Statistical Learning– MATH 6333
Set 5 (Support Vector Machines - SVM)

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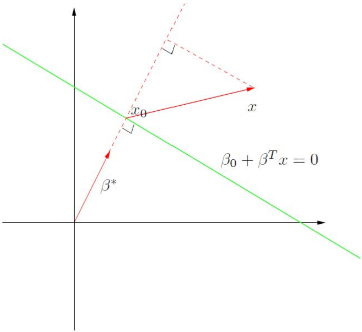
* Last updated October 27, 2021

Recall ...

From linear algebra ...

- $\beta^* = \frac{\beta}{||\beta||}$ is orthonormal to the separating hyperplane

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



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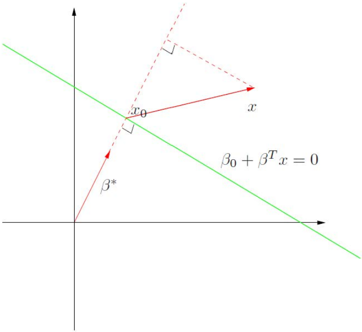
  for any $x_0, x_1 \in L$.



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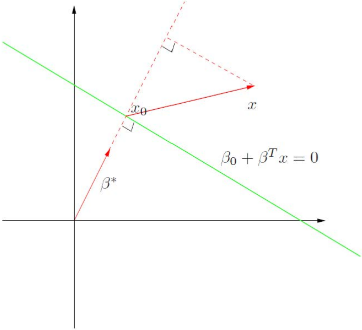

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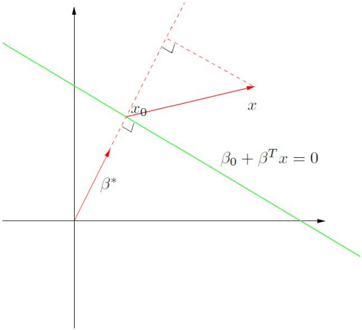
- Note that, signed distance of $x_1 \in L$ is zero.



Recall ...

From linear algebra ...

- The "actual" distance between two hyperplanes

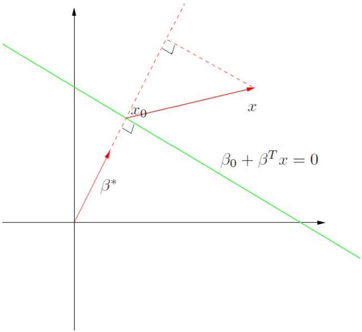
$$L_1 = \{x : \beta_{0,1} + x^T\beta = 0\}$$

and

$$L_2 = \{x : \beta_{0,2} + x^T\beta = 0\}$$

is

$$\frac{|\beta_{0,1} - \beta_{0,2}|}{||\beta||}$$



Other Classification Methods

Other Classification Methods

1. Maximal Margin Classifier (*aka* Optimal Separating Hyperplane)
2. Support Vector Classifier (*aka* Soft Margin Classifier)
3. Support Vector Machine
4. Flexible Discriminant Methods

Separating Hyperplanes - Maximal Margin Classifier

Maximal Margin Classifier

aka Optimal Separating Hyperplanes

OSH maximizes the margins (signed distances M) of the slab

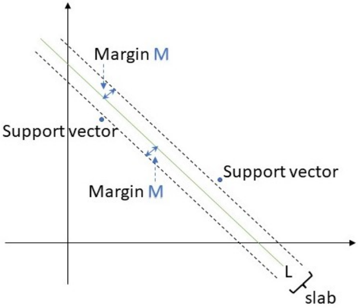
- Solve

$$\max_{\beta_0,\beta} M$$

subject to

$$\frac{1}{\|\beta\|} y_i(\beta_0 + x_i^T \beta) \geq M$$

for $i = 1, 2, \ldots, N$.



- Set $\|\beta\| = \frac{1}{M}$

Maximal Margin Classifier

aka Optimal Separating Hyperplanes

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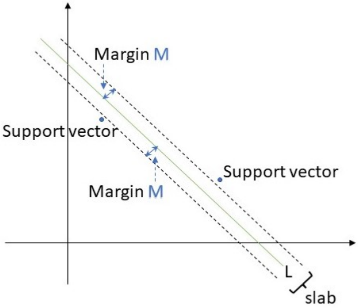


Maximal Margin Classifier

aka Optimal Separating Hyperplanes

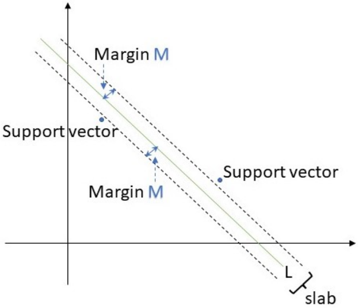
- Then the problem becomes equivalent to the convex optimization problem

$$\min_{\beta_0,\beta} \frac{1}{2} \|\beta\|^2$$

subject to

$$y_i(\beta_0 + x_i^T\beta) \geq 1$$

for $i = 1, 2, \ldots, N$.



Maximal Margin Classifier

aka Optimal Separating Hyperplanes

- Step 1: is the Lagrange problem to

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

where

$$L_p = \frac{1}{2}\|\beta\|^2 - \sum_{i=1}^{N} \alpha_i (y_i(\beta_0 + x_i^T \beta) - 1)$$

s.t. $\alpha_i \geq 0$

- Setting derivatives equal to zero leads to

$$\sum_{i=1}^{N} \alpha_i y_i = 0 \text{ and } \sum_{i=1}^{N} \alpha_i y_i x_i = \beta$$

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Maximal Margin Classifier

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- Substituting with those into L_p we get

$$L_p = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j x_i^T x_j$$

Maximal Margin Classifier

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- Step 2: Using Wolfe dual optimization, the problem becomes

$$\max_{\alpha_i} L_D$$

where

$$L_D = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j x_i^T x_j$$

subject to (the Karush-Kuhn-Tucker conditions)

$$\sum_{i=1}^{N} \alpha_i y_i = 0 \text{ and } \sum_{i=1}^{N} \alpha_i y_i x_i = \beta$$

$$\alpha_i \geq 0$$

and

$$\alpha_i (y_i (\beta_0 + x_i^T \beta) - 1) = 0$$

for $i = 1, 2, \ldots, N$.

Maximal Margin Classifier

aka Optimal Separating Hyperplanes

- Here, β depends on α through the KKT conditions.
- If optimal $\alpha_i = 0$, then $y_i(\beta_0 + x_i^T \beta) - 1 > 0$ and so the point is not on the margin line.
- If $\alpha_i > 0$, then $y_i(\beta_0 + x_i^T \beta) - 1 = 0$ and so the point is on the margin line and which will contribute to the values of β that will make up the decision boundary based on this support points on the slab's boundaries.
- Separation will occur according to $\hat{G}(x) = sign(\hat{\beta}_0 + x^T \hat{\beta})$.
- where $\hat{\beta} = \sum_{i \in \partial slab} \alpha_i^* y_i x_i$ and $\hat{\beta}_0 = y_i - x_i^T \hat{\beta}$ for any $i \in \partial slab$

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Maximal Margin Classifier

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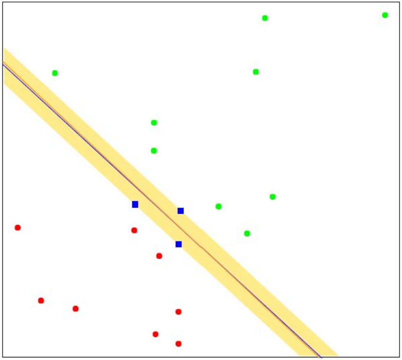
Example (Simulated data in $\mathbb{R}^2$)



The blue line is the OHS and the red line is due to logistic regression.

Separating Hyperplanes - Support Vector Classifier

Support Vector Classifier

aka Soft Margin Classifier

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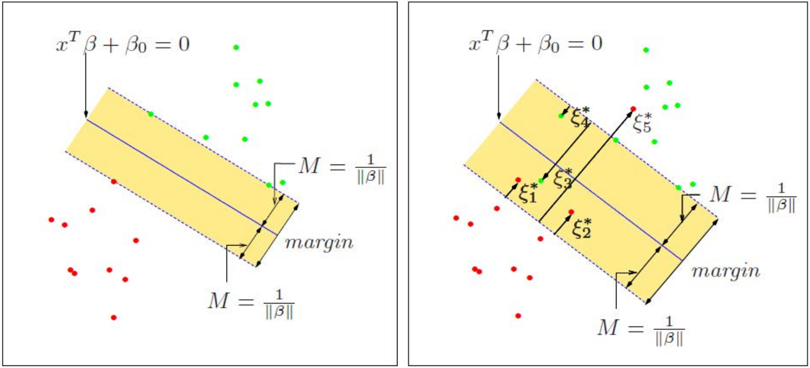

Maximal Margin Classifier works for the left panel with $y_i(x_i^T\beta + \beta_0) \geq 1$ since the points are linearly separable. But it is not the case in the right panel where $y_i(x_i^T\beta + \beta_0) < 1$. Adding *slack* variables $\xi_i \geq 0$ gives $y_i(x_i^T\beta + \beta_0) + \xi_i \geq 1$.

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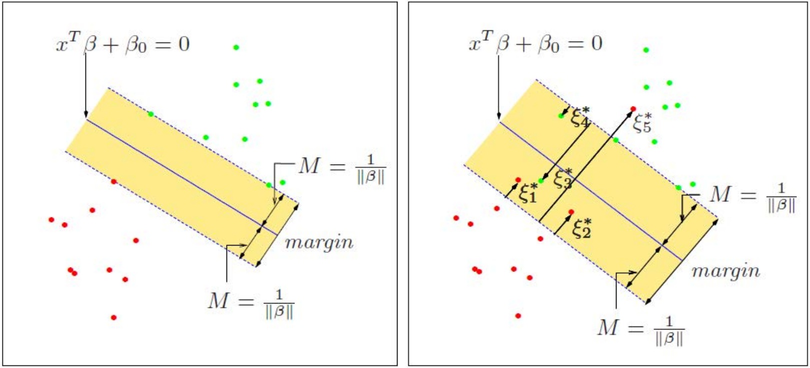

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If the vectors are not linearly separable. Let ξ_i is the smallest such that $y_i(x_i^T\beta + \beta_0) + \xi_i = 1$ and

- if $\xi_i = 0$, then $y_i(x_i^T\beta + \beta_0) = 1$ so it is accurately classified point, otherwise

$$y_i(x_i^T\beta + \beta_0) = 1 - \xi_i$$

- if $0 < \xi_i \leq 1$, then $0 \leq y_i(x_i^T\beta + \beta_0) < 1$ so it is "also" accurately classified point. Yet, that point (vector) has violated the margin.
- if $\xi_i > 1$, then $y_i(x_i^T\beta + \beta_0) < 0$, and so it is inaccurately classified point. That point (vector) is on the wrong side of the hyperplane.

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Support Vector Classifier

aka Soft Margin Classifier

- Thus, the misclassification rate is $\sum_{i=1}^{N} I(\xi_i > 1)$.
- It makes sense to include it in the optimization problem by minimizing $\sum_{i=1}^{N} I(\xi_i > 1)$.
- But, $\sum_{i=1}^{N} I(\xi_i > 1)$ is not differentiable in ξ_i.
- However, since $I(\xi_i > 1) \leq \xi_i$ for all i then it is sufficient to minimize $\sum_{i=1}^{N} \xi_i$.

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Support Vector Classifier

aka Soft Margin Classifier

- So the optimization problem becomes

$$\min_{\beta_0,\beta,\xi} \frac{1}{2}\|\beta\|^2 + C\sum_{i=1}^{N}\xi_i$$

subject to

$$y_i(\beta_0 + x_i^T\beta) + \xi_i \geq 1$$

and

$$\xi_i \geq 0$$

for $i = 1, 2, \ldots, N$.

- Where $C > 0$ is a tuning parameter that is the reciprocal of the cost the problem can afford from misclassification.
- When $C = \infty$, the cost is zero and only solution is the zero solution.

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$$L_p = \frac{1}{2}\|\beta\|^2 + C\sum_{i=1}^{N}\xi_i - \sum_{i=1}^{N}\alpha_i(y_i(\beta_0 + x_i^T\beta) + \xi_i - 1) - \sum_{i=1}^{N}\mu_i\xi_i$$

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

s.t. the Lagrange multipliers $\alpha_i, \mu_i \geq 0$ and the slack variables $\xi_i \geq 0$.

- Setting derivatives equal to zero leads to

$$\sum_{i=1}^{N}\alpha_i y_i = 0 \text{ and } \sum_{i=1}^{N}\alpha_i y_i x_i = \beta \text{ and } C - \alpha_i - \mu_i = 0 \text{ for all } i$$

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- Substituting with those into L_p we get

$$L_p = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j x_i^T x_j$$

- Note that since $C = \alpha_i + \mu_i$, then $0 \le \alpha_i \le C$.

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$$0 \leq \alpha_i \leq C$$

and

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and $\mu_i \xi_i = 0$ for $i = 1, 2, \ldots, N$.

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- Again, β depends on optimal α^* through the KKT conditions.
- If optimal $\alpha_i^* = 0$, then $\mu_i = C$ and $\xi_i = 0$ and so $y_i(\beta_0 + x_i^T\beta) - 1 > 0$. Thus, the point/vector is not on the margin line.
- If optimal $0 < \alpha_i^* < C$, then $\mu_i \neq 0$ and $\xi_i = 0$ and so $y_i(\beta_0 + x_i^T\beta) - 1 = 0$. Thus, the point/vector is on the margin line and α_i^* will contribute to the values of β that will make up the decision boundary. Those points are called margin support vectors.
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aka Soft Margin Classifier

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- If optimal $\alpha_i^* = C$, then $\mu_i = 0$ and $\xi_i \geq 0$ and so $y_i(\beta_0 + x_i^T\beta) + \xi_i - 1 = 0$.
  - If $\xi \leq 1$, the point/vector beyond the margin line but before the hyperplane. Those points are called non-margin support vectors. (A violator but accurately classified.)
  - If $\xi > 1$, the point/vector beyond the hyperplane. (A misclassification.)
- with $\hat{\beta} = \sum_{i \in slab} \alpha_i^* y_i x_i$ and $\hat{\beta}_0 = y_i - x_i^T\hat{\beta}$ for any $i \in slab$
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$$\hat{G}(x) = sign(\hat{\beta}_0 + x^T\hat{\beta}) = sign(\hat{\beta}_0 + \sum_{i \in slab} \alpha_i^* y_i x_i^T x)$$

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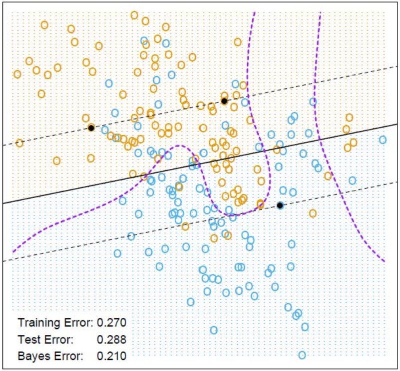

$C = 10000$

The broken purple curve is the Bayes decision boundary. 62% observations are support points.

Support Vector Classifier

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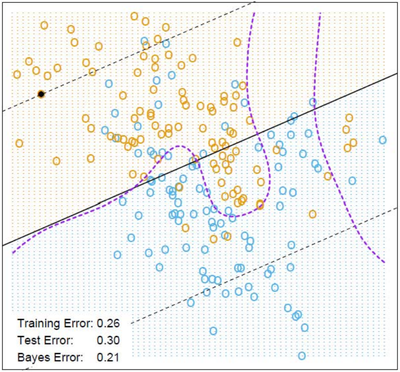

$C = 0.01$

The broken purple curve is the Bayes decision boundary. 85% observations are support points.

Regression and Kernels

Regression and Kernels

- Let $\{h_m(x), m = 1, 2, \ldots, M\}$ be a set of basis transformations, each of which maps $\mathbb{R}^p$ into $\mathbb{R}$, e.g.
  1. $h_m(x) = X_m$, X_j, X_j^2, X_iX_j, $\log(X_j)$
  2. piece-wise constants $h_m(x) = c_m I(L_m \leq X < U_m)$ with $-\infty = L_1 < U_1 \leq L_2 < U_2 \leq L_3 < \cdots \leq L_M < U_M = \infty$
  3. $h_m(x) = \sum_{i \in A_m} c_{m,i} X_i$ for some set A_m
  4. h_m is a polynomial or spline function
- A regression function

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

is a linear function in h_m in the new $M-$ dimensional space

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Regression and Kernels

- whose estimate is

$$\hat{f}(x) = \hat{\beta}_0 + \sum_{m=1}^{M} \hat{\beta}_m h_m(x)$$

where parameters β_0 and β are estimated by minimizing the L_2-penalized objective function

$$RSS_\lambda(\beta_0, \beta) = \sum_{i=1}^{N} L(y_i, f(x_i)) + \lambda \sum_{m=1}^{M} \beta_m^2$$

with $M > N$.

- L could be the squared loss function $L(x, y) = (x - y)^2$
- thus, after estimating β_0 a priori (let us set $\hat{\beta}_0 = 0$ for simplicity) ...

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Regression and Kernels

- the objective function is

$$RSS_\lambda(\beta) = (y - X_h\beta)^T(y - X_h\beta) + \lambda||\beta||^2$$

where the $N \times M$ matrix

$$X_h = \begin{pmatrix} h_1(x_1) & h_2(x_1) & \cdots & h_M(x_1) \\ h_1(x_2) & h_2((x_2) & \cdots & h_M(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ h_1(x_N) & h_2(x_N) & \cdots & h_M(x_N) \end{pmatrix}$$

is of the model $y = X_h\beta$

Regression and Kernels

- The penalized least squares solution is determined by differentiation of $RSS_\lambda(\beta)$ and setting the result equal to zero

$$-X_h^T(y - X_h\beta) + \lambda\beta = 0$$

$$-X_h X_h^T(y - X_h\beta) + \lambda X_h\beta = 0$$

and so for $\lambda > 0$

$$\hat{y} = X_h\hat{\beta} = (X_h X_h^T + \lambda I)^{-1} X_h X_h^T y$$

- The $N \times N$ matrix $X_h X_h^T$ has the ij^{th} elements

$$\sum_{m=1}^{M} h_m(x_i)h_m(x_j) = h(x_i)^T h(x_j) = \underbrace{< h(x_i), h(x_j) >}_{\text{inner product}}$$

which requires a total of N^2M calculations.

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Regression and Kernels

- Thus, for a new x_*,

$$\hat{f}(x_*) = h(x_*)^T \hat{\beta} = \sum_{i=1}^{N} \hat{\alpha}_i h(x_*)^T h(x_i)$$

  where $\hat{\alpha}_i = (X_h X_h^T + \lambda I)^{-1} y_i$

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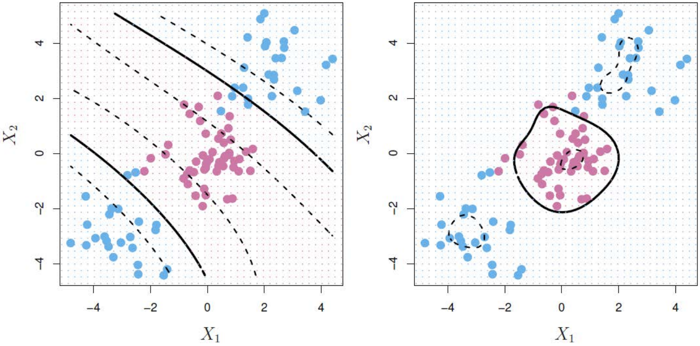
Non-linear Classification via Support Vector Machine

Support Vector Machine

Example (Simulated data in $\mathbb{R}^2$)



Left panel: using a polynomial of degree 3 kernel and right panel: using radial kernel.

Support Vector Machine

- In the linear classification case, SVC uses

$$\hat{G}(x) = sign(\hat{\beta}_0 + x^T\hat{\beta}) = sign(\hat{\beta}_0 + \sum_{i \in slab} \alpha_i^* y_i \underbrace{x_i^T x}_{\text{inner product}})$$

- In the non-linear classification case, SVC uses

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for some $\{h_m(x), m = 1, 2, \ldots, M\}$ set of basis transformations. Note that $0 < \alpha_i^* < C$ for $i \in slab$.

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Support Vector Machine

- In general classification case, SVM is a SVC that uses kernels so that

$$\hat{G}(x) = sign(\hat{\beta}_0 + \sum_{i \in slab} \alpha_i^* y_i \underbrace{K(x_i, x)}_{\text{kernel}})$$

and the previously described optimization problem in SVC is still valid.
- DIY analytically Show that $\hat{G}$ described using the kernel is the decision rule obtained via the optimization problem described in SVC.
- If we don't use penalized objective functions (the regularization parameter $\lambda = 0$), then we need the symmetric kernel K to be positive definite function.

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Support Vector Machine

- K is positive definite if there exists a function h such $K(x_i, x_j) =< h(x_i), h(x_j) >$
- Mercer's condition: A symmetric real-valued function $K(x, y)$ is said to satisfy Mercer's condition, if for all $L_2(\mathbb{R}^p)$ real-valued functions g,

$$\int_{\mathbb{R}^p} \int_{\mathbb{R}^p} K(x, y) g(x) g(y) dx dy \geq 0$$

- Theorem: Let $K(x, y)$ be a symmetric real-valued function. There exists a function h such $K(x, y) =< h(x), h(y) >$ if and only if K satisfies Mercer's condition.

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- Mercer-Hilbert Schmidt Theorem: Let $K(x, y)$ be a symmetric real-valued function that satisfies Mercer's condition, then there exists a set of orthonormal eigenfunctions $\{v_i(x)\}_{i=1}^{\infty}$ such that

$$\int_{\mathbb{R}^p} K(x, y) v_i(y) dy = \lambda_i v_i(x)$$

for $i = 1, 2, \ldots, \infty$, and

$$K(x, y) = \sum_{j=1}^{\infty} \lambda_j v_j(x) v_j(y)$$

.

- Thus, define $h_j(x) = \sqrt{\lambda_j} v_j(x)$ so that

$$K(x, y) = < h(x), h(y) >$$

Support Vector Machine

- Mercer-Hilbert Schmidt Theorem: Let $K(x, y)$ be a symmetric real-valued function that satisfies Mercer's condition, then there exists a set of orthonormal eigenfunctions $\{v_i(x)\}_{i=1}^{\infty}$ such that

$$\int_{\mathbb{R}^p} K(x, y) v_i(y) dy = \lambda_i v_i(x)$$

for $i = 1, 2, \ldots, \infty$, and

$$K(x, y) = \sum_{j=1}^{\infty} \lambda_j v_j(x) v_j(y)$$

.

- Thus, define $h_j(x) = \sqrt{\lambda_j} v_j(x)$ so that

$$K(x, y) = < h(x), h(y) >$$

Support Vector Machine

Popular Kernels in SVM are:

- Polynomial kernel of degree d

$$K(x, y) = (1 + \sum_{i=1}^{p} x_i y_i)^d$$

- (Gaussian) Radial kernel (strong local support)

$$K(x, y) = \exp(-\gamma \sum_{i=1}^{p} (x_i - y_i)^2)$$

- (Laplace) Radial kernel (weak local support)

$$K(x, y) = \exp(-\gamma \sum_{i=1}^{p} |x_i - y_i|)$$

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Support Vector Machine

Popular Kernels in SVM are:

- Cauchy kernel

$$K(x, y) = \gamma \frac{1}{1 + \sum_{i=1}^{p} (x_i - y_i)^2}$$

- Neural kernel

$$K(x, y) = \tanh(\kappa_1 \sum_{i=1}^{p} x_i y_i + \kappa_2)$$

Support Vector Machine

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Support Vector Machine

Example

Consider the polynomial kernel of degree 2, for $x, y \in \mathbb{R}^2$

$$\begin{aligned} K(x, y) &= (1 + x_1 y_1 + x_2 y_2)^2 \\ &= 1 + x_1^2 y_1^2 + 2x_1 y_1 + 2x_1 y_1 x_2 y_2 + 2x_2 y_2 + x_2^2 y_2^2 \\ &= h(x)^T h(y) \end{aligned}$$

such that $h(x) = (1, x_1^2, \sqrt{2}x_1, \sqrt{2}x_1 x_2, \sqrt{2}x_2, x_2^2) \in \mathbb{R}^6$

Support Vector Machine

- SVM uses

$$\hat{G}(x) = sign(\hat{\beta}_0 + \sum_{i \in slab} \alpha_i^* y_i \underbrace{K(x_i, x)}_{\text{kernel}})$$

  such that $0 < \alpha_i^* < C$ for $i \in slab$.
- If C is large then most of $\xi_i = 0$ and that leads to wiggly boundary in the input space (an overfitting situation).
- If C is small then most of α_i are small and so is $\hat{\beta} = \sum_{i \in slab} \alpha_i^* y_i h(x_i)$ and that leads to smooth boundary.

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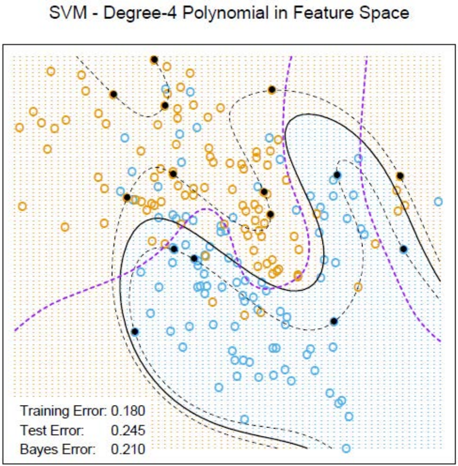
Support Vector Machine

Example (Simulated data in $\mathbb{R}^2$)



$C = 1$. The broken purple curve is the Bayes decision boundary.

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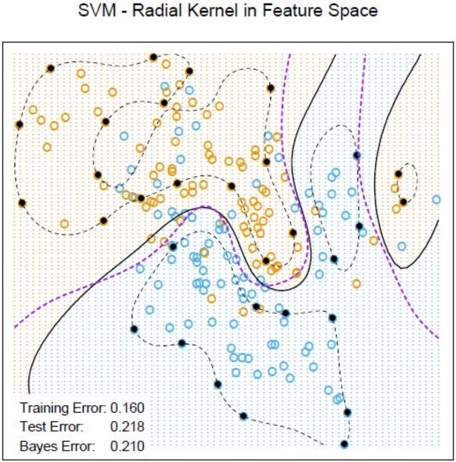

$C = 1$. It closer to Bayes optimal. The broken purple curve is the Bayes decision boundary.

SVM for more than two classes

Support Vector Machine

- One-versus-one classification:
  In a C_2^K round-robin, two classes k, k' play against each other coded $y_k + 1$ and $y_{k'} = -1$ and tally the classifications of x_* and assign it at the end of to the class with the highest number of classifications/votes.

- One-versus-all classification:
  Here, one class k (with $y_k = +1$) plays against the rest $K - 1$ classes (with $y_{[1,K]-\{k\}} = -1$) and estimate $f_k(x)$. Then use $\hat{G}(x_*) = argmax_k f_k(x_*)$.

Notation: $[1, K] = \{1, 2, \ldots, K\}$

Support Vector Machine

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SVM's relationship to Hinge Loss function and others

Support Vector Machine

In case of,
linear ($f(x) = \beta_0 + x^T\beta$) or nonlinear ($f(x) = \beta_0 + h(x)^T\beta$) classification problems

- The optimization problem is

$$\min_{\beta_0,\beta,\xi} \frac{1}{2}\|\beta\|^2 + C\sum_{i=1}^{N}\xi_i$$

  subject to

$$y_i(\beta_0 + x_i^T\beta) + \xi_i \geq 1$$

  and

$$\xi_i \geq 0$$

  for $i = 1, 2, \ldots, N$.

- The constraints are equivalent to the constraint

$$\xi_i \geq [1 - y_i f(x_i)]_+$$

  giving are the smallest value attainable by ξ_i for all i.

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Support Vector Machine

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where $C > 0$.

- Setting $C = \frac{1}{2\lambda}$, it further becomes

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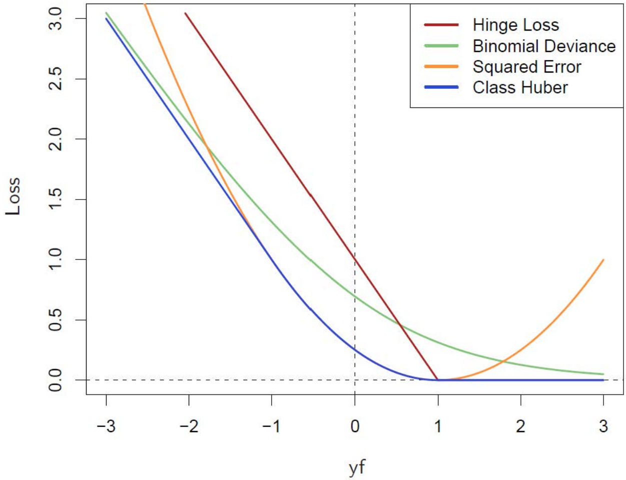
$$\min_{\beta_0,\beta} \sum_{i=1}^{N} \underbrace{[1 - y_i f(x_i)]_+}_{\text{hinge loss function}} + \lambda\|\beta\|^2$$

which is an L_2 regularized problem with a new loss function (hinge loss function) that allows no contribution from the non-support vectors.

Support Vector Machine



Note: $y_i f(x_i) > 1$ is for accurately classified points, and using hinge loss function, makes their contribution nil.

Support Vector Machine

- Minimizing the L_2-penalized objective function

$$RSS_\lambda(\beta_0, \beta) = \sum_{i=1}^{N} L(y_i, f(x_i)) + \lambda \sum_{m=1}^{M} \beta_m^2$$

  with $M > N$.
- L could take other forms for other functional forms of f

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Support Vector Machine

Loss Function	$L[y, f(x)]$	Minimizing Function
Binomial Deviance	$\log[1 + e^{-yf(x)}]$	$f(x) = \log \frac{\Pr(Y=+1\|x)}{\Pr(Y=\text{-}1\|x)}$
SVM Hinge Loss	$[1 - yf(x)]_+$	$f(x) = \text{sign}[\Pr(Y=+1\|x) - \frac{1}{2}]$
Squared Error	$[y - f(x)]^2 = [1 - yf(x)]^2$	$f(x) = 2\Pr(Y=+1\|x) - 1$
"Huberised" Square Hinge Loss	$-4yf(x)$, $yf(x) < \text{-}1$; $[1 - yf(x)]_+^2$ otherwise	$f(x) = 2\Pr(Y=+1\|x) - 1$

Also, ...

L_2-Regularized Logistic Regression

- Recall, the L_2-Regularized Logistic Regression for any $f(x)$ is due to the maximization problem

$$max_\beta \sum_{i=1}^{N} \left[\tilde{y}_i f(x_i) - \log(1 + e^{f(x_i)})\right] - \lambda \sum_{j=1}^{p} \beta_j^2$$

for $\tilde{y}_i = 0, 1$

- which is easily transformed into ± 1 using $\tilde{y}_i = \frac{y_i+1}{2}$ for $y_i = -1, +1$
- $\tilde{y}_i f(x_i) - \log(1 + e^{f(x_i)}) = -\log(1 + e^{y_i f(x_i)})$
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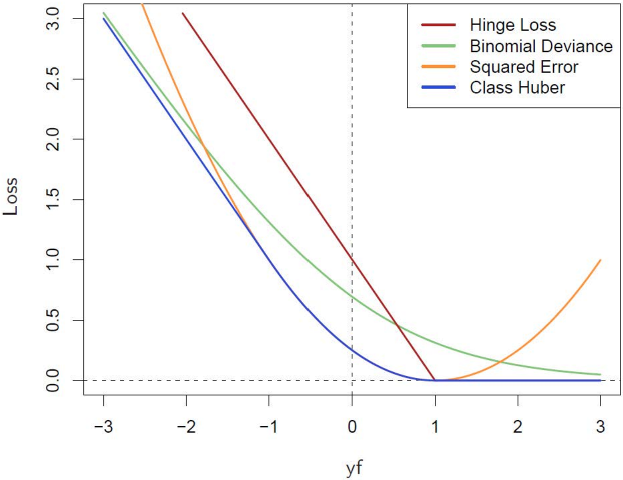
Support Vector Machine



Note: $y_i f(x_i) > 1$ is for accurately classified points, and using binomial deviance (in a logistic regression approach), makes their contribution positive but very small.

Support Vector Machine

Example (SA Heart Disease)

DIY in R

1. Carry out SVC classification using *e1071*. It is svm with Kernel="linear"
2. Carry out SVM classification using *e1071*. Use kernel = "polynomial" and kernel = "radial"
3. To evaluate the performance of the classifiers: use the receiver operating characteristic (ROC) curve using *ROCR*.

Support Vector Machine

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Please study the different methods in the ISL book. See also SVM with multiple classes.

End of Set 5