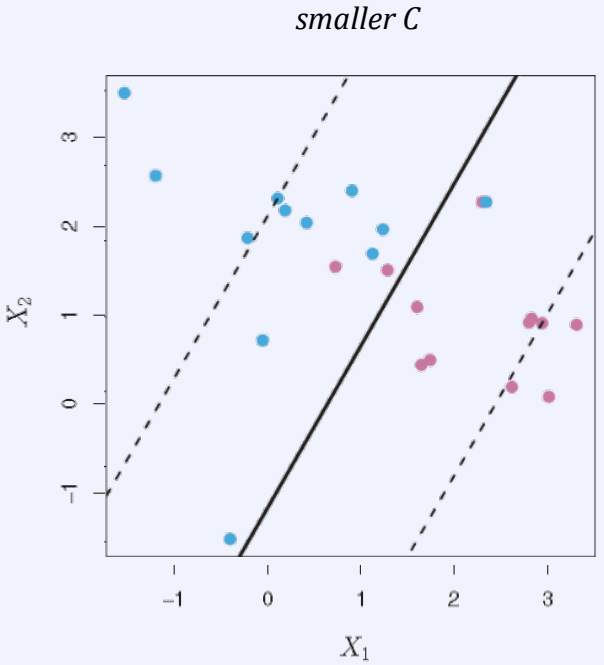

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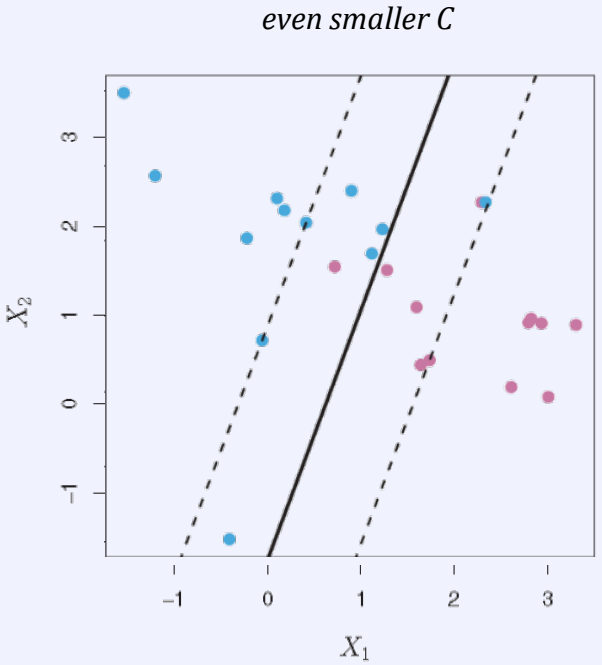

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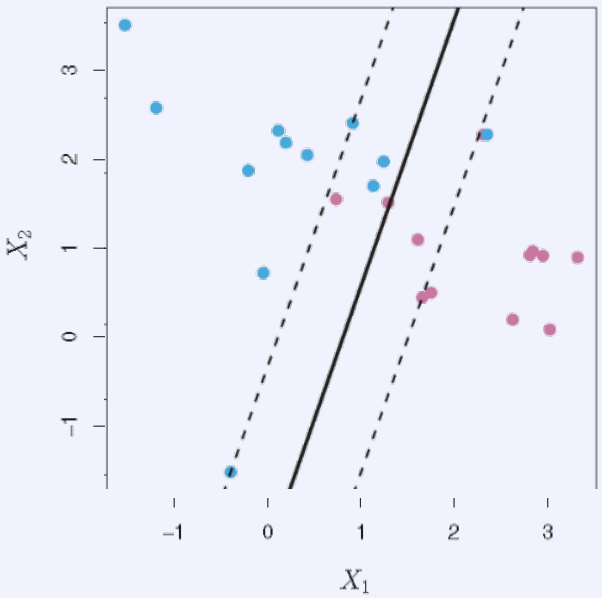
As C increases, we become more tolerant to violations

very small C



(ISLR 9.2.2)

The Margin and the Support Vectors

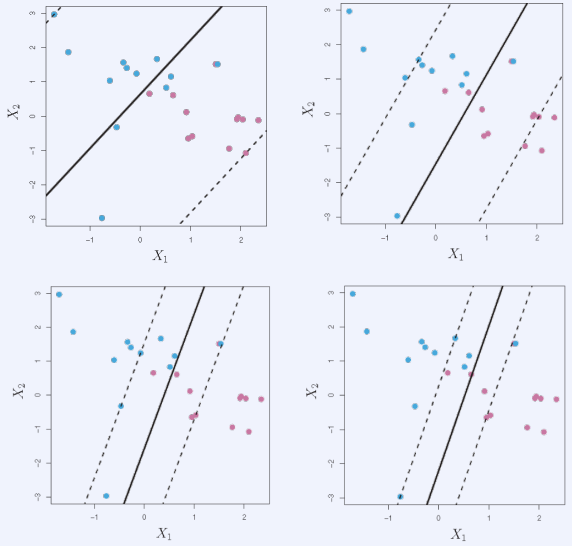
We choose C via cross-validation

For the soft-margin classifier support vectors all either lie exactly on the margin or on the wrong side of the margin

- intuition: only changing those points affects the hyperplane
- C controls the bias-variance tradeoff
- with large C the margin is wide and there are many support vectors
  - low variance and potentially high bias
- with small C the margin is thin and there are a few support vectors
  - high variance and small bias

The fact that correctly classified points far away from the hyperplane do not affect the classifier is a property of the support-vector classifier

as C decreases we become less tolerant to violations



Nonlinear Decision Boundaries

Sometimes, data is inherently nonlinear

- then there is no soft margin that will do the trick
- we need a nonlinear version of support vector machines
- we could add nonlinear features to the feature space, e.g. $X_1, X_1^2, X_2, X_2^2, \dots, X_p, X_p^2$ instead of $X_1, X_2, \dots, X_p$
- the resulting optimization program would become

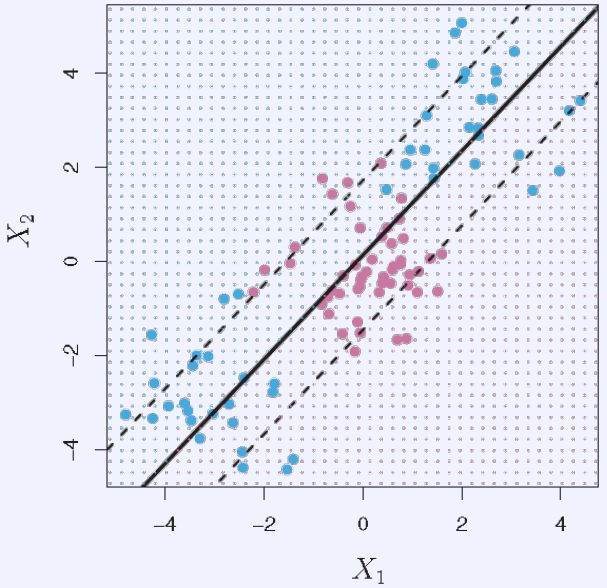
$$\max_{\beta_0,\beta_{11},\beta_{12},\dots\beta_{p1},\beta_{p2},\epsilon_1,\dots,\epsilon_n,M} M$$

$$\text{subject to } \epsilon_i \geq 0, \sum_{i=1}^{n} \epsilon_i \leq C, \sum_{j=1}^{p} \sum_{k=1}^{2} \beta_{jk}^2 = 1$$

$$y_i\left(\beta_0 + \sum_j^p \beta_{j1} x_{ij} + \sum_{j=1}^{p} \beta_{j2} x_{ij}^2\right) \geq M(1-\epsilon_i),\ i = 1, \dots n$$

- we could add higher-order, interaction terms, or use functions other than polynomials

the true boundary is non-linear



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The Kernel Trick

With **support vectors machines (SVMs)** there is a different very elegant trick – the **kernel trick**

- builds on the optimization procedure for SVMs, which we will not detail
- it suffices to say that the linear support vector classifier can be rewritten as $f(x^*) = \beta_0 + \sum_{i=1}^{n} \alpha_i \langle x^*, x_i \rangle$
- $\langle x^*, x_i \rangle = \sum_{j=1}^{p} x_j^* x_{ij}$ is the inner product,
- and the α_i are parameters that result from the training

set of support vectors

Important: Only the α_i for the support vectors are nonzero $f(x^*) = \beta_0 + \sum_{i \in S} \alpha_i \langle x^*, x_i \rangle$

The Kernel Trick

Only the α_i for the support vectors are nonzero $f(x^*) = \beta_0 + \sum_{i \in S} \alpha_i \langle x^*, x_i \rangle$

- to calculate α_i and β_0 we only need $\frac{n(n-1)}{2}$ inner products $\langle x_i, x_{i'} \rangle$ between all pairs of training points
- the actual coordinates of the training observations or the test point are never needed!

We can generalize inner products to (nonlinear) kernels $K(x_i, x_{i'})$

- a kernels quantifies the similarity between two data points
- a simple linear kernel is $K(x_i, x_{i'}) = \langle x_i, x_{i'} \rangle$
- it quantifies similarity in terms of the standard (Pearson) correlation

Nonlinear Kernels

Two popular choices:

- The polynomial kernel with degree d

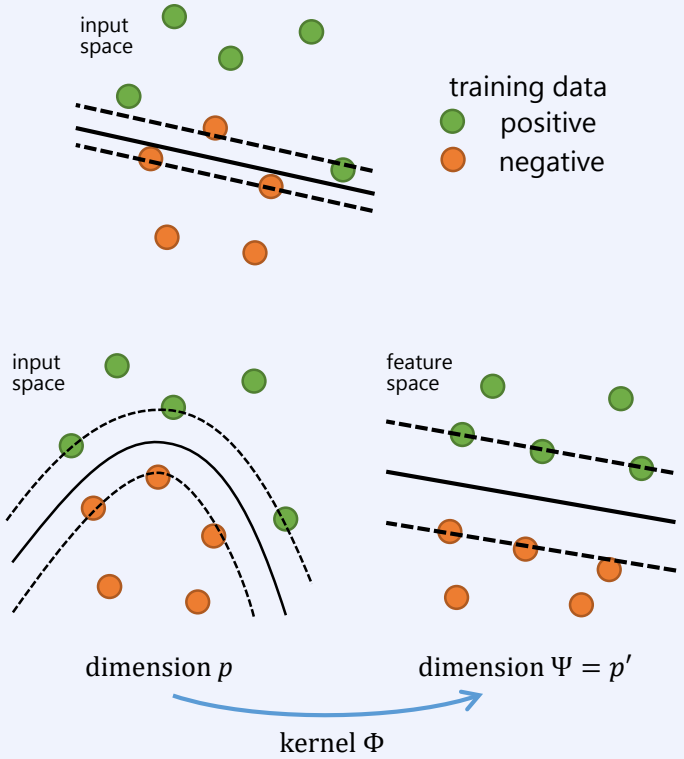
  $K(x_i, x_{i'}) = \left(1 + \sum_{j=1}^{p} \langle x_{ij}, x_{i'j} \rangle\right)^d$

- The radial-basis kernel

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

- in general, a kernel is any symmetric and positive definite function[1] of its two arguments

A VERY important theorem says that for any kernel K there is a function $\Phi: \mathbb{R}^p \to \Psi$ such that $K(x_i, x_j) = \langle \Phi(x_i), \Phi(x_j) \rangle$

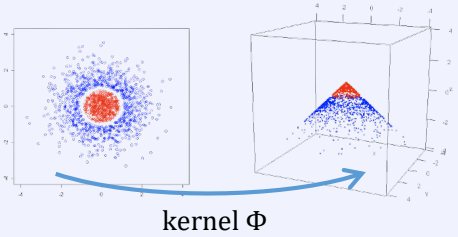


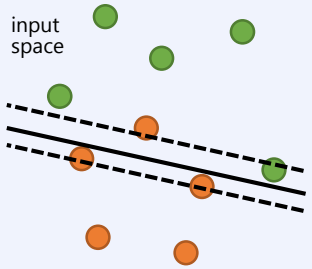
1) i.e. for any non-zero real vector $(c, \ldots, c_N)$ we have $\sum_{i=1}^{N} \sum_{j=1}^{N} c_i c_j K(X_i, X_j) > 0$

Reproducing Kernel Hilbert Space (RKHS)

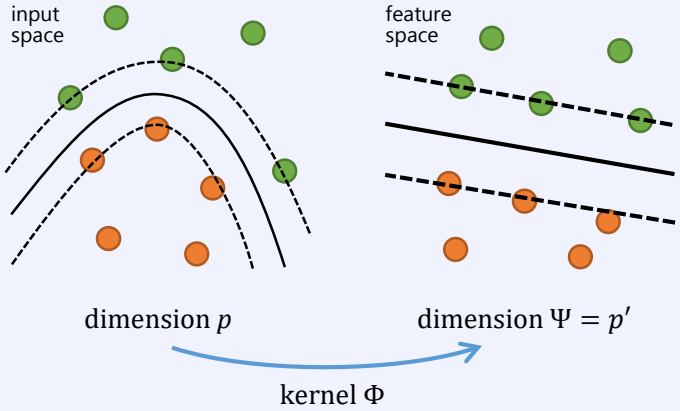
Applying the kernel actually means performing an inner product in some space Ψ, the so-called RKHS

- neither Φ nor Ψ generally can (or need) be constructed in a computationally usable form
- however in some cases, they can, e.g., for $p = 2$ and the polynomial kernel with $d = 2$, we have dim $\Psi = p' = 6$ and
  $\Phi_1(X) = 1, \quad \Phi_2(X) = \sqrt{2}X_1, \quad \Phi_3(X) = \sqrt{2}X_2$
  $\Phi_4(X) = X_1^2, \quad \Phi_5(X) = X_2^2, \quad \Phi_6(X) = \sqrt{2}X_1X_2$
- for the radial basis kernel, p' is infinite[1]





training data
positive
negative



1) Steinwart et al (2006) (ISLR 9.3.2)

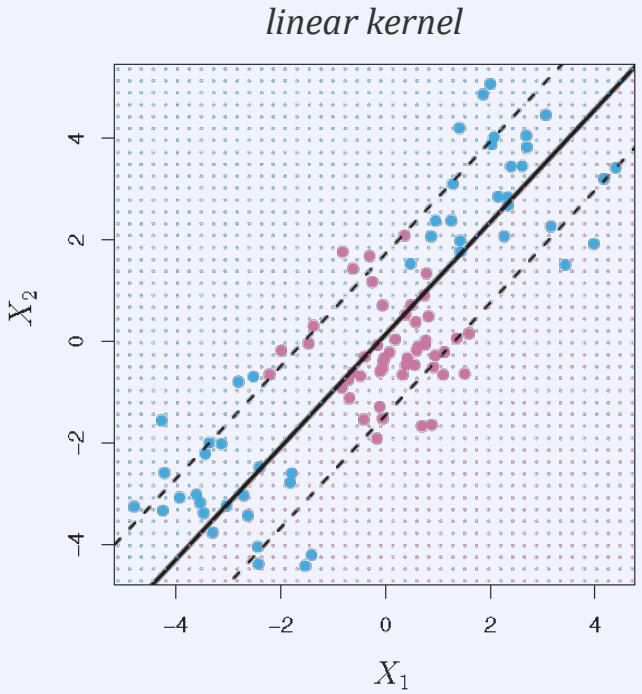
The Radial Basis Kernel

If our test point x^* is far from the training point x_i then $\sum_{j=1}^{p}\left(x_j^* - x_{ij}\right)^2$ will be large, so the kernel value $\exp\left(-\gamma \sum_{j=1}^{p}\left(x_j^* - x_{ij}\right)^2\right)$ will be tiny

- thus x_i will not influence the value of $f(x^*)$ by much

Since the class label is based on the sign of $f(x^*)$ the radial basis kernel thus has very local behavior

- γ controls the locality
- decreasing γ increases locality



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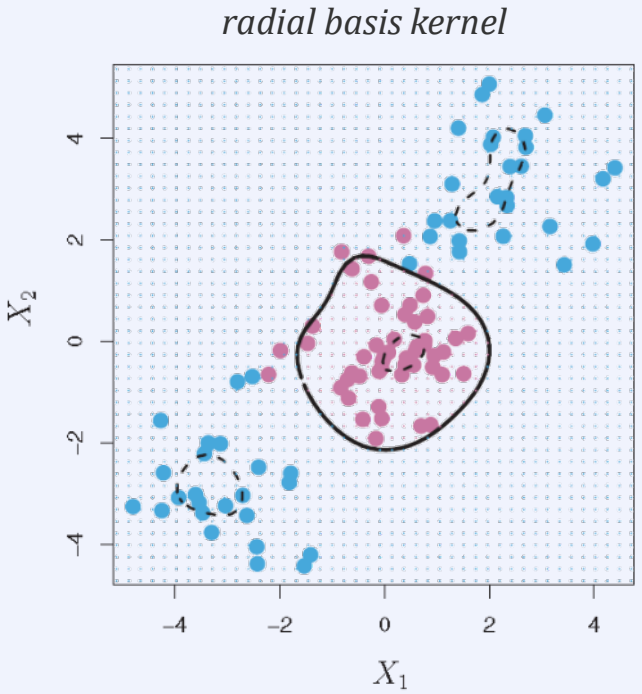


(ISLR 9.3.2)

Advantages of Kernels

To calculate the SVM you only need the kernel matrix for the pairs of training points

- in contrast, enlarging the feature space is computationally expensive

Can be applied to arbitrary observations that are not vectors: graphs, strings, molecules, etc.

The kernel trick can also be used with other statistical learning methods such as LDA or PCA

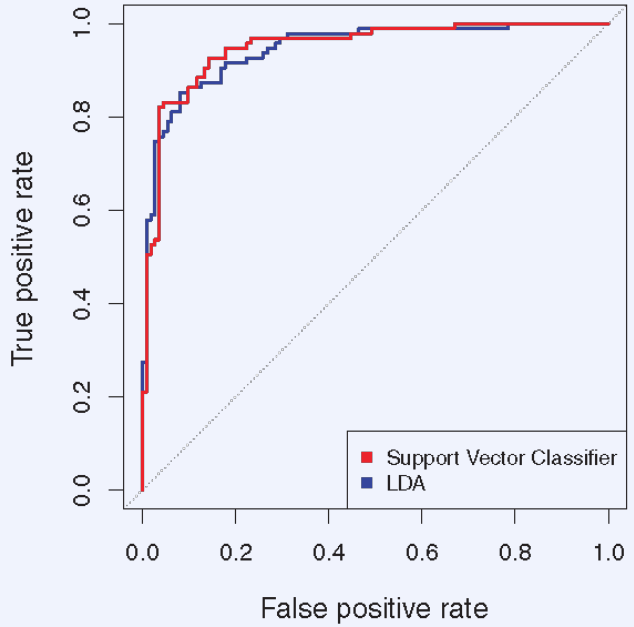
Application to the Heart Disease Data

- 13 predictors are used for classification
- binary target: whether an individual has heart disease
- 207 training, 90 test observations

Comparison of LDA and linear SVM

- use a threshold on $f(x)$ to parameterize SVM
- use a threshold on the linear discriminant to parameterize LDA
- similar performance on the training data

*ROC curve for classification performance on the **Heart** dataset – training data*



(ISLR 9.3.3)

Application to the Heart Disease Data

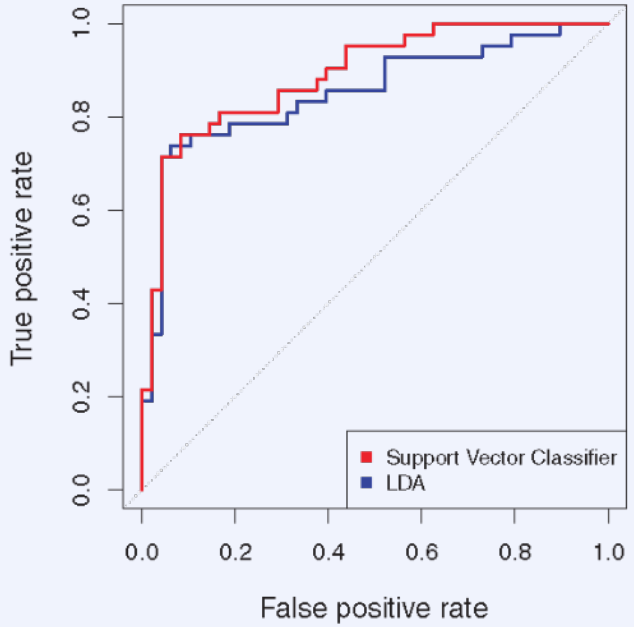
- 13 predictors are used for classification
- binary target: whether an individual has heart disease
- 207 training, 90 test observations

Comparison of LDA and linear SVM

- use a threshold on $f(x)$ to parameterize SVM
- use a threshold on the linear discriminant to parameterize LDA
- similar performance on the training data

- SVM outperforms LDA on the test set – generalizes better

*ROC curve for classification performance on the **Heart** dataset – test data*



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Comparison of linear and nonlinear (radial basis kernel) support vector classifiers

- $\gamma = 10^{-1}$ is best on the training set

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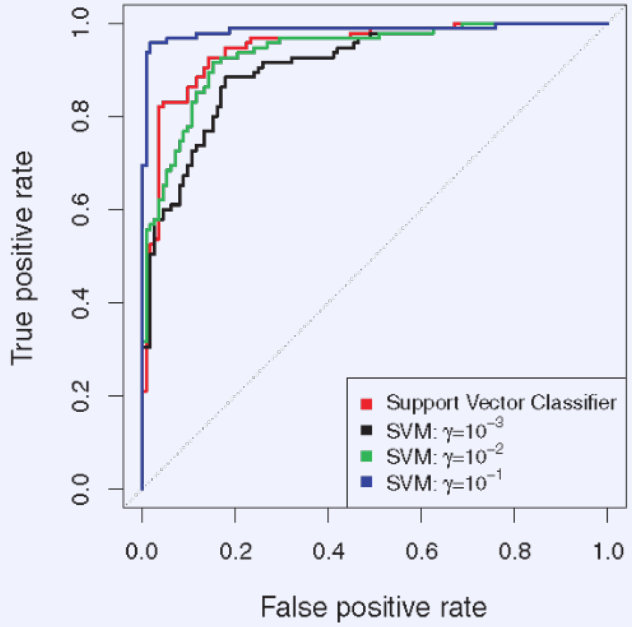

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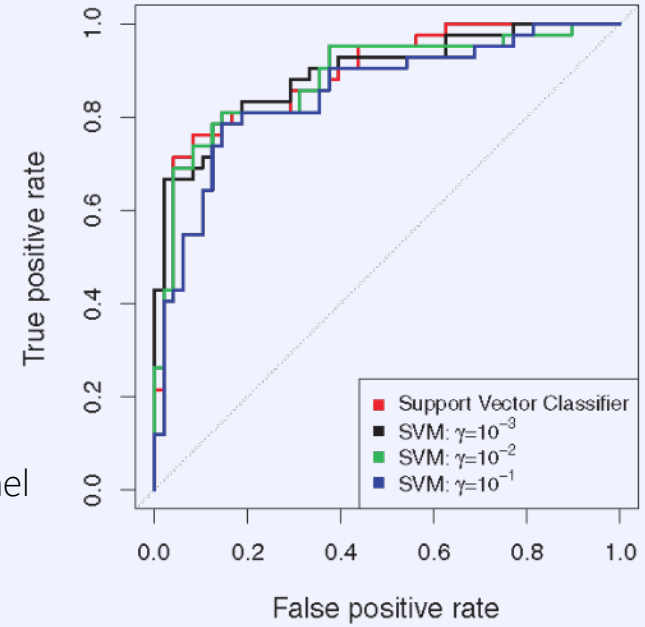
Comparison of linear and nonlinear (radial basis kernel) support vector classifiers

- $\gamma = 10^{-1}$ is best on the training set

- $\gamma = 10^{-1}$ is worst on the training set
- this amounts to a very local kernel which incurs high variance
- other nonlinear kernels perform comparably with the linear kernel

*ROC curve for classification performance on the **Heart** dataset – test data*



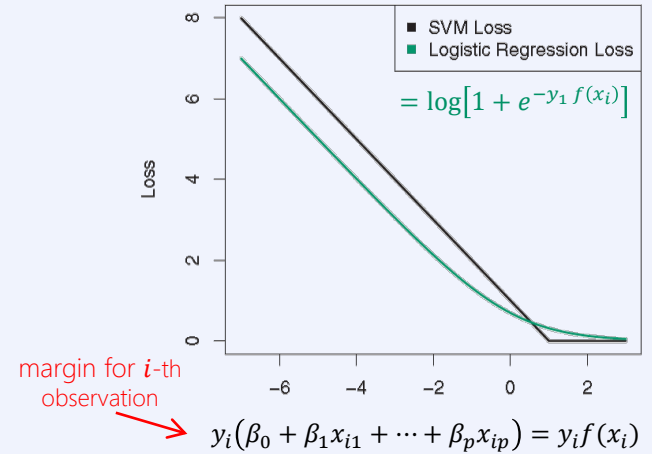
(ISLR 9.3.3)

Relationship to Logistic Regression

The SVM optimization problem can be rewritten as

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

- this has a general form of a regularized regression $\min_{\beta_0,\beta_1,\ldots,\beta_p}\{L(\mathbf{X},\mathbf{y},\beta)+\lambda P(\beta)\}$ with loss L and penalty P



SVM uses the same penalty as in ridge regression, but a different loss function, called **hinge** loss

- similar to that used in logistic regression, thus both classifiers often give similar results
- with better separation, SVM is better, with more overlap logistic regression tends to be better

The budget C for margin violations is inversely proportional to the penalty parameter λ

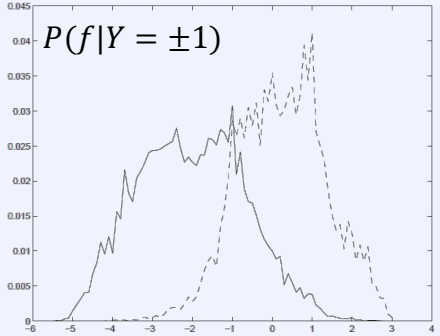
Posterior Probabilities from SVMs

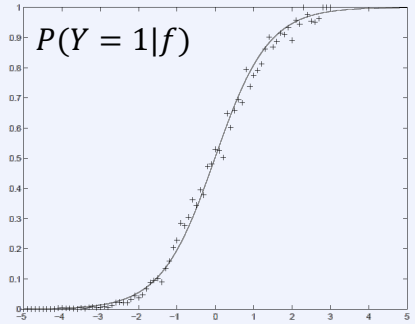
Turning SVM output into ROC curves

- compute posterior probability of the input belonging to class 0 and 1 respectively using the formula $P(y = 1|x) = \frac{1}{1+\exp(Af(x)+B)}$ where $f(x)$ is the SVM output
- A and B are parameters that are trained discriminatively

The original distributions are not Gaussian and ragged

- but, logistic fit works well





(Platt, J. C. (1999). In Advances in Large Margin Classifiers. A. J. Smola et al., eds., MIT Press: 61-74.)

Multiclass classification

Standard SVM cannot handle multiple classes. We show strategies to address the issue.

- they can be generally applied anytime a binary classifier is the only option

One-vs-rest: Train K SVM models for K classes, where each SVM is being trained for classification of one class against all the remaining ones.

- winner is then the class, where the distance from the hyperplane is maximal

One-vs-one: train $\binom{K}{2}$ classifiers (all possible pairings) and evaluate all

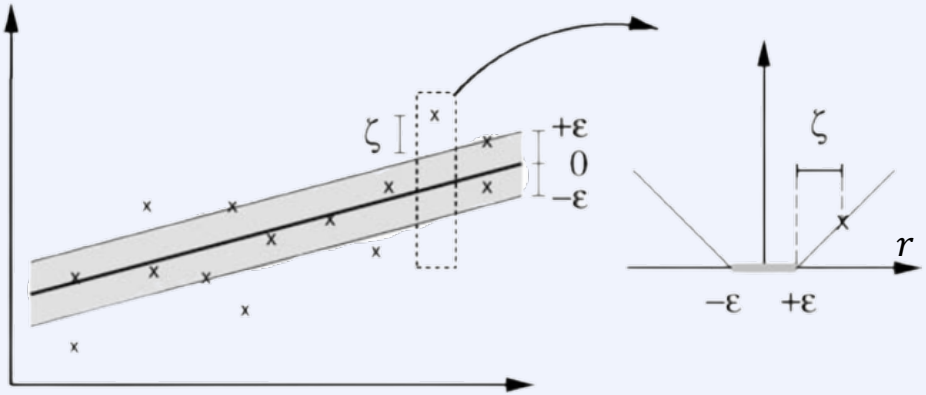
- winner is the class with the majority vote
- votes can be weighted according to the distance from the margin

One-class SVM: an unsupervised algorithm to learn a decision function for novelty detection

Support Vector Machines for Regression

Want to fit a linear model $f(x) = x^T\beta + \beta_0$ such that all data points lie inside a margin of width ϵ of the regression hyperplane

- impose a square penalty on model complexity



The loss function is the ϵ-insensitive $V_\epsilon(r)$

- only data points **on or outside** the tube change the model (this is different from classification)
- these are the support vectors
- kernels distort the tube

(Smola and Schölkopf. A Tutorial on Support Vector Regression. 1998)

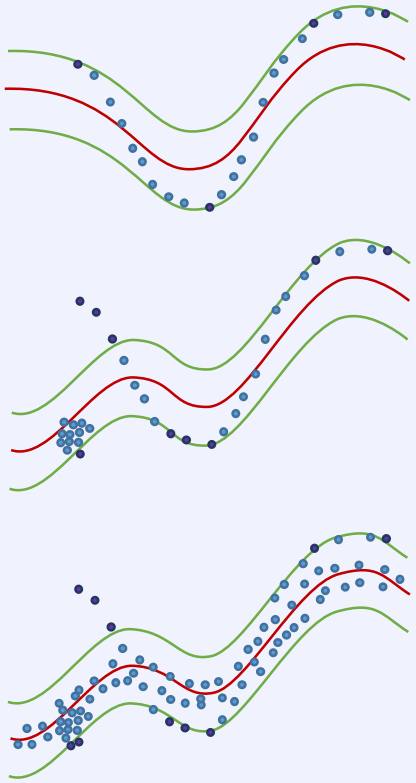
Example SVR with a Radial Basis Kernel

SVR with RBF kernel on synthetic data

- Green lines show the ϵ-boundaries
- Blue points represent data instance
- Marked blue points are the support vectors

The fitted model adapts well to the structure of the data

Introducing new datapoints changes the model only if they are outside or on the ϵ-boundary



(Smola and Schölkopf. A Tutorial on Support Vector Regression. 1998)

Summary

The main ideas behind SVMs is to find the max-margin hyperplane that separate the data

Hard SVM requires that all training data is correctly separated by can overfit

Soft SVM allows violations of the margin up to a budget C to get a better hyperplane overall

We can rewrite the SVM classifier only in terms of inner products – replacing those with a kernel is the kernel trick which allow us to efficiently introduce non-linearity

- the kernel trick is an important general idea that also applies to LDA, PCA and other models

Linear SVM is similar to logistic ridge regression but uses a hinge loss instead