MATH 680 Computation Intensive Statistics

November 27, 2019

SVM

1 Optimal separating hyperplanes

Consider two-class classification problem, where we find a **hyperplane** or affine set L defined by the equation $f(x) = \beta_0 + \beta^\top x = 0$. The classifier is $\text{sign}(x^\top \beta + \beta_0)$. It has some properties:

1. For any x_1 and x_2 lying in L
$$\beta^\top (x_1 - x_2) = 0$$
and hence $\beta^\star = \beta / \|\beta\|$ is the vector normal to the surface of L.

2. For any point x_0 in L, $\beta^\top x_0 = -\beta_0$.

3. The signed distance of any point x to L is
$$\begin{aligned}\beta^{\star\top}(x - x_0) = \frac{\beta^\top}{\|\beta\|}(x - x_0) &= \frac{1}{\|\beta\|}(\beta^\top x + \beta_0) \\ &= \frac{1}{\|f'(x)\|} f(x).\end{aligned}$$

Now we find a separating hyperplane by maximizing the distance of correctly classified points to the decision boundary.

For any point i, if

- $y_i = +1$ while $\hat{y}_i = f(x_i) = x_i^\top \beta + \beta_0 > 0$
- $y_i = -1$ while $\hat{y}_i = f(x_i) = x_i^\top \beta + \beta_0 < 0$

we say this point i is correctly classified. For both cases, $y_i(x_i^\top \beta + \beta_0) > 0$. We only interested in the solutions for which all data points are correctly classified, so that $y_i(x_i^\top \beta + \beta_0) > 0$ for $i = 1, \ldots, n$ (**This is because now we considered the separable case**). The **distance** of x_i to the decision surface is given by

$$\frac{y_i(\beta^\top x_i + \beta_0)}{\|\beta\|}$$

The **margin** M is given by the perpendicular distance from the hyperplane to the closest point x_i. We want to maximize the margin. Thus the maximum margin solution is

$$\max_{(\beta,\beta_0)} M$$
$$\text{subject to } \frac{1}{\|\beta\|} y_i(\beta^\top x_i + \beta_0) \geq M, \; i = 1, \ldots, N. \tag{1}$$

Observe that any positively scaled $\beta \to \kappa\beta$ and $\beta_0 \to \kappa\beta_0$ would satisfy the inequality constraint:

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

Therefore we can arbitrarily set $\|\beta\| = 1/M$. Thus (1) can be simplified to

$$\min_{\beta,\beta_0} \frac{1}{2}\|\beta\|^2$$
$$\text{subject to } y_i(\beta^\top x_i + \beta_0) \geq 1, \; i = 1, \ldots, N.$$

This is a convex quadratic optimization problem, in which we minimize a quadratic function subject to a set of linear inequality constraints. The corresponding **Lagrangian** is

$$L(\beta, \beta_0, \alpha) = \frac{1}{2}\|\beta\|^2 + \sum_{i=1}^{N} \alpha_i [1 - y_i(\beta^\top x_i + \beta_0)], \tag{2}$$

with $\alpha_i \geq 0$. Setting $\frac{\partial L}{\partial \beta_0}$ and $\frac{\partial L}{\partial \beta}$ to zero, we obtain (stationarity)

$$\beta = \sum_{i=1}^{N} \alpha_i y_i x_i, \tag{3}$$

$$0 = \sum_{i=1}^{N} \alpha_i y_i, \tag{4}$$

and substituting these in (2) we obtain the **Lagrange dual function** $L_D(\alpha) = \min_{(\beta,\beta_0)} L(\beta, \beta_0, \alpha)$

$$\max_{\alpha} L_D(\alpha) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2}\sum_{i=1}^{N}\sum_{k=1}^{N} \alpha_i \alpha_k y_i y_k x_i^\top x_k$$
$$\text{subject to } \alpha_i \geq 0 \text{ and } \sum_{i=1}^{N} \alpha_i y_i = 0. \tag{5}$$

The solution of β^*, β_0^* and α^* of the above primal and dual problem must satisfy the Karush-Kuhn-Tucker conditions, which include **stationarity:** (3) and (4), **dual feasibility:** (5) and **complementary slackness:**

$$\alpha_i^* [y_i(x_i^\top \beta^* + \beta_0^*) - 1] = 0 \, \forall i,$$

from which we see that

- If $\alpha_i^* > 0$, then $y_i(x_i^\top \beta^* + \beta_0^*) = 1$, x_i is on the boundary of the margin.
- If $y_i(x_i^\top \beta^* + \beta_0^*) > 1$, x_i is not on the boundary of the margin, and $\alpha_i^* = 0$.

We see that the solution vector β^* and β_0^* is defined in terms of a linear combination of the support point x_i, where corresponding $\alpha_i^* > 0$. To predict new data points using the trained model, we evaluate the sign $\text{sign}(f(x)) = \text{sign}(x^\top \beta^* + \beta_0^*)$. Plug in (3), we get

$$f(x) = \sum_{i=1}^{N} \alpha_i^* y_i \langle x_i, x \rangle + \beta_0^*. \tag{6}$$

Data points with $\alpha_i > 0$, are called **support vector;** Data points with $\alpha_i = 0$, plays no role in (6).

2 Overlapping class distributions

For the general data set, there is no $x^\top \beta + \beta_0 = 0$ to perfectly separate class "+1" from class "−1".

The original optimization problem is

$$\max_{(\beta,\beta_0)} M$$
$$\text{subject to } \frac{1}{\|\beta\|} y_i(\beta^\top x_i + \beta_0) \geq M, \, i = 1, \dots, N. \tag{7}$$

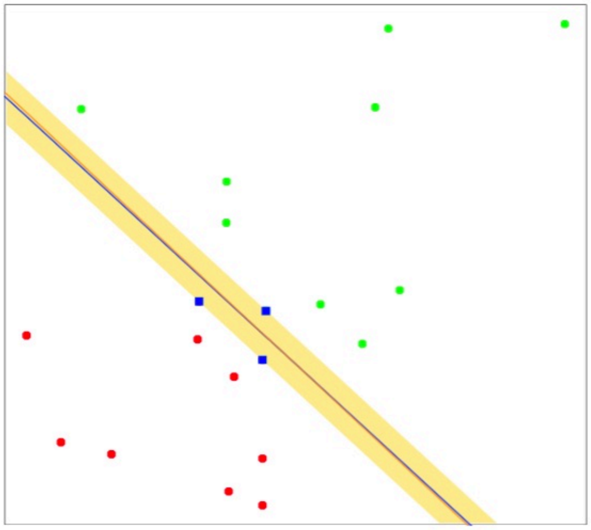


Figure 1: The same data as in Figure **??**. The shaded region delineates the maximum margin separating the two classes. There are three support points indicated, which lie on the boundary of the margin, and the optimal separating hyperplane (blue line) bisects the slab. Included in the figure is the boundary found using logistic regression (red line), which is very close to the optimal separating hyperplane.

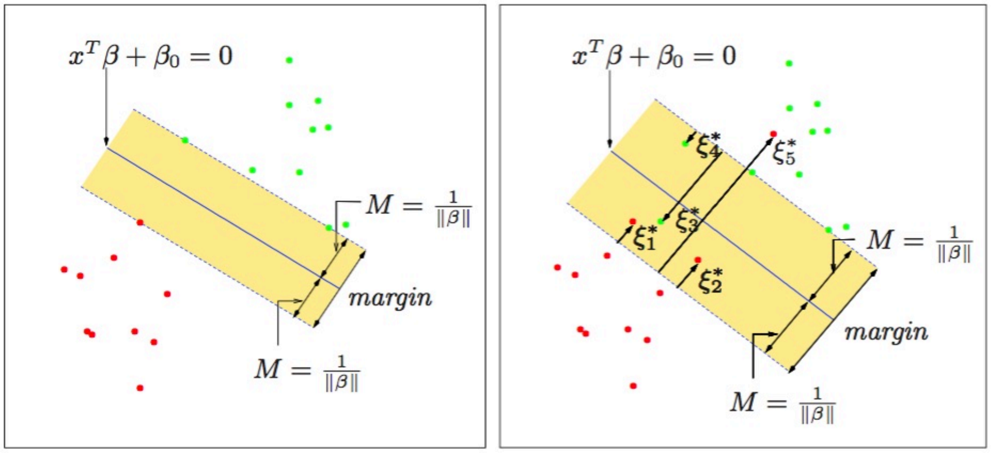


Figure 2: Support vector classifiers. The left panel shows the separable case. The decision boundary is the solid line, while broken lines bound the shaded maximal margin of width $2M = 2/\|\beta\|$. The right panel shows the nonseparable (overlap) case. The points labeled $\xi_j^\star$ are on the wrong side of their margin by an amount $\xi_j^\star = M\xi_j$; points on the correct side have $\xi_j^\star = 0$. The margin is maximized subject to a total budget $\sum \xi_j \leq constant$. Hence $\sum \xi_j^\star$ is the total distance of points on the wrong side of their margin.

Suppose now that the classes overlap in feature space. We now allow for some points to be on the wrong side of the margin. Define the **slack variables** $\xi = (\xi_1, \xi_2, \ldots, \xi_N)$. There is a natural way to modify the constraint in (7):

$$\frac{1}{\|\beta\|} y_i(\beta^\top x_i + \beta_0) \geq M(1 - \xi_i) \qquad \forall i,\ \xi_i \geq 0,\ \sum_{i=1}^{N} \xi_i \leq \text{const.}$$

Misclassifications occur when $\xi_i > 1$. Define $M = 1/\|\beta\|$, we get

$$\begin{aligned} &\min_{\beta, \beta_0} \frac{1}{2}\|\beta\|^2 \\ \text{subject to } & y_i(\beta^\top x_i + \beta_0) \geq 1 - \xi_i \qquad \forall i,\ \xi_i \geq 0,\ \sum_{i=1}^{N} \xi_i \leq \text{const.} \end{aligned}$$

The problem is quadratic with linear inequality constraints, hence is convex optimization problem. For convenience, we re-express it as

$$\min_{\beta, \beta_0} \frac{1}{2}\|\beta\|^2 + C\sum_{i=1}^{N} \xi_i \tag{8}$$

$$\text{subject to } y_i(\beta^\top x_i + \beta_0) \geq 1 - \xi_i \qquad \forall i,\ \xi_i \geq 0$$

We know that

$$\begin{aligned} & y_i(x_i^\top \beta + \beta_0) + \xi_i \geq 1,\ \forall i \\ & \xi_i \geq 0 \\ \iff & (1 - \xi_i - y_i(x_i^\top \beta + \beta_0)) \leq 0,\ \forall i, \\ & -\xi_i \leq 0. \end{aligned}$$

We obtain the **<u>Lagrangian</u>** as

$$L(\beta, \beta_0, \xi, \mu, \alpha) = \frac{1}{2}\|\beta\|^2 + C\sum_{i=1}^{n} \xi_i + \sum_{i=1}^{N} \alpha_i \left[(1 - \xi_i) - y_i(x_i^\top \beta + \beta_0)\right] - \sum_{i=1}^{N} \mu_i \xi_i. \tag{9}$$

$$
\begin{aligned}
\frac{\partial L}{\partial \beta} &= \beta - \sum_{i=1}^{N} \alpha_i y_i x_i = 0 \qquad (10)\\
\frac{\partial L}{\partial \beta_0} &= -\sum_{i=1}^{N} \alpha_i y_i = 0\\
\frac{\partial L}{\partial \xi_i} &= C - \alpha_i - \mu_i = 0\\
&\iff \begin{cases} \alpha_i = C - \mu_i \\ \sum_{i=1}^{N} \alpha_i y_i = 0 \\ \sum_{i=1}^{N} \alpha_i y_i x_i = \beta \end{cases} \qquad (11)
\end{aligned}
$$

and $\alpha_i \geq 0,\ \mu_i \geq 0,\ \xi_i \geq 0\ \forall i$. Plug in (11) into (9) we get the **Lagrange dual function** as $L_D(\mu, \alpha) = \min_{\beta, \beta_0, \xi} L(\beta, \beta_0, \xi, \mu, \alpha)$.

$$
\begin{aligned}
L_D(\mu, \alpha) &= \frac{1}{2} \left\| \sum_{i=1}^{N} \alpha_i y_i x_i \right\|_2^2 + \sum_{i=1}^{N} \alpha_i (1 - y_i (x_i^\top \beta + \beta_0))\\
&= \frac{1}{2} \left\| \sum_{i=1}^{N} \alpha_i y_i x_i \right\|_2^2 + \sum_{i=1}^{N} \alpha_i - \left(\sum_{i=1}^{N} \alpha_i y_i x_i \right)^\top \left(\sum_{i=1}^{N} \alpha_i y_i x_i \right)\\
&= -\frac{1}{2} \left\| \sum_{i=1}^{N} \alpha_i y_i x_i \right\|_2^2 + \sum_{i=1}^{N} \alpha_i\\
&= \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j x_i^\top x_j.
\end{aligned}
$$

We find that $\alpha_i \geq 0,\ \mu_i \geq 0$ and $\alpha_i = C - \mu_i$ implies $0 \leq \alpha_i \leq C$. We therefore maximize

$$
\begin{aligned}
L_D = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j x_i^\top x_j \qquad (12)\\
\text{subject to } 0 \leq \alpha_i \leq C,\ \sum_{i=1}^{N} \alpha_i y_i = 0.
\end{aligned}
$$

Maximizing the dual problem (12) is a simpler convex quadratic programming problem than the primal (8), and can be solved with standard techniques.

Let's check the K.K.T. conditions to gain more insight:

$$Stationarity : \quad \begin{cases} \alpha_i = C - \mu_i \\ \sum_{i=1}^{N} \alpha_i y_i = 0 \\ \sum_{i=1}^{N} \alpha_i y_i x_i = \beta \end{cases} \tag{13}$$

$$\begin{matrix} Complementary \\ slackness \end{matrix} : \quad \begin{cases} \alpha_i(y_i(x_i^\top \beta + \beta_0) - (1 - \xi_i)) = 0 \\ \mu_i \xi_i = 0 \end{cases} \tag{14}$$

$$\begin{matrix} Primal \\ feasibility \end{matrix} : \quad \begin{cases} y_i(x_i^\top \beta + \beta_0) - (1 - \xi_i) \geq 0 \\ \xi_i \geq 0 \end{cases} \tag{15}$$

$$\begin{matrix} Dual \\ feasibility \end{matrix} : \quad \begin{cases} \alpha_i \geq 0 \\ \mu_i \geq 0 \end{cases} \tag{16}$$

From (10) we see that the solution for β has the form

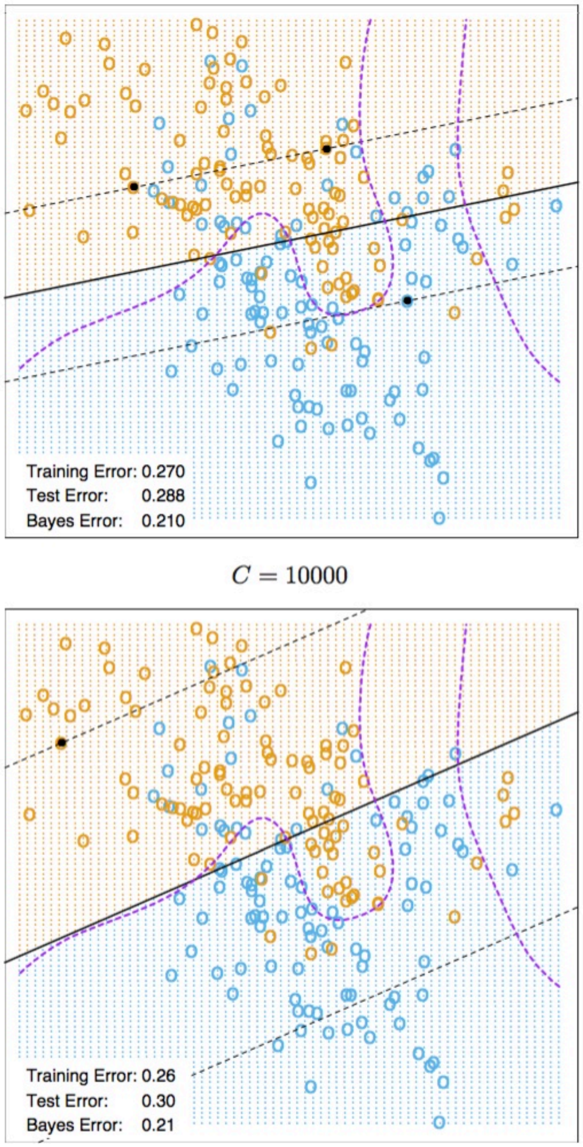
$$\hat{\beta} = \sum_{i=1}^{N} \hat{\alpha}_i y_i x_i = \sum_{i:\alpha_i \neq 0} \alpha_i y_i x_i$$

with nonzero coefficient $\hat{\alpha}_i$ only for those observations i for which the constraints in (15) are exactly met. i.e.

- If $y_i(x_i^\top \beta + \beta_0) - (1 - \xi_i) > 0$ then $\alpha_i = 0$.
- If $\alpha_i \neq 0$, $y_i(x_i^\top \beta + \beta_0) - (1 - \xi_i) = 0$. These observations are called the **support vectors**. We have two scenarios for $\alpha_i \neq 0$, :
  - If $\xi_i = 0$, then x_i lies exactly on the margin and by (13) and (14), we get $\alpha_i \in (0, C]$.
  - If $\xi_i > 0$, then by (14) $\mu_i = 0$, then by (13) $\alpha_i = C$.

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

$$\hat{G}(x) = \text{sgn}(x^\top \hat{\beta} + \hat{\beta}_0).$$



$C = 10000$

Figure 3: The linear support vector boundary for the mixture data example with two overlapping classes, for two different values of C. The broken lines indicate the margins, where $f(x) = \pm 1$. The support points $(\alpha_i > 0)$ are all the points on the wrong side of their margin. The black solid dots are those support points falling exactly on the margin $(\xi_i = 0, \alpha_i > 0)$. In the upper panel 62% of the observations are support points, while in the lower panel 85% are. The broken purple curve in the background is the Bayes decision boundary.

3 Support Vector Machines and Kernels

The **Lagrange dual function** has the form

$$L_D(\alpha) = \sum_{i=1}^N \alpha_i - \frac{1}{2}\sum_{i=1}^N\sum_{j=1}^N \alpha_i\alpha_j y_i y_j \langle x_i, x_j\rangle,$$

and produce the classifier

$$\begin{aligned} &\text{sgn}(x^\top \beta + \beta_0)\\ =&\text{sgn}(\beta_0 + x^\top \sum_i \alpha_i y_i x_i)\\ =&\text{sgn}(\beta_0 + \sum_i \alpha_i y_i \langle x, x_i\rangle). \end{aligned}$$

so the computation and use of the fitted SVM only requires $\langle x_i, x_j\rangle$. The support vector classifier described so far finds linear boundaries in the input feature space. As with other linear methods, we can make the procedure more flexible by enlarging the feature space using basis expansions such as polynomials or splines. Now we can perform similar inner product operation for the transformed feature vectors $h(x_i)$, $h(x_i) = (h_1(x_i), h_2(x_i), \ldots, h_M(x_i))$, $i = 1, \ldots, n$, where each $x_i \in \mathbb{R}^p$ is transformed to $h(x_i) \in \mathbb{R}^M$.

$$L_D(\alpha) = \sum_{i=1}^N \alpha_i - \frac{1}{2}\sum_{i=1}^N\sum_{j=1}^N \alpha_i\alpha_j y_i y_j \langle h(x_i), h(x_j)\rangle,$$

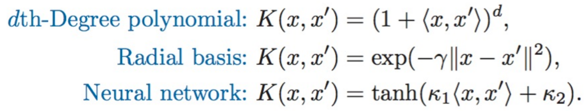
Generally linear boundaries in the enlarged space achieve better training-class separation, and translate to nonlinear boundaries in the original space.

$$\begin{aligned} f(x) =& h(x)^\top \beta + \beta_0\\ =& \sum_{i=1}^n \alpha_i y_i \langle h(x), h(x_i)\rangle + \beta_0. \end{aligned}$$

In fact, we need not specify the transformation $h(x)$ at all, but require only knowledge of the kernel function

$$K(x, x') = \langle h(x), h(x')\rangle$$

that computes inner products in the transformed space. K should be a symmetric positive (semi-) definite function; Three popular choices for K in the SVM literature are



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

Replace $\langle x_i, x_j\rangle$ with $K(x_i, x_j)$. We require $K(x_i,x_j) = \exp(-\gamma\|x_i - x_j\|^2) > 0$. Then SVM dual becomes

$$\begin{aligned}
&\max \sum_{i=1}^{N}\alpha_i - \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{n}\alpha_i\alpha_j y_i y_j K(x_i,x_j) \\
&\text{s.t. } 0 \le \alpha_i \le C \\
&\sum_{i=1}^{N}\alpha_i y_i = 0.
\end{aligned}$$

and the solution can be written as

$$\hat{f}(x) = \sum_{i=1}^{N}\hat{\alpha}_i y_i K(x, x_i) + \hat{\beta}_0.$$

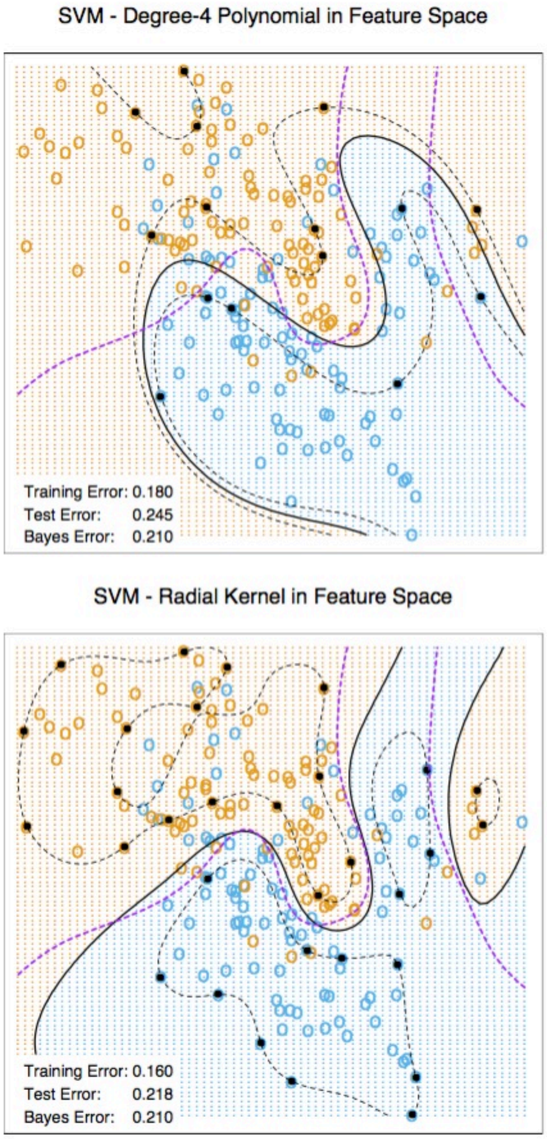
Consider for example a feature space with two inputs X_1 and X_2, and a polynomial kernel of degree 2. Then

$$\begin{aligned}
K(X,X') &= (1+\langle X,X'\rangle)^2 \\
&= (1+X_1X_1'+X_2X_2')^2 \\
&= 1+2X_1X_1'+2X_2X_2'+(X_1X_1')^2+(X_2X_2')^2+2X_1X_1'X_2X_2'.
\end{aligned}$$

Then $M = 6$, and if we chose $h_1(X) = 1$, $h_2(X) = \sqrt{2}X_1$, $h_3(X) = \sqrt{2}X_2$, $h_4(X) = X_1^2$, $h_5(X) = X_2^2$, $h_6(X) = \sqrt{2}X_1X_2$, then $K(X,X') = \langle h(X), h(X')\rangle$.

4 The SVM as A Penalization Method

The SVM with overlapping class distributions is



SVM - Degree-4 Polynomial in Feature Space

SVM - Radial Kernel in Feature Space

Figure 4: Two nonlinear SVMs for the mixture data. The upper plot uses a 4th degree polynomial kernel, the lower a radial basis kernel (with $\gamma = 1$). In each case C was tuned to approximately achieve the best test error performance, and $C = 1$ worked well in both cases. The radial basis kernel performs the best (close to Bayes optimal), as might be expected given the data arise from mixtures of Gaussians. The broken purple curve in the background is the Bayes decision boundary.

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

$$\text{subject to } y_i(\beta^\top x_i + \beta_0) \geq 1 - \xi_i \qquad \forall i,\ \xi_i \geq 0$$

We can also eliminate the linear inequality constraints.

$$\begin{aligned} &\forall i,\ \xi_i \geq 0 \text{ and } \xi_i \geq 1 - y_i(x_i^\top \beta + \beta_0) \\ \iff &\max(1 - y_i(x_i^\top \beta + \beta_0), 0) \leq \xi_i. \end{aligned}$$

Given (β, β_0), $\sum_i \xi_i$ should be minimized, therefore the optimal value $\xi_i^\star$ should have the property that $\xi_i^\star = \max(1 - y_i(x_i^\intercal \beta^\star + \beta_0^\star), 0)$. Then,

$$\begin{aligned} (\beta^\star, \beta_0^\star) &= \arg\min_{(\beta,\beta_0)} \frac{1}{2}\|\beta\|_2^2 + C\sum_i \max(1 - y_i(x_i^\intercal \beta + \beta_0), 0) \\ &= \arg\min_{(\beta,\beta_0)} \sum_{i=1}^{n} \max(1 - y_i(x_i^\intercal \beta + \beta_0), 0) + \lambda\|\beta\|_2^2. \end{aligned}$$

Let $\phi_{\text{hinge}} = \max(1-t, 0) = (1-t)_+$ and $f(x) = x^\top \beta + \beta_0$. The problem becomes

$$\min \sum_{i=1}^{N} \phi_{\text{hinge}}(y_i f(x_i)) + \lambda\|\beta\|_2^2. \tag{17}$$

If the data are separable, then the limit of $\hat{\beta}_\lambda$ in (17) as $\lambda \to 0$ defines the optimal separating hyperplane. Compare it with logistic regression:

$$\min \sum_{i=1}^{N} \phi_{\text{logit}}(y_i f(x_i))^2 + \lambda\|\beta\|_2^2.$$

where $y_i = \pm 1$, and $\phi_{\text{logit}}(t) = \log(1 + \exp(-t))$. This error function is also plotted in Figure 5 and we see that it has a similar form to the support vector error function. The key difference is that the flat region in $\phi_{\text{hinge}}(t) = (1-t)_+$ leads to sparse solutions.

Both the logistic error and the hinge loss can be viewed as continuous approximations to the misclassification error. Another continuous error function that has sometimes been used to solve classification problems

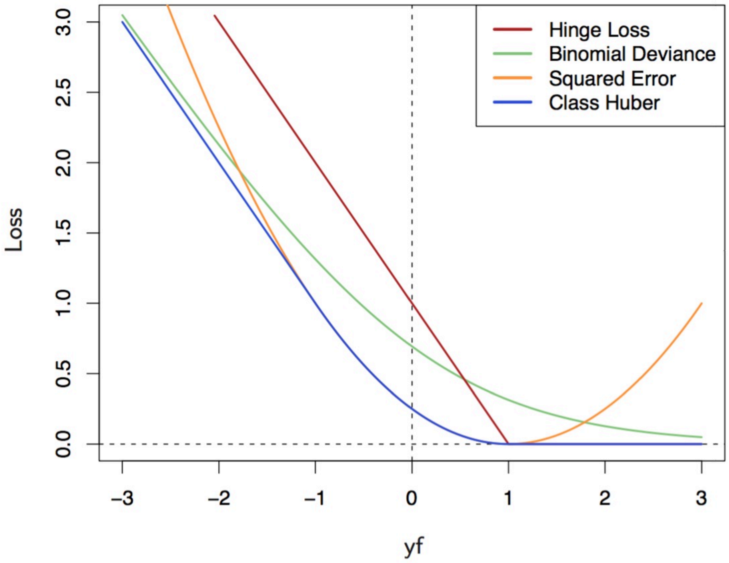


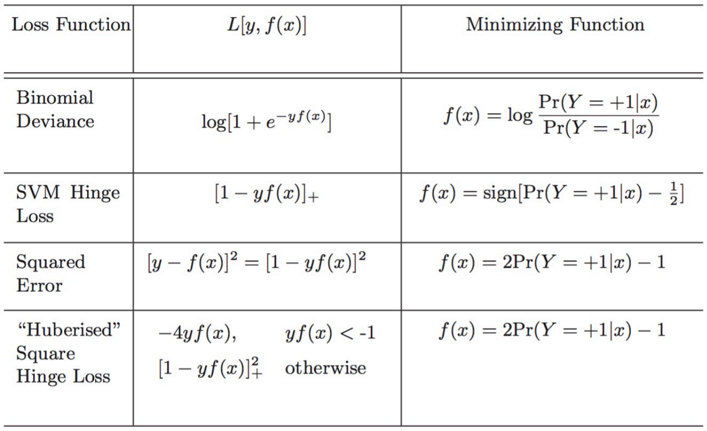
Figure 5: The support vector loss function (hinge loss), compared to the negative log-likelihood loss (binomial deviance) for logistic regression, squared-er- ror loss, and a “Huberized” version of the squared hinge loss. All are shown as a function of yf rather than f, because of the symmetry between the $y = +1$ and $y = -1$ case. The deviance and Huber have the same asymptotes as the SVM loss, but are rounded in the interior. All are scaled to have the limiting left-tail slope of -1.

is the squared error, which is again plotted in Figure 5. It has the property, however, of placing increasing emphasis on data points that are correctly classified but that are a long way from the decision boundary on the correct side. Such points will be strongly weighted at the expense of misclassified points, and so if the objective is to minimize the misclassification rate, then a monotonically decreasing error function would be a better choice.

5 Kernel Regression

Now we extended the model

$$\min \sum_{i=1}^{N} \phi(y_i, f(x_i))^2 + \lambda \|\beta\|_2^2.$$



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	$-4yf(x), \quad yf(x) < \text{-}1$ $[1 - yf(x)]_+^2 \quad \text{otherwise}$	$f(x) = 2\Pr(Y = +1\|x) - 1$

Figure 6: The population minimizers for the different loss functions in Figure 5. Logistic regression uses the binomial log-likelihood or deviance. Linear discriminant analysis uses squared-error loss. The SVM hinge loss estimates the mode of the posterior class probabilities, whereas the others estimate a linear transformation of these probabilities.

to the kernel case. We consider the problem

$$\hat{f}(x) = \arg\min_{f \in \mathbb{H}_K} \sum_{i=1}^{n} \phi(y_i, f(x_i)) + \lambda \|f\|_{\mathbb{H}_K}^2, \tag{18}$$

We express $f(x)$ in a finite-dimensional subspace spanned by kernel functions on observational data, i.e.,

$$f(x) = \sum_{i=1}^{n} \alpha_i K(x_i, x), \tag{19}$$

for some $\{\alpha_i\}_{i=1}^n \subset \mathbb{R}$. By (19) and the reproducing property of RKHS we have

$$\|f\|_{\mathbb{H}_K}^2 = \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j K(\mathbf{x}_i, \mathbf{x}_j). \tag{20}$$

Based on (19) and (20) we can rewrite the minimization problem (18) in a finite-dimensional space

$$\{\hat{\alpha}_i\}_{i=1}^n = \arg\min_{\{\alpha_i\}_{i=1}^n} \sum_{i=1}^{n} \phi\left(y_i, \sum_{j=1}^{n} \alpha_j K(x_i, x_j)\right) + \lambda \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j K(x_i, x_j). \tag{21}$$

The corresponding estimator is $\hat{f}(x) = \sum_{i=1}^n \hat{\alpha}_i K(x_i, x)$.