Support vector machines and kernelization

-Statistical Machine Learning-

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An overview

Outline of optimization steps

1. Formulate constrained form of problem
2. Convert to (primal) Langragian form
3. Take all relevant (sub)-derivatives and set to zero
4. Substitute these conditions back into primal Langrangian $\longrightarrow$ dual Lagrangian

   (This forms a lower bound on the solution to the constrained primal form of objective)
5. Form Karush-Kuhn-Tucker (KKT) conditions for inequality constraints
6. Examine the conditions for strong duality which implies that the primal and dual forms have the same solution

   (The usual method is via Slater's condition, which says strong duality holds if it is a convex program with non-empty constraint region)

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..

Optimal separating hyperplane

Reminder: The Wolfe dual, which gets maximized over α, produces the optimal separating hyperplane

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

(this is all subject to $\alpha_i \geq 0$)

A similar result holds after the introduction of slack variables

(e.g. support vector classifiers)

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

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

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

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

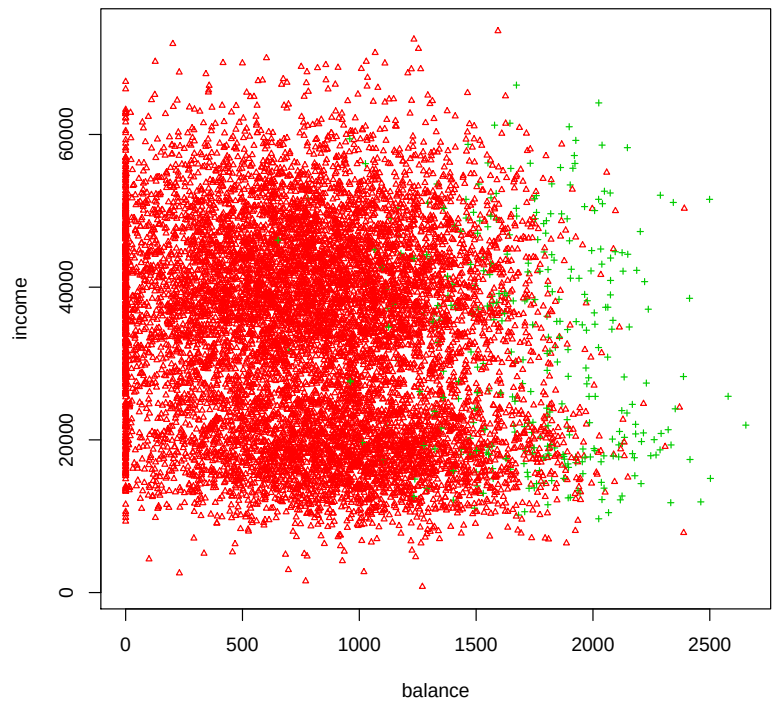
Again, we have the features enter only as

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

Logistic regression: transformations

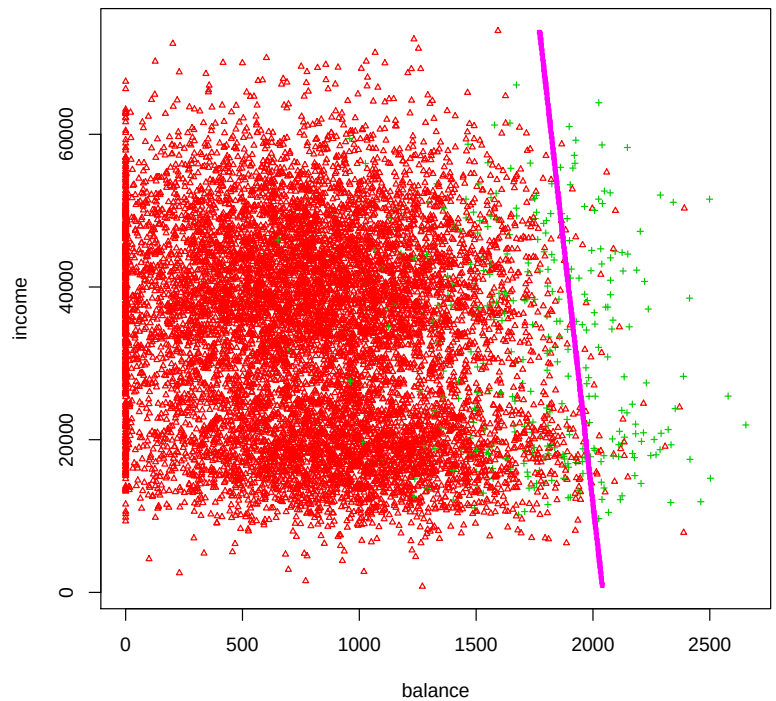
Let's look at the default data in "Introduction to Statistical Learning"

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



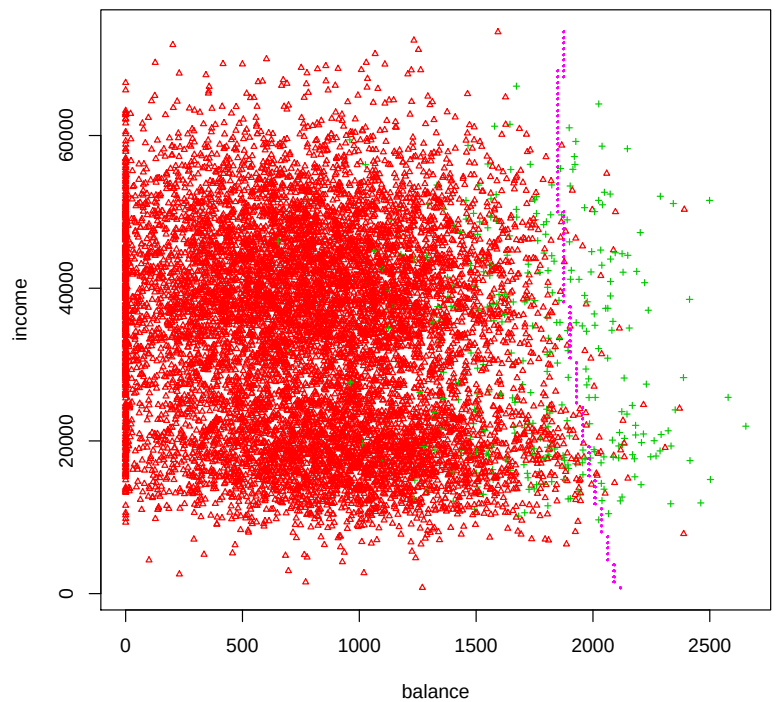
Logistic regression: transformations

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



Logistic regression: transformations

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



Conclusion: A Linear rule in a transformed space can have a nonlinear boundary in the original features

Logistic regression: transformations

Reminder: The logistic model: untransformed

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

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

This is linear in the feature space

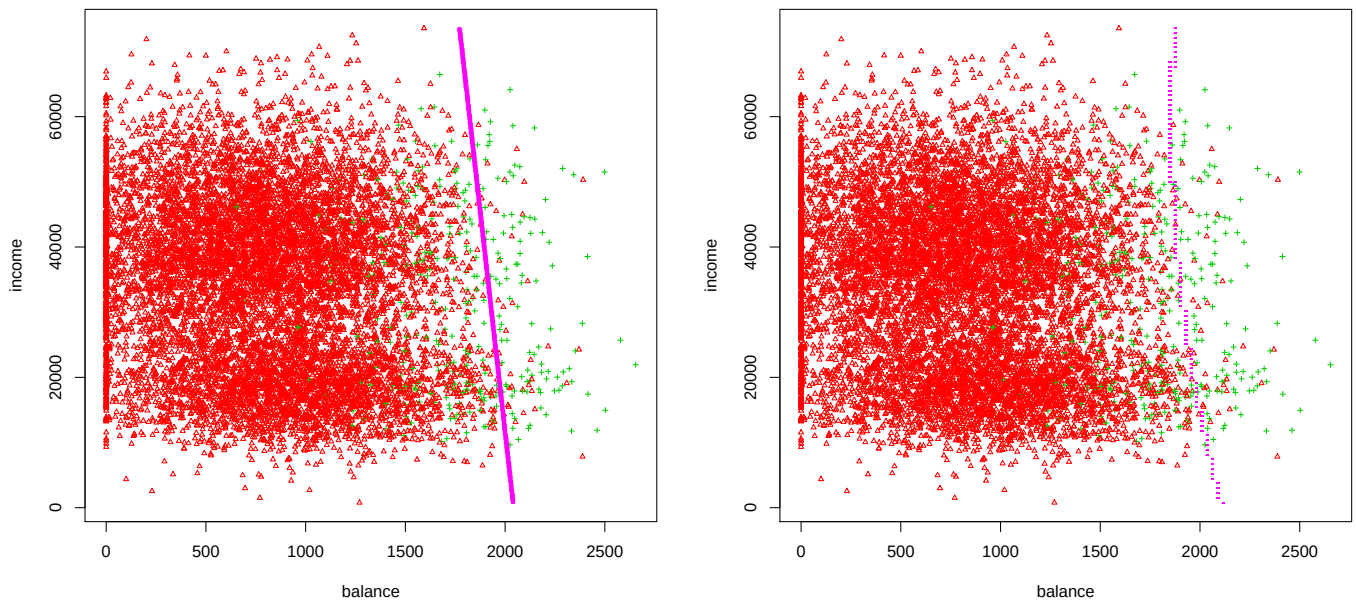
Logistic regression: transformations

Adding the polynomial transformation $\Phi(X) = (X_1, X_2, X_2^2)$:

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

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

This is nonlinear in the feature space!



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 (Example: Solving the least squares problem takes something like np^2 computations)
- We need to regularize to prevent overfitting

Can we form them in an automated fashion?

Kernel Methods

Three related methods

The following are seemingly disparate methods

- Smoothness penalization: Regularizing a loss function with a penalty on smoothness

  (Example: Smoothing splines)
- Feature creation: Imposing a feature mapping $\Phi : \mathbb{R}^p \to \mathcal{A}$ thus creating new features e.g. via polynomials or interactions

  (Example: Regression splines or polynomial regression)
- Gaussian processes: Modeling the regression function as a Gaussian process with a given mean and covariance

  (Example: Gaussian process regression)

It turns out these concepts are all the same and each forms a reproducing kernel Hilbert space (RKHS)

(Many of these ideas are in Wahba (1990). It was introduced to the ML community in Vapnik et al. (1996) and summarized in a nice review paper in Hofmann et al. (2008))

Kernel methods

Suppose $k : \mathcal{A} \times \mathcal{A} \to \mathbb{R}$ is a positive definite kernel

(This means $\int \int k(x, y) f(x) f(y) dx dy > 0$)

To be concrete, think of $\mathcal{A} = \mathbb{R}^p$

(However, any set of objects will do as long as an inner product can be defined)

Let's consider the space of functions generated by the completion of

$$\mathcal{H}_k = \{k(\cdot, y) : y \in \mathbb{R}^p\}$$

(This, loosely speaking, is all functions of the form $f(x) = \sum_{j=1}^{J} \alpha_j k(x, y_j)$)

Nonnegative definite matrices

Let $A \in \mathbb{R}^{p \times p}$ be a symmetric, nonnegative definite matrix:

$$z^\top A z \geq 0 \text{ for all } z \text{ and } A^\top = A$$

Then, A has an eigenvalue expansion

$$A = UDU^\top = \sum_{j=1}^{p} d_j u_j u_j^\top$$

where $d_j \geq 0$

Observation: Each such A, generates a new inner product

$$\langle z, z' \rangle = z^\top z' = z^\top \underbrace{I}_{\text{Identity}} z'$$

$$\langle z, z' \rangle_A = z^\top A z'$$

(If we enforce A to be positive definite, then $\langle z, z \rangle_A = ||z||_A^2$ is a norm)

Nonnegative definite matrices

Suppose A_i^j is the (i, j) entry in A, and A_i is the i^{th} row

$$Az = \begin{bmatrix} A_1^\top \\ \vdots \\ A_p^\top \end{bmatrix} z = \begin{bmatrix} A_1^\top z \\ \vdots \\ A_p^\top z \end{bmatrix}$$

Note: Multiplication by A is really taking inner products with its rows.

Hence, A_i is called the (multiplication) kernel of matrix A

Kernel methods

$k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a symmetric, nonnegative definite kernel

Write the eigenvalue expansion of k as

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

- $\theta_j \geq 0$ (nonnegative definite)
- $\left|\left|(\theta_j)_{j=1}^{\infty}\right|\right|_2^2 = \sum_{j=1}^{\infty} \theta_j^2 < \infty$
- The ϕ_j are orthogonal eigenfunctions: $\int \phi_j \phi_{j'} = \delta_{j,j'}$

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

We can write any $f \in \mathcal{H}_k$ with two constraints

- $f(X) = \sum_{j=1}^{\infty} f_j \phi_j(X)$
- $\langle f, f \rangle_{\mathcal{H}_k} = ||f||_{\mathcal{H}_k}^2 = \sum_{j=1}^{\infty} f_j^2 / \theta_j < \infty$

Kernel methods via regularization

After specifying a kernel function[1] k, we can define an estimator via

$$\min_{f \in \mathcal{H}_k} \hat{\mathbb{P}} \ell_f + \lambda ||f||^2_{\mathcal{H}_k}$$

This is a (potentially) infinite dimensional optimization problem

(hard, especially with a computer)

It can be shown that the solution has the form

$$f(X) = \sum_{i=1}^{n} \beta_i k(X, X_i)$$

(This is known as the representer theorem)

[1] Or crucially and equivalently a set of eigenfunctions and eigenvalues

Kernel methods via regularization

$$f(X) = \sum_{i=1}^{n} \beta_i k(X, X_i)$$

The terms $k(X, X_i)$ are the representers, as

$$\langle k(\cdot, X_i), f \rangle_{\mathcal{H}_k} = f(X_i)$$

and $\mathcal{H}_k$ is called a reproducing kernel Hilbert space (RKHS) as

$$\langle k(\cdot, X_i), k(\cdot, X_{i'}) \rangle_{\mathcal{H}_k} = k(X_i, X_{i'})$$

Kernel methods via regularization

Due to these properties, we can write the optimization problem as

$$\min_{\beta} \hat{\mathbb{P}} \ell_{\mathbb{K}\beta} + \lambda \beta^\top \mathbb{K} \beta$$

where $\mathbb{K} = [k(X_i, X_{i'})]$

This provides a prescription for forming an incredibly rich suite of estimators:

Choose a

- kernel k
- loss function ℓ

and then minimize

Kernel methods via regularization: Example

Suppose that $\ell_{\mathbb{K}\beta}(Z) = (Y - \mathbb{K}\beta)^2$

Then:

$$\hat{\beta} = \underset{\beta}{\text{argmin}}\, \hat{\mathbb{P}}\ell_{\mathbb{K}\beta} + \lambda\beta^\top \mathbb{K}\beta = (\mathbb{K} + \lambda I)^{-1} Y$$

and

$$\hat{f} = \mathbb{K}\hat{\beta} = \mathbb{K}(\mathbb{K} + \lambda I)^{-1} Y = (\lambda \mathbb{K}^{-1} + I)^{-1} Y$$

are the fitted values

(This should be compared with the notes on ridge regression)

Kernel: Example

Back to polynomial terms/interactions:

Form

$$k_d(X, X') = (X^\top X' + 1)^d$$

k_d has $M = \binom{p+d}{d}$ eigenfunctions

These span the space of polynomials in $\mathbb{R}^p$ with degree d

Kernel: Example

Example: Let $d = p = 2 \Rightarrow M = 6$ and

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

where

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

Important: These equalities are everything that makes kernelization work!

Kernel: Conclusion

Let's recap:

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

- 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)# n = 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

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

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

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

General kernel machines

After specifying a kernel function, it can be shown that many procedures have a solution of the form

$$f(X) = \sum_{i=1}^{n} \gamma_i k(X, X_i)$$

For some $\gamma_1, \ldots, \gamma_n$

Also, this is equivalent to performing the method in the space given by the eigenfunctions of k

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

Also, (the) feature map is

$$\Phi = [\phi_1, \ldots, \phi_p, \ldots]$$

Kernel SVMs

Hence (and luckily) specifying Φ itself unnecessary,

(Luckily, as many kernels have difficult to compute eigenfunctions)

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

Some common choices for SVMs:

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

  (For example, $b = 2$ and $\tau = 1/(2\sigma^2)$ 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:

$$h(X) = \Phi(X)^\top \beta + \beta_0 = \sum_{i=1}^{n} \alpha_i Y_i \langle \Phi(X), \Phi(X_i) \rangle + \beta_0$$

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

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

SVMs via penalization

SVMs via penalization

NOTE: SVMs can be derived from penalized loss methods

The support vector classifier optimization problem:

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

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

Consider the alternative program:

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

These optimization problems are the same!

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

SVMs via penalization

The loss part is the hinge loss function

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

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

It has one major advantage, however: convexity

Surrogate losses: convex relaxation

Looking at

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

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 (in $u = h(X)Y$)

A common trick is to approximate the nonconvex objective with a convex one

(This is known as convex relaxation with a surrogate loss function)

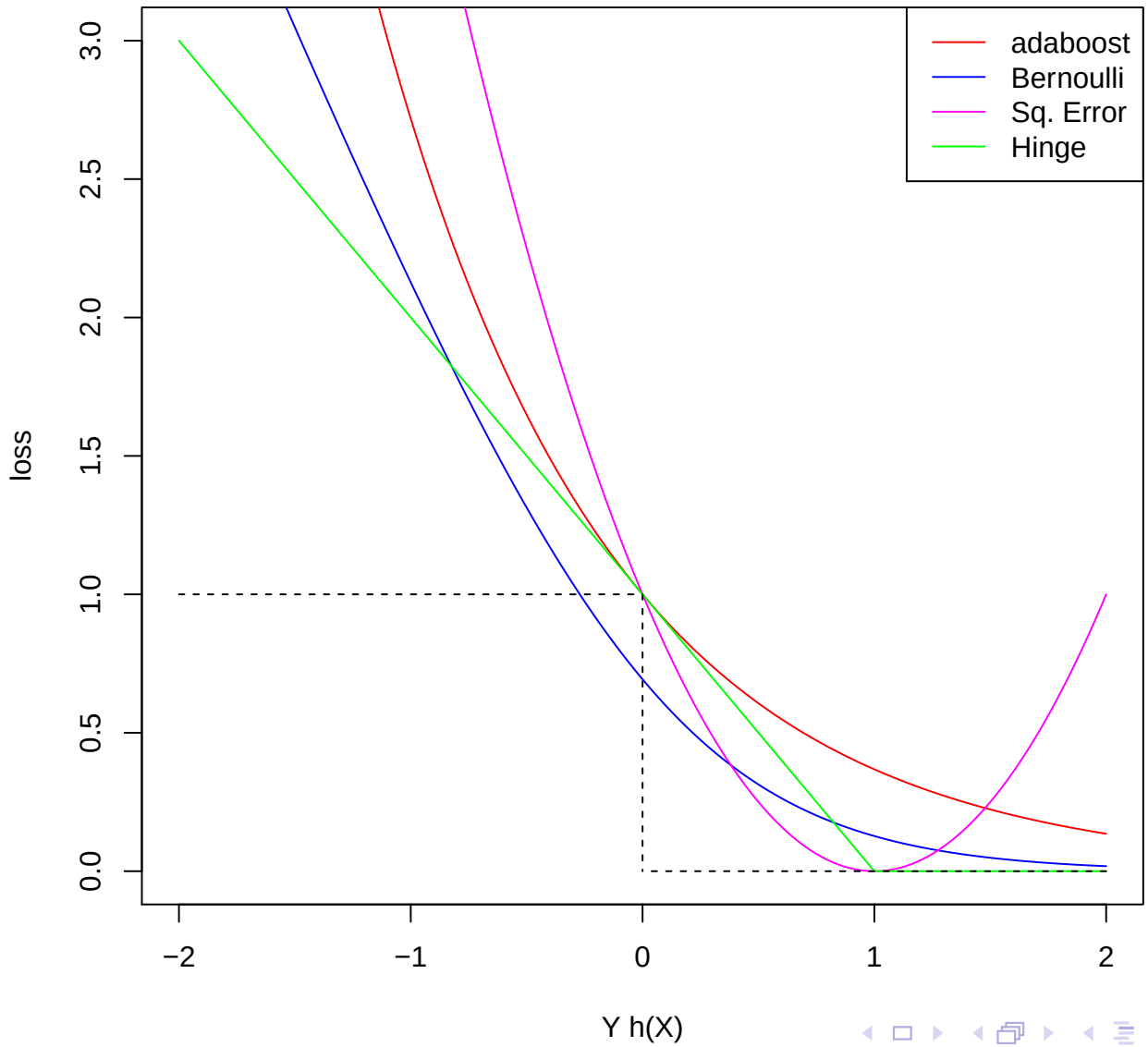
Surrogate losses

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

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

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

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

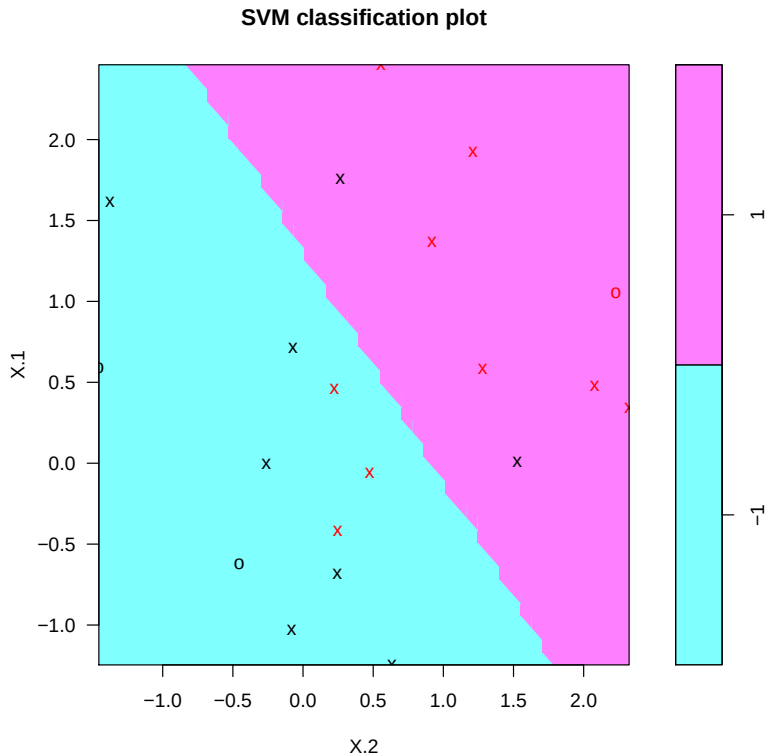
Path algorithm: `svmpath`

For a nice comparison of these approaches, see "Support vector machines in R"

(`http://www.jstatsoft.org/v15/i09/paper`)

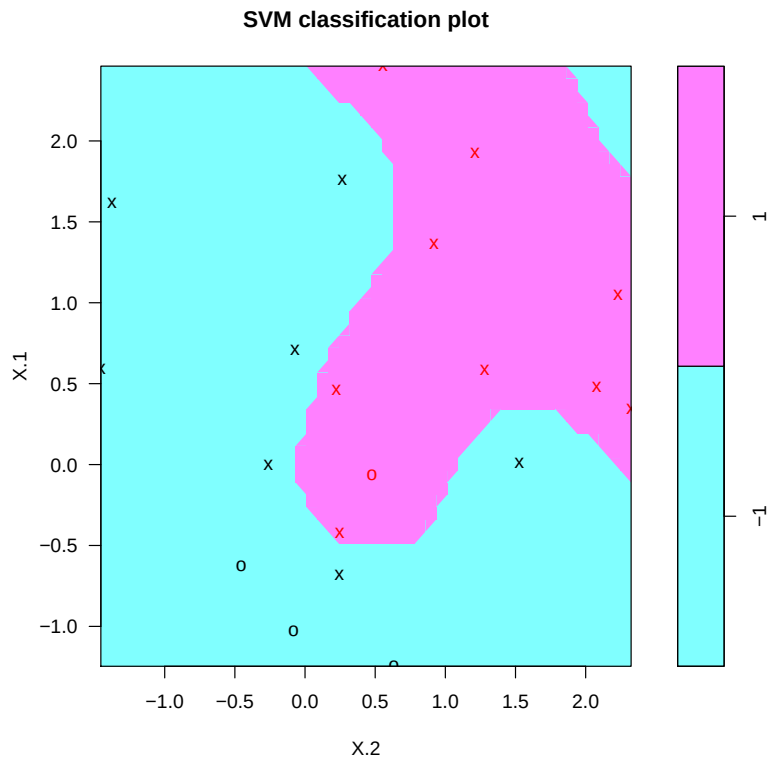
SVM example

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



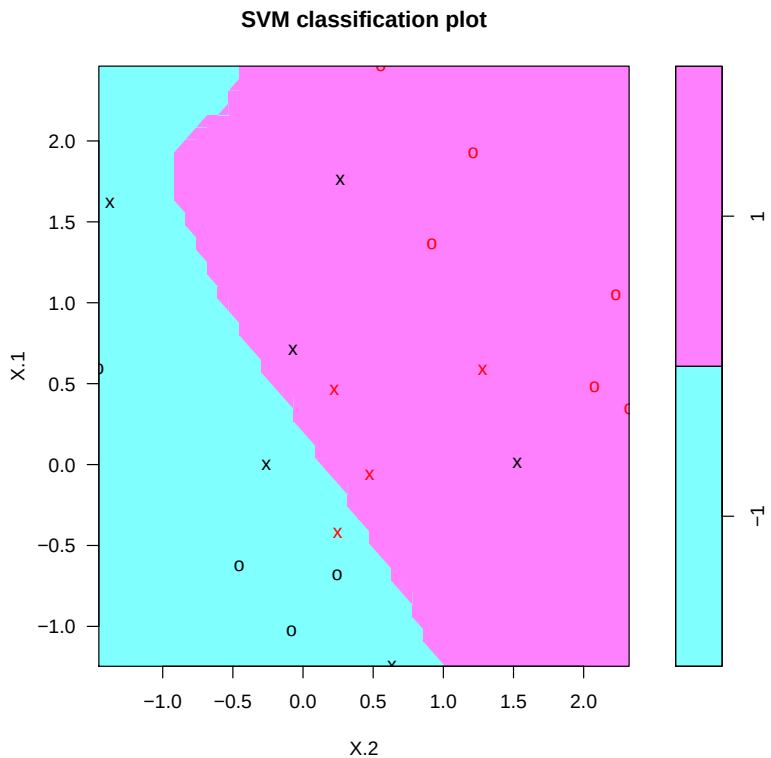
SVM example

```
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)))
```

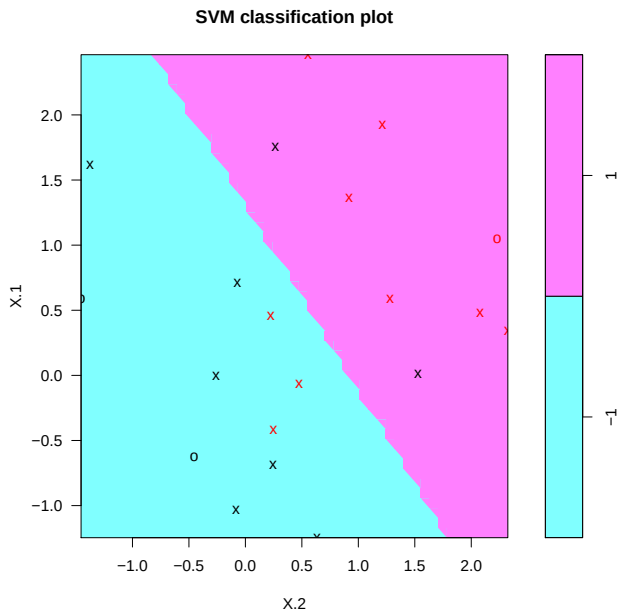


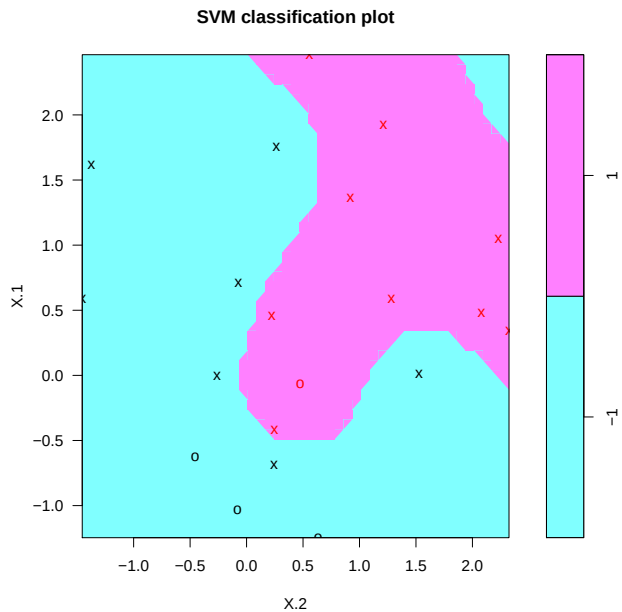
SVM example

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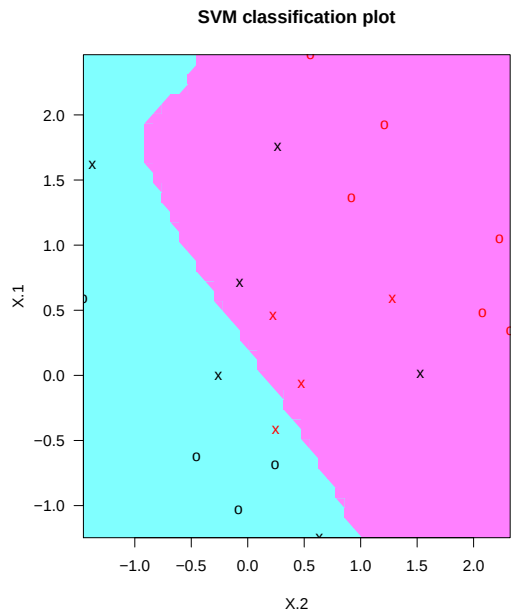
SVM classification plot
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0.5
0.0
−0.5
−1.0
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0

Multiclass classification

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 $\hat{g}_k(X)$ 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 $\hat{g}(X) = \arg\max_g \hat{G}$

This approach uses all the class information, but can be slow

Multiclass SVMs: One-versus-all

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

(This is compared with $G(G-1)/2$ comparisons for one-versus-one)

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

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

(Note that these strategies can be applied to any classifier)