Support vector machines 1

-Introduction to Data Science-

ISL Chapter 9.1 and 9.2

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Optimal separating hyperplanes

A main initiative in early computer science was to find separating hyperplanes among groups of data

The issue is that if there is a separating hyperplane, there is an infinite number

An optimal separating hyperplane can be generated by finding support points and bisecting them.

(The book calls the optimal separating hyperplane the maximum margin classifier)

Basic linear geometry

A hyperplane in $\mathbb{R}^p$ is given by

$$\mathcal{H} = \{X \in \mathbb{R}^p : f(X) = \beta_0 + \beta^\top X = 0\}$$

1. The vector β is normal to $\mathcal{H}$

   (To see this, let $X, X' \in \mathcal{H}$. Then $\beta^\top (X - X') = 0$)
2. Important: If $||\beta||_2 = 1$, then for any point $X \in \mathbb{R}^p$, the (signed) length of its orthogonal complement to $\mathcal{H}$ is $f(X)$

Support vector machines (SVM)

Let $Y_i \in \{-1, 1\}$

(It is common with SVMs to code Y this way. With logistic regression, Y is commonly phrased as $\{0, 1\}$ due to the connection with Bernoulli trials)

We will generalize this to supervisors with more than 2 levels at the end

A classification rule induced by a hyperplane is

$$g(X) = \mathrm{sgn}(X^\top \beta + \beta_0) = \mathrm{sgn}(f(X))$$

Separating hyperplanes

Our classification rule is based on a hyperplane $\mathcal{H}$

$$g(X) = \operatorname{sgn}(X^\top \beta + \beta_0)$$

A correct (training) classification: $f(X_i)Y_i > 0$ & $g(X_i)Y_i > 0$

The signed distance to $\mathcal{H}$ is $f(X) = X^\top \beta + \beta_0$

Under classical separability, we can find a function f such that $Y_i f(X_i) > 0$

(That is, makes perfect classifications via $g(X) = \operatorname{sgn}(f(X))$)

The larger the quantity $Y_i f(X_i)$, the more separated the classes

Optimal separating hyperplane

This idea can be encoded in the following convex program

$$\max_{\beta_0,\beta} M \text{ subject to}$$

$$Y_i f(X_i) \geq M \text{ for each } i \quad \text{and} \quad ||\beta||_2 = 1$$

Intuition:

- We know that $Y_i f(X_i) > 0 \Rightarrow g(X_i) = Y_i$. Hence, larger $Y_i f(X_i) \Rightarrow$ "more" correct classification
- For "more" to have any meaning, we need to normalize β, thus the other constraint

Optimal separating hyperplane

Taking another look at the optimization problem:

$$\max_{\beta_0,\beta} M \text{ subject to}$$

$$\underbrace{Y_i f(X_i) \geq M \text{ for each } i \quad \text{and} \quad ||\beta||_2 = 1}_{\text{Combine: } \frac{Y_i f(X_i)}{||\beta||_2} \geq M \text{ for each } i}$$

(Note that this is the same as $Y_i f(X_i) \geq M\,||\beta||_2$)

For any $a > 0$, if we form $af(X)$, the constraint still holds:

$$Y_i(a\beta_0 + a\beta^\top X_i) \geq ||a\beta||_2\, M$$

Hence, without any loss of generality, we can set

$$||\beta||_2\, M \overset{\text{set}}{=} 1 \leftrightarrow \left(M = \frac{1}{||\beta||_2} \quad \text{and} \quad Y_i f(X_i) \geq 1 \right)$$

Optimal separating hyperplane

Using these insights, we form the equivalent program

$$\min_{\beta_0,\beta} \frac{1}{2}\,||\beta||_2^2 \text{ subject to}$$

$$Y_i f(X_i) \geq 1 \text{ for each } i$$

(FACTS: $\operatorname{argmin} ||\beta||_2 = \operatorname{argmin} \frac{1}{2}\,||\beta||_2^2$ and $\max M = \min ||\beta||_2$ as $M = \frac{1}{||\beta||_2}$)

Hence, the margin around the hyperplane has width $\frac{1}{||\beta||_2}$

This is still a convex optimization program

(quadratic criterion, linear inequality constraints)

Optimal separating hyperplane

Again, we can convert this constrained optimization problem into a Lagrangian

$$\min_{\beta,\beta_0} \frac{1}{2}||\beta||_2^2 - \sum_{i=1}^{n} \alpha_i [Y_i(X_i^\top \beta + \beta_0) - 1]$$

(It is subtraction as the constraint is $\geq$ while lasso is $\leq$)

In contrast to the lasso problem, there are now n Lagrangian parameters $\alpha_1, \ldots, \alpha_n$

(There are n constraints, after all)

Everything is nice and smooth $\rightarrow$ take derivatives to optimize

Also: A general fact is that at the minimum,

$$\alpha_i [Y_i f(X_i) - 1] = 0 \qquad \text{for all } i = 1, \ldots, n$$

(This comes from the Karush-Kuhn-Tucker conditions for constrained optimization)

Optimal separating hyperplane

$$\frac{1}{2}||\beta||_2^2 - \sum_{i=1}^{n} \alpha_i [Y_i(X_i^\top \beta + \beta_0) - 1]$$

Derivatives with respect to β and β_0 imply that:

- $\beta = \sum_{i=1}^{n} \alpha_i Y_i X_i$
- $0 = \sum_{i=1}^{n} \alpha_i Y_i$

Substituting these equations back into the Lagrangian

$$\max_{\alpha_1, \ldots, \alpha_n} \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{k=1}^{n} \alpha_i \alpha_k Y_i Y_k X_i^\top X_k$$

(this is all subject to $\alpha_i \geq 0$. This is known as the Wolfe dual. Note that this is a maximization problem. There is some optimization theory going on here that I'm skipping known as strong duality and Slatter's condition)

Optimal separating hyperplane

Observe: Two important facts from the preceding slides:

$$\alpha_i[Y_i f(X_i) - 1] = 0 \qquad \text{for all } i = 1, \ldots, n$$

and

$$Y_i f(X_i) \geq 1 \text{ for each } i$$

Therefore,

- $\alpha_i = 0$, which happens if the constraint $Y_i f(X_i) > 1$
  (That is, when the constraint is non binding)
- $\alpha_i > 0$, which happens if the constraint $Y_i f(X_i) = 1$
  (That is, when the constraint is binding)

Optimal separating hyperplane

Taking this relationship

$$\alpha_i[Y_i f(X_i) - 1] = 0$$

and

$$\beta = \sum_{i=1}^{n} \alpha_i Y_i X_i$$

we see that, for $i = 1, \ldots, n$,

- The points (X_i, Y_i) such that $\alpha_i > 0$ are support vectors
- The points (X_i, Y_i) such that $\alpha_i = 0$ are irrelevant

(Compare this idea to logistic regression which uses the exact same form of classifier ($\mathrm{sgn}(f(X))$) but the fitted function always depends on all of the observations)

Support vector classifier

Support vector classifier

Of course, we can't realistically assume that the data are linearly separated (even in a transformed space)

In this case, the previous program has no feasible solution

We need to introduce slack variables, ξ, that allow for overlap among the classes

(ξ is pronounced "k-see" or sometimes "zai")

These slack variables allow for us to encode training misclassifications into the optimization problem

Support vector classifier

$$\min_{\beta_0,\beta,\xi} \frac{1}{2}||\beta||_2^2 \quad \text{subject to}$$

$$Y_i f(X_i) \geq 1 \underbrace{(1-\xi_i), \xi_i \geq 0, \sum \xi_i \leq t}_{new}, \ \text{for each } i$$

(Convex optimization program. Equations 9.12-15 in ISL)

This can be rewritten as

$$\min_{\beta_0,\beta,\xi} \frac{1}{2}||\beta||_2^2 + \lambda \sum \xi_i \quad \text{subject to}$$

$$Y_i f(X_i) \geq 1 - \xi_i, \xi_i \geq 0, \ \text{for each } i$$

Note that

- t or λ are the tuning parameters

  (The literature usually refers to it as a cost parameter)
- The separable case corresponds to $t = 0$ or $\lambda = \infty$

SVMs: slack variables

Once we find $\hat{\beta}(\lambda)$ and $\hat{\beta}_0(\lambda)$ by solving the previous program, we make a classifier via

$$\hat{f}_\lambda(X) = \mathrm{sgn}(\hat{\beta}(\lambda)^\top X + \hat{\beta}_0(\lambda)) = \mathrm{sgn}(\hat{f}(X))$$

The slack variables give us insight into the problem

- If $\xi_i = 0$, then that observation is on correct side of the margin
- If $\xi_i \in (0, 1]$, then that observation is on the incorrect side of the margin, but still correctly classified
- If $\xi_i > 1$, then that observation is incorrectly classified

SVMs: tuning parameter

We can think of t as a budget for the problem

If $t = 0$, then there is no budget and we won't tolerate any margin violations

If $t > 0$, then no more than $\lfloor t \rfloor$ observations can be misclassified

A larger t then leads to larger margins

(we allow more margin violations)

SVMs: tuning parameter

Further intuition:

Like the optimal hyperplane, only observations that violate the margin determine $\mathcal{H}$

A large t allows for many violations, hence many observations factor into the fit

A small t means only a few observations do

Hence, t calibrates a bias/variance trade-off, as expected

In practice, t or λ gets selected via cross-validation

SVMs: tuning parameter

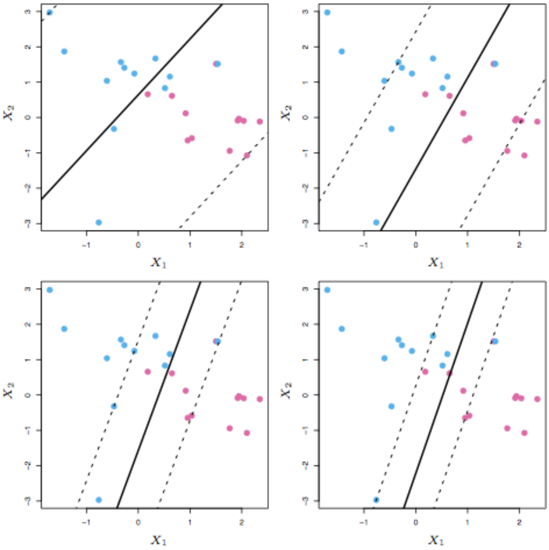


Figure 9.7 in ISL

Support vector classifier in R

A common package to use is e1071

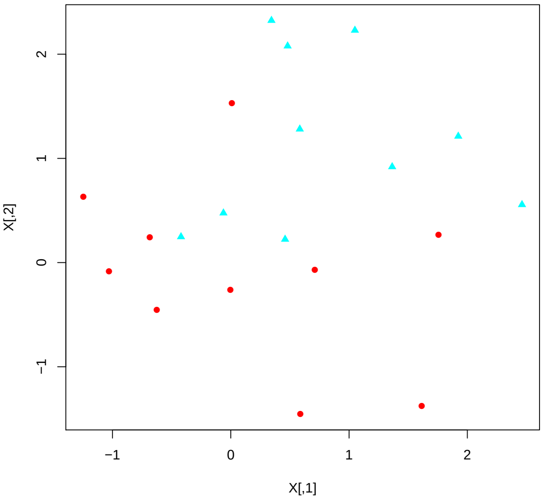
```
X = matrix(rnorm(20*2),ncol=2)
Y = c(rep(-1,10),rep(1,10))
X[Y == 1,] = X[Y == 1,] + 1

col = rep(0,length(Y))
col[Y == -1] = rainbow(2)[1]
col[Y == 1] = rainbow(2)[2]

pch = rep(0,length(Y))
pch[Y == -1] = 16
pch[Y == 1] = 17

plot(X,col=col,pch=pch)
```

Support vector classifier in R



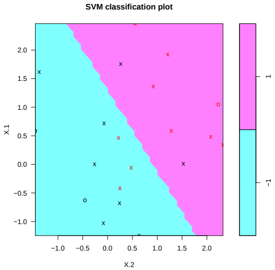
Support vector classifier in R

```
library(e1071)
dat  =data.frame(X=X, Y=as.factor(Y))
svmfit=svm(Y~., data=dat, kernel="linear", cost=cost)
```

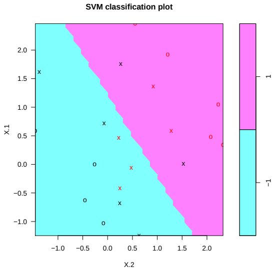
IMPORTANT: Their definition of cost is the Lagrangian version, which we defined as λ

Hence, a small cost means a large t and a wider margin

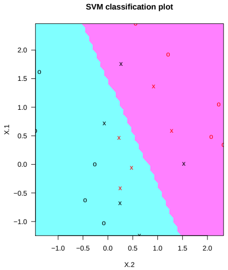
Support vector classifier in R



cost $= .1$



cost $= 1$

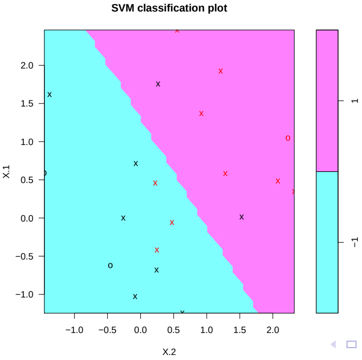


cost $= 10$

Support vector classifier in R

```
tune.out = tune(svm,Y~.,data=dat,kernel="linear",
     ranges=list(cost=c(0.001, 0.01, 0.1, 1,5,10,100)))
best.model = tune.out$best.model
```

Note that best.model is an svm object:



Next time: Kernel methods

Intuition: Many methods have linear decision boundaries

We know that sometimes this isn't sufficient to represent data

Example: Sometimes we need to included a polynomial effect or a log transform in multiple regression

Sometimes, a linear boundary, but in a different space makes all the difference..