Support vector machines and kernelization

-Statistical Learning and Data Mining-

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Optimal separating hyperplane

Reminder: The optimal separating hyperplane is produced by maximizing

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

subject to $\alpha_i \geq 0$

A similar result holds after the introduction of slack variables

(e.g. support vector classifiers. In fact, the only difference is $\alpha_i \leq \lambda$ for each i)

Important: The features only enter via

$$X^\top X' = \langle X, X' \rangle$$

(Kernel) ridge regression

Reminder: Suppose we want to predict at X, then

$$\hat{f}(X) = X^\top \hat{\beta}_{\mathrm{ridge}}(\lambda) = X^\top \mathbb{X}^\top (\mathbb{X}\mathbb{X}^\top + \lambda I)^{-1} Y$$

Also,

$$\mathbb{X}\mathbb{X}^\top = \begin{bmatrix} \langle X_1, X_1 \rangle & \langle X_1, X_2 \rangle & \cdots & \langle X_1, X_n \rangle \\ & \vdots & & \\ \langle X_n, X_1 \rangle & \langle X_n, X_2 \rangle & \cdots & \langle X_n, X_n \rangle \end{bmatrix}$$

and

$$X^\top \mathbb{X}^\top = [\langle X, X_1 \rangle, \langle X, X_2 \rangle, \cdots, \langle X, X_n \rangle]$$

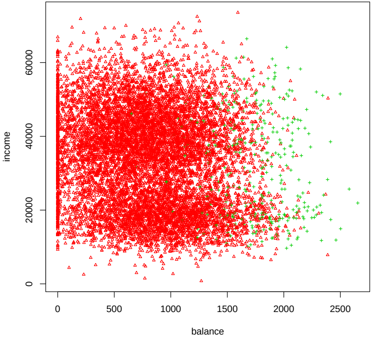
Again, we have the features enter only as

$$\langle X, X' \rangle = X^\top X'$$

Logistic regression: transformations

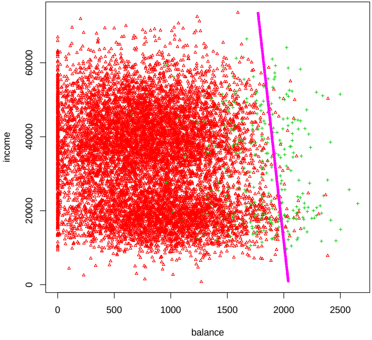
Let's look at the default data in ISL

In particular, we will look at default status as a function of balance and income



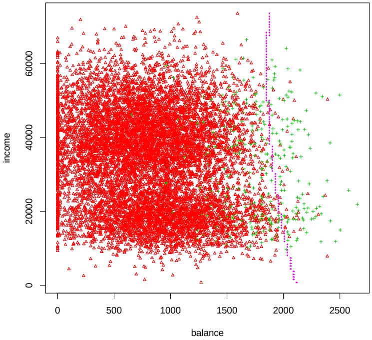
Logistic regression: transformations

```
out.glm  = glm(default~balance + income,family='binomial')
```



Logistic regression: transformations

```
out.glm  = glm(default~balance + income +
                  I(income^2),family='binomial')
```



Conclusion: Linear rules in a transformed space can have nonlinear decisions in original features

Logistic regression: transformations

Reminder: The logistic model: untransformed

$$\begin{aligned}\operatorname{logit}(\mathbb{P}(Y = 1|X)) &= \beta_0 + \beta^\top X \\ &= \beta_0 + \beta_1 \text{balance} + \beta_2 \text{income}\end{aligned}$$

The decision boundary is the hyperplane $\{X : \beta_0 + \beta^\top X = 0\}$

This is linear in the feature space

Logistic regression: transformations

Adding the polynomial transformation:

$$\Phi(X) = (\phi_1(X), \phi_2(X), \phi_3(X)) = (x_1, x_2, x_2^2)$$

$$\begin{aligned} \mathrm{logit}(\mathbb{P}(Y = 1|X)) &= \beta_0 + \beta^\top \Phi(X) \\ &= \beta_0 + \beta_1 \mathrm{balance} + \beta_2 \mathrm{income} + \beta_3 \mathrm{income}^2 \end{aligned}$$

Decision boundary is still a hyperplane $\{X : \beta_0 + \beta^\top \Phi(X) = 0\}$

This is nonlinear in the original x_1, x_2 feature space, but is linear in terms of $\Phi(X)$!

Logistic regression: transformations

Of course, as we include more transformations,

- We need to choose the transformations manually
- Computations can become difficult if we aren't careful
- We need to regularize to prevent overfitting

Can we form them in an automated fashion?

Kernel Methods

Kernel: Example

Back to polynomial terms/interactions $\Phi(X) = (x_1, x_2, x_2^2)$:

What if instead we could form a (kernel) function that produces these polynomial terms automatically?

We can!

$\rightarrow$ Form $k(X, X') = (X^\top X' + 1)^d$

This kernel implicitly forms all polynomials/interactions up to degree d

Kernel: Example

Example: Let $d = p = 2$

$$
\begin{aligned}
k(u, v) &= 1 + 2u_1 v_1 + 2u_2 v_2 + u_1^2 v_1^2 + u_2^2 v_2^2 + 2u_1 u_2 v_1 v_2 \\
&= \sum_{k=1}^{M} \Phi_k(u)\Phi_k(v) \qquad \qquad (M = 6) \\
&= \Phi(u)^\top \Phi(v) \\
&= \langle \Phi(u), \Phi(v) \rangle
\end{aligned}
$$

where

$$
\Phi(v)^\top = [1, \sqrt{2}v_1, \sqrt{2}v_2, v_1^2, v_2^2, \sqrt{2}v_1 v_2]
$$

Important: These equalities are everything that makes kernelization work!

Kernel: Conclusion

Let's recap:

$$\begin{aligned} k(u, v) &= 1 + 2u_1v_1 + 2u_2v_2 + u_1^2v_1^2 + u_2^2v_2^2 + 2u_1u_2v_1v_2 \\ &= \langle \Phi(u), \Phi(v) \rangle = \Phi(u)^\top \Phi(v) \end{aligned}$$

where

$$\Phi(v)^\top = [1, \sqrt{2}v_1, \sqrt{2}v_2, v_1^2, v_2^2, \sqrt{2}v_1v_2]$$

- Some methods only involve features via inner products $X^\top X' = \langle X, X' \rangle$

  (We've explicitly seen two: ridge regression and support vector classifiers)
- If we make transformations of X to $\Phi(X)$, the procedure depends on $\Phi(X)^\top \Phi(X') = \langle \Phi(X), \Phi(X') \rangle$
- Crucial: We can compute this inner product via the kernel:

$$k(X, X') = \langle \Phi(X), \Phi(X') \rangle$$

Kernel: Conclusion

Instead of creating a very high dimensional object via transformations, choose a kernel k

Now, the only thing left to do is form the outer product of kernel evaluations

$$\mathbb{K} = [k(X_i, X_{i'})]_{1 \leq i, i' \leq n}$$

```
X = c(1,2,3)
k = function(x,y){ return(x + y + x*y)}
> outer(X,X,k)
     [,1] [,2] [,3]
[1,]    3    5    7
[2,]    5    8   11
[3,]    7   11   15
```

(Kernel) SVMs

Kernel SVM

Recall:

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

Derivatives with respect to β and β_0 imply:

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

Write the solution function

$$f(X) = \beta_0 + \beta^\top X = \beta_0 + \sum_{i=1}^{n} \alpha_i Y_i X_i^\top X$$

Kernelize the SVC $\Rightarrow$ support vector machine (SVM):

$$f(X) = \beta_0 + \sum_{i=1}^{n} \alpha_i Y_i k(X_i, X)$$

General kernel machines

We can write the eigenvalue expansion of k as

$$k(x,y)=\sum_{j=1}^{\infty}\theta_j\phi_j(x)\phi_j(y)$$

(This is called Mercer's theorem, and such a k is called a Mercer kernel)

Replacing inner products with kernel evaluations is equivalent to performing the unkernelized method in the space given by the eigenfunctions of k with feature map $\Phi=[\phi_1,\ldots,\phi_p,\ldots]$

Polynomial Example:

$$\begin{aligned}k(u,v)&=1+2u_1v_1+2u_2v_2+u_1^2v_1^2+u_2^2v_2^2+2u_1u_2v_1v_2\\&=\sum_{k=1}^{M}\Phi_k(u)\Phi_k(v),\end{aligned}$$

where: $\Phi(v)^\top=[1,\sqrt{2}v_1,\sqrt{2}v_2,v_1^2,v_2^2,\sqrt{2}v_1v_2]$

Kernel SVMs

Hence (and luckily) specifying Φ itself unnecessary,

We need only define the kernel that is symmetric, positive definite

Some common choices for SVMs:

- Polynomial: $k(X, X') = (1 + X^\top X')^d$
- Radial basis: $k(X, X') = e^{-\tau ||X - X'||_b^b}$

(For example, $b = 2$ and $\tau = \sigma^{-2}/2$ is (proportional to) the Gaussian density)

Kernel SVMs: Summary

Reminder: the solution form for SVM is

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

Kernelized, this is

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

Therefore, the induced hyperplane is:

$$\begin{aligned} f(X) = \Phi(X)^\top \beta + \beta_0 &= \sum_{i=1}^{n} \alpha_i Y_i \langle \Phi(X), \Phi(X_i) \rangle + \beta_0 \\ &= \sum_{i=1}^{n} \alpha_i Y_i k(X, X_i) + \beta_0 \end{aligned}$$

The final classification is still $\hat{g}(X) = \mathrm{sgn}(\hat{f}(X))$

SVMs via penalization

SVMs via penalization

Note: SVMs can be derived from penalized loss methods

The support vector classifier optimization problem:

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

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

Consider the alternative optimization problem:

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

These optimization problems are the same!

(With the relation: $2\lambda = 1/\tau$)

SVMs via penalization

The loss part is the hinge loss function

$$\ell(f(X), Y) = [1 - Yf(X)]_+$$

The hinge loss approximates the zero-one loss function underlying classification

It has one major advantage, however: convexity

Surrogate losses

Looking at

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

It is tempting to minimize (analogous to linear regression)

$$\sum_{i=1}^{n} \mathbf{1}(Y_i \neq \hat{g}(X_i)) + \tau \, ||\beta||_2^2$$

However, this is nonconvex

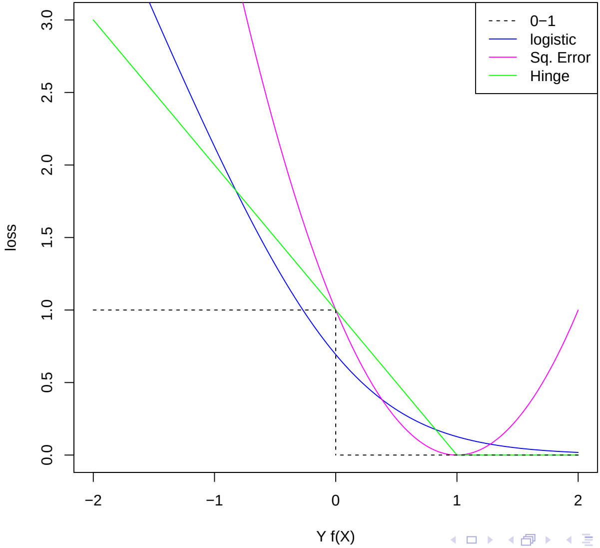
Surrogate losses

Idea: We can use a surrogate loss that mimics this function while still being convex

It turns out we have already done that! (twice times)

- Hinge: $[1 - Yf(X)]_+$
- Logistic: $\log(1 + e^{-Yf(X)})$

Comparing loss functions



SVMs in practice

General functions: The basic SVM functions are in the C++ library libsvm

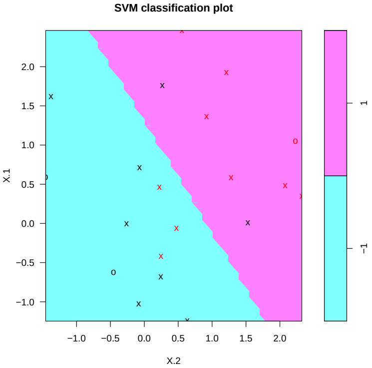
R package: The R package e1071 calls libsvm

Path algorithm: `svmpath`

For a nice comparison of these approaches, see "Support vector machines in R"
(http://www.jstatsoft.org/v15/i09/paper)

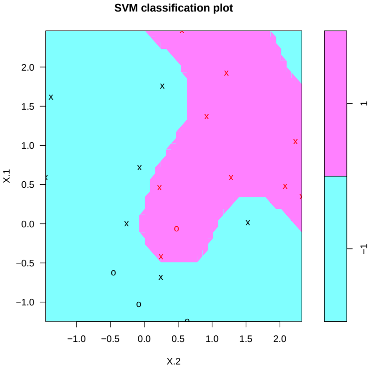
SVM EXAMPLE

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



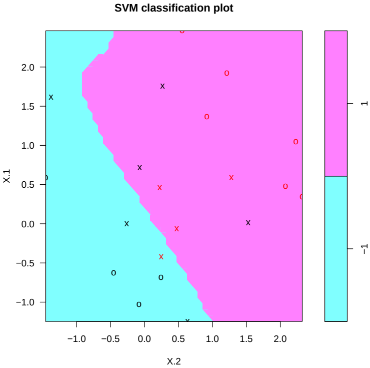
SVM example

```
tune.out = tune(svm,Y~.,data=dat,kernel="radial",
        gamma=c(1,2),
        ranges=list(cost=c(0.001, 0.01, 0.1, 1,5,10,100)))
```

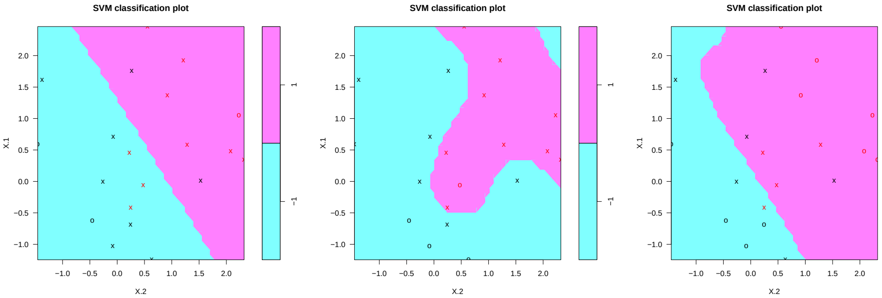


SVM EXAMPLE

```
tune.out = tune(svm,Y~.,data=dat,kernel="polynomial",
        degree=c(3,5,10),
        ranges=list(cost=c(0.001, 0.01, 0.1, 1,5,10,100)))
```



SVM EXAMPLE



SVM classification plot
SVM classification plot
SVM classification plot
X.1
X.2
−1.0 −0.5 0.0 0.5 1.0 1.5 2.0
1
−1

Multiclass SVMs

Multiclass SVMs

Sometimes, it becomes necessary to do multiclass classification

There are two main approaches:

- One-versus-one
- One-vesus-all

Multiclass SVMs: One-versus-one

Here, for G possible classes, we run $G(G-1)/2$ possible pairwise classifications

For a given test point X, we find $\hat{f}_k(X)$ for $k = 1, \ldots, G(G-1)/2$ fits

The result is a vector $\hat{G} \in \mathbb{R}^G$ with the total number of times X was assigned to each class

We report $\hat{f}(X) = \arg\max_g \hat{G}$

This approach leverages all the class information, but can be REALLY slow

(It does have the advantage of only using at any one time the training observations i such that Y_i has either of two classes we are considering)

Multiclass SVMs: One-vesus-all

Here, we fit only G SVMs by respectively collapsing over all size $G - 1$ subsets of $\{1, \ldots, G\}$

Take all $\hat{h}_g(X)$ for $g = 1, \ldots, G$, where class g is coded 1 and "the rest" is coded -1

Assign $\hat{f}(X) = \arg\max_g \hat{h}_g(X)$