Classification using Generalized Partial Least Squares

Beijing Ding
Robert Gentleman
April 24, 2017

Introduction

The gpls package includes functions for classification using generalized partial least squares approaches. Both two-group and multi-group (more than 2 groups) classifications can be done. The basic functionalities are based on and extended from the Iteratively ReWeighted Least Squares (IRWPLS) by Marx (1996). Additionally, Firth’s bias reduction procedure (Firth, 1992a,b, 1993) is incorporated to remedy the nonconvergence problem frequently encountered in logistic regression. For more detailed description of classification using generalized partial least squares, refer to Ding and Gentleman (2005).

The glpls1a function

The glpls1a function carries out two-group classification via IRWPLS(F). Whether or not to use Firth’s bias reduction is an option (br=T). The X matrix shouldn’t include an intercept term.

```r
> library(gpls)
> set.seed(123)
> x <- matrix(rnorm(20),ncol=2)
> y <- sample(0:1,10,TRUE)
> ## no bias reduction
> glpls1a(x,y,br=FALSE)

Call:
NULL

Coefficients:
Intercept  X:1  X:2
-2.3122  -0.5069  -0.4529

> ## no bias reduction and 1 PLS component
> glpls1a(x,y,K.prov=1,br=FALSE)
```
Call:
NULL

Coefficients:
Intercept X:1 X:2
-2.2916 -0.3650 -0.5377

> ## bias reduction
> glpls1a(x,y,br=TRUE)

Call:
NULL

Coefficients:
Intercept X:1 X:2
-1.4319 -0.1549 -0.2760

K.prov specifies the number PLS components to use. Note that when K.prov is no specified, the number of PLS components are set to be the smaller of the row and column rank of the design matrix.

The glpls1a.cv.error and glpls1a.train.test.error functions

The glpls1a.cv.error calculates leave-one-out classification error rate for two-group classification and glpls1a.train.test.error calculates test set error where the model is fit using the training set.

> ## training set
> x <- matrix(rnorm(20),ncol=2)
> y <- sample(0:1,10,TRUE)
> ## test set
> x1 <- matrix(rnorm(10),ncol=2)
> y1 <- sample(0:1,5,TRUE)
> ## no bias reduction
> glpls1a.cv.error(x,y,br=FALSE)

$error
[1] 0.6

$error.obs
[1] 1 2 4 7 9 10

> glpls1a.train.test.error(x,y,x1,y1,br=FALSE)
The glpls1a.mlogit and glpls1a.logit.all functions

The glpls1a.mlogit carries out multi-group classification using MIRWPLS(F) where the baseline logit model is used as counterpart to glpls1a for two group case. glpls1a.logit.all carries out multi-group classification by separately fitting $C$ two-group classification using glpls1a separately
for $C$ group vs the same baseline class (i.e. altogether $C + 1$ classes). This separate fitting of logit is known to be less efficient but has been used in practice due to its more straightforward implementation.

Note that when using `glplsl1a.mlogit`, the X matrix needs to have a column of one, i.e. intercept term.

```r
> x <- matrix(rnorm(20), ncol=2)
> y <- sample(1:3, 10, TRUE)
> ## no bias reduction and 1 PLS component
> glplsl1a.mlogit(cbind(rep(1,10), x), y, K.prov=1, br=FALSE)

$coefficients

   [,1]     [,2]
[1,] -0.7689747 -0.0370627
[2,]  2.1926005 -4.2015007
[3,]  0.5442713 -0.9331431

$convergence
[1] FALSE

$niter
[1] 100

$bias.reduction
[1] FALSE

> glplsl1a.logit.all(x, y, K.prov=1, br=FALSE)

$coefficients

   [,1]     [,2]
[1,] -2.339152  1.029019
[2,]  2.906929 -9.000959
[3,]  0.579930 -1.387408

> ## bias reduction
> glplsl1a.mlogit(cbind(rep(1,10), x), y, br=TRUE)

$coefficients

   [,1]     [,2]
[1,]  1.0327659  0.41635681
[2,]  1.2298647 -2.58869374
[3,]  0.4357512 -0.08656436

$convergence
[1] TRUE
```
$niter
[1] 36

$bias.reduction
[1] TRUE

> glpls1a.logit.all(x,y,br=TRUE)

$coefficients
[,1]     [,2]
[1,] -1.1433739 0.5402162
[2,]  1.3337074 -2.9934497
[3,]  0.5325446 -0.2234683

> The glpls1a.mlogit.cv.error function

The glpls1a.mlogit.cv.error calculates leave-one-out error for multi-group classification using (M)IRWPLS(F). When the mlogit option is set to be true, then glpls1a.mlogit is used, else glpls1a.logit.all is used for fitting.

> x <- matrix(rnorm(20),ncol=2)
> y <- sample(1:3,10,TRUE)
> ## no bias reduction
> glpls1a.mlogit.cv.error(x,y,br=FALSE)

$error
[1] 0.6

$error.obs
[1] 3 4 5 7 9 10

> glpls1a.mlogit.cv.error(x,y,mlogit=FALSE,br=FALSE)

$error
[1] 0.5

$error.obs
[1] 3 4 5 7 10

> ## bias reduction
> glpls1a.mlogit.cv.error(x,y,br=TRUE)

$error
[1] 0.6
> glpls1a.mlogit.cv.error(x,y,mlogit=FALSE,br=TRUE)

$\text{error.obs}$
[1] 3 4 5 7 9 10

> glpls1a.mlogit.cv.error(x,y,mlogit=FALSE,br=TRUE)

$\text{error}$
[1] 0.5

$\text{error.obs}$
[1] 3 4 5 7 10

> 0.1 Fitting Models to data

Here we demonstrate the use of gpls on some standard machine learning examples. We first make use of the Pima Indian data from the MASS package.

> library(MASS)
> m1 = glpls(type~., Pima.tr)
> p1 = predict(m1, Pima.te[-8])
> ##when we get to the multi-response problems
> data(iris3)
> Iris <- data.frame(rbind(iris3[,1], iris3[,2], iris3[,3]),
+ Sp = rep(c("s","c","v"), rep(50,3)))
> train <- sample(1:150, 75)
> table(Iris$Sp[train])

       c  s  v 23 27 25

> ## your answer may differ
> ## c  s  v
> ## 22 23 30
> z <- lda(Sp ~ ., Iris, prior = c(1,1,1)/3, subset = train)
> predict(z, Iris[-train,])$class

[1] s s s s s s s s s s s s s s s c c c c c c c c c c c c c c c c c c c c c
[39] c c c c c c c c c c c c c c c c c v v v v v v v v v v v v v c v v v v v v c c c v v v v v v v v
Levels: c s v

> References


