9: Discrimination and Classification

John H Maindonald

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Ideas and issues illustrated by the graphs in this vignette

The methods illustrated here have the character of regression models where the outcome is categorical, one of g classes. For example, the `fgl` dataset has measurements of each on nine physical properties, for 214 samples of glass that are classified into six different glass types.

Note: The versions of Figures 9.9 and 9.10 that are shown in Section 2 are for a substantially reduced number of points, relative to the text *Statistically Informed Data Mining.*

```
# To include the figures, change `showFigs <- FALSE`
# to `showFigs <- TRUE` in the source `.Rnw` file,
# and regenerate the PDF.
#
showFigs <- FALSE
```

1 Code for the Figures

```
fig9.1 <- function(plotit=TRUE){
    fgl.lda <- lda(type ~ ., data=fgl)
    scores <- predict(fgl.lda)$x
    library(lattice)
    gph <- xyplot(scores[,2] ~ scores[,1], groups=fgl$type,
                  xlab="Discriminant 1", ylab="Discriminant 2",
                  aspect=1, scales=list(tck=0.4),
                  auto.key=list(columns=3),
                  par.settings=simpleTheme(alpha=0.6, pch=1:6))
    gph
}
```

```r
fig9.2 <- function(){
    gph <- xyplot(length ~ breadth, groups=species, data=cuckoos,
                  type=c("p"), auto.key=list(space="right"), aspect=1,
                  scales=list(tck=0.5), par.settings=simpleTheme(pch=16))
    LDmat <- cuckoos.lda$scaling
    ld1 <- LDmat[,1]
    ld2 <- LDmat[,2]
    gm <- sapply(cuckoos[, c("length", "breadth")], mean)
    av1 <- gm[1] + ld1[2]/ld1[1]*gm[2]
    av2 <- gm[1] + ld2[2]/ld2[1]*gm[2]
    assign('av1', av1, pos=1)
    assign('av2', av2, pos=1)
    assign('ld1', ld1, pos=1)
    assign('ld2', ld2, pos=1)
    addlayer <- latticeExtra::layer(panel.abline(av1, -ld1[2]/ld1[1], lty=1),
                                    panel.abline(av2, -ld2[2]/ld2[1], lty=2))
    gph + addlayer
}
```

```r
fig9.3 <- function(){
    ## This will show decision boundaries
    gph <- xyplot(length ~ breadth, groups=species, data=cuckoos,
                  type=c("p"), auto.key=list(space="right"), aspect=1,
                  scales=list(tck=0.5), par.settings=simpleTheme(pch=16))
    x <- pretty(cuckoos$breadth, 20)
    y <- pretty(cuckoos$length, 20)
    Xcon <- expand.grid(breadth=x, length=y)
    cucklda.pr <- predict(cuckoos.lda, Xcon)$posterior
    cuckqda.pr <- predict(cuckoos.qda, Xcon)$posterior
    m <- match("wren", colnames(cucklda.pr))
    ldadiff <- apply(cucklda.pr, 1, function(x)x[m]-max(x[-m]))
    qdadiff <- apply(cuckqda.pr, 1, function(x)x[m]-max(x[-m]))
    addlayer1 <- latticeExtra::as.layer(contourplot(ldadiff ~ breadth*length,
                                      at=c(-1,0,1), labels=c("", "lda",""),
                                      label.style="flat",
                                      data=Xcon), axes=FALSE)
    addlayer2 <- latticeExtra::as.layer(contourplot(qdadiff ~ breadth*length,
                                     at=c(-1,0,1), labels=c("", "qda",""),
                                     label.style="flat",
                                     data=Xcon), axes=FALSE)
    gph + addlayer1 + addlayer2
}
```

```
fig9.4 <- function(seed=47){
  opar <- par(xpd=TRUE)
  ## xpd=TRUE allows labels to extend outside of figure region
    b.rpart <- rpart(rfac ~ cig+poll, data=bronchitis)
    plot(b.rpart, uniform=TRUE)
    text(b.rpart)
  par(opar)
}
```

```
fig9.5 <- function(){
    b001.rpart <- rpart(rfac ~ cig+poll, cp=0.001, minsplit=15,
                    data=bronchitis)
    plotcp(b001.rpart)
}
```

```
fig9.6 <-
function () {
plot.root <- function(text='Reduction in "error" (Gini) = 20.55',
                      cutoff="cig<4.375", left="138/11", rt="28/35",
                      xlef=0.15, xrt=0.85,
                      treetop=0.85, treebot=0.1){
    par(mar=rep(0,4))
    plot(0:1, 0:1, axes=F, xlab="",ylab="", type="n")
    lines(c(xlef,xlef, xrt,xrt), c(.1,treetop,treetop,.1))
    lines(c(.5,.5),c(-0.01,0.01)+treetop)
    chh <- strheight("O")
    text(.5, treetop+chh, cutoff)
    text(c(xlef,xrt), rep(.1-chh,2), c(left,rt))
    legend(x=0.5, y=1, xjust=0.5, yjust=1, xpd=TRUE,
       legend=text, bg='gray')
}
    par(fig=c(0,0.5,0,1))
    plot.root(text='Decrease in "error" = 20.55',
              cutoff="cig<4.375", left="138/11", rt="28/35",
              treetop=0.6, treebot=0.1)
    par(fig=c(0.5,1,0,1), new=TRUE)
    plot.root(text='Decrease in "error" = 2.90',
              cutoff="poll<58.55", left="98/16", rt="68/30",
              treetop=0.6, treebot=0.1)
}
```

```
fig9.7 <-
function ()
{
    set.seed(31)   # Reproduce the trees shown
    opar <- par(mfrow=c(3,3), xpd=TRUE)
    num <- 1:nrow(bronchitis)
    for(i in 1:9){
        useobs <- sample(num, replace=TRUE)
        dset <- bronchitis[useobs, ]
        b.rpart <- rpart(rfac ~ cig+poll, data=dset,
                         control=rpart.control(maxdepth=2))
        plot(b.rpart, uniform=TRUE)
        text(b.rpart, xpd=TRUE, cex=1.2)
    }
    par(mfrow=c(1,1))
    par(opar)
}
```

```
fig9.8 <- function(){
    bronchitis <-
      within(bronchitis,
             rfac <- factor(r, labels=c("abs","pres")))
    parset <- simpleTheme(pch=1:2)
    bronchitis.rf <- randomForest(rfac ~ cig+poll, proximity=TRUE,
                                  data=bronchitis)
    points <- cmdscale(1-bronchitis.rf$proximity)
    gph <- xyplot(points[,2] ~ points[,1], groups=bronchitis$rfac,
                  xlab="Axis 1", ylab="Axis 2",
                  par.settings=parset, aspect=1,
                  auto.key=list(columns=2))
    gph
    }
```

```
fig9.9 <- function(nn0 = c(3596, 900, 600, 400, 270, 180, 120, 90, 60, 40),
                   repeats=5, seed=NULL, testlong=NULL, plotit=TRUE){
if(!is.null(seed))set.seed(seed)
if(is.null(testlong)){
## ---- vary-noninsure ----
testInsure <- matrix(0, ncol=repeats, nrow=length(nn0))
for(i in 1:repeats){
  j<-0
  for(n0 in nn0){
    j<-j+1
    testInsure[j, i] <- bestsize(n0)
  }
}
attr(testInsure, "dimnames") <- list(n0=nn0, Repeat=1:repeats)
## Long version of data frame
testlong <- data.frame(test=as.vector(testInsure),
                       n0=rep(nn0, repeats),
                       gp=rep(1:repeats, rep(length(nn0),repeats)))
}
if(!plotit)return(invisible(testlong))
## Plot data
nn0 <- unique(testlong[,"n0"])
ndistinct <- length(nn0)
if(ndistinct >= 4){
test.gam <- gam(test ~ s(log(n0), k=min(ndistinct,3)), data=testlong)
plot(test.gam, se=T, residuals=T, pch=1, xaxt="n",
     xlab="n0, in 'sampsize=c(n0, 226)'",
     ylab="# insurances, best 400 test",
     shift=mean(fitted(test.gam)))
axis(1, at=log(nn0), labels=paste(nn0), las=3)
} else
{
    plot(test ~ log(n0), data=testlong, pch=1, xaxt="n",
    xlab="n0, in 'sampsize=c(n0, 226)'",
    ylab="# insurances, best 400 test")
    mtext(side=3, line=0.5, expression(
          "Curve is fitted only if there are " >= " 4 distinct values of n0"))
}
invisible(testlong)
}
```

```
fig9.10 <- function(nn0 = c(3596, 900, 600, 400, 270, 180, 120, 90, 60, 40),
                    repeats=5, seed=NULL, heldlong=NULL, plotit=TRUE){
if(!is.null(seed))set.seed(seed)
if(is.null(heldlong)){
## ---- vary-held ----
heldInsure <- matrix(0, ncol=repeats, nrow=length(nn0))
for(i in 1:repeats){
  j<-0
  for(n0 in nn0){
    j<-j+1
    heldInsure[j, i] <- bestsize(n0, nselect=800,
                                 x=ticShown[, -c(1,86)],
                                 y=ticShown[, 86],
                                  xtest=ticHeld[, -c(1,86)],
                                  ytest=ticHeld[, 86])
  }
}
attr(heldInsure, "dimnames") <- list(n0=nn0, Repeat=1:repeats)
## ---- plot-held ----
heldlong <- data.frame(insure=as.vector(heldInsure),
                       n0=rep(nn0, repeats),
                       gp=rep(1:repeats, rep(length(nn0),repeats)))
}
if(!plotit)return(invisible(heldlong))
## Plot data
nn0 <- unique(heldlong[,"n0"])
ndistinct <- length(nn0)
if(ndistinct>=4){
held.gam <- gam(insure ~ s(log(n0), k=min(ndistinct-1,3)), data=heldlong)
plot(held.gam, se=T, residuals=T, pch=1, xaxt="n",
     xlab="n0, in 'sampsize=c(n0, 348)'",
     ylab="# insurances, best 800 prospects",
     shift=mean(fitted(held.gam)))
} else
{
    plot(insure ~ log(n0), data=heldlong, pch=1, xaxt="n",
    xlab="n0, in 'sampsize=c(n0, 226)'",
    ylab="# insurances, best 400 test")
    mtext(side=3, line=0.5, expression(
          "Curve is fitted only if there are " >= " 4 distinct values of n0"))
}
axis(1, at=log(nn0), labels=paste(nn0), las=3)
invisible(heldlong)
}
```

```
compareTargets <-
function(rfobj, prior1, prior2){
    nam1 <- deparse(substitute(prior1))
    nam2 <- deparse(substitute(prior2))
    print(c(nam1,nam2))
    err <- rfobj$confusion[,3]
    err1 <- sum(err*prior1)/sum(prior1)
    err2 <- sum(err*prior2)/sum(prior2)
    errvec <- c(err, err1,err2)
    names(errvec) <- c("error-good", "error-bad", nam1, nam2)
    errvec
  }
```

```r
bestsize <- function(n0=226, mtry=9, nselect=400,
                     x=tictrain[, -c(1,86)], y=tictrain[, 86],
                     xtest=tictest[, -c(1,86)], ytest=tictest[, 86])
{
  tic.rf <- randomForest(x=x, y=y,
                         xtest=xtest, ytest=ytest,
                         sampsize=c(n0,226),
                         mtry=mtry, data=data)
  nrbest <- order(tic.rf$test$votes[,2],
                  decreasing=TRUE)[1:nselect]
  buy <- sum(ytest[nrbest]=="insurance")
  buy
}
```

```r
ldaErr <- function(train.lda=spam01.lda, train=spam01, test=spam2,
                   traingp=spam01[,'type'], testgp=spam2[,'type']){
    trainCV.lda <- update(train.lda, CV=TRUE)
    prior01 <- train.lda$prior
    ldaRates <- c(loo=1-confusion(traingp,
                           trainCV.lda$class,
                           printit=NULL)$overall,
              trainerr=1-confusion(traingp,
                                   predict(train.lda)$class,
                                   printit=NULL)$overall,
              testerr=1-confusion(testgp,
                                  predict(train.lda,
                                          newdata=test)$class,
                                  prior=prior01, printit=NULL)$overall)
     ldaRates
}
```

```r
rpartErr <- function(train.rp=spam01.rp, train=spam01, test=spam2,
                     outcome='type'){
    cptab <- train.rp$cptable
    nbest <- which.min(cptab[,"xerror"])
    rnprop <- prop.table(table(train.rp$y))
    xcv <- cptab[nbest,"xerror"] * min(rnprop)
    trainerr <- cptab[nbest,"rel error"] * min(rnprop)
    class2 <- predict(train.rp, newdata=test, type="class")
    testerr <- 1-confusion(test[, outcome], class2, printit=FALSE,
                         prior=rnprop)$overall
    c(cverror=xcv, trainerror=trainerr, testerror=testerr)
}
```

```r
rfErr <- function(train.rf=spam01.rf, train=spam01, test=spam2,
                  outcome='type'){
    trainClass <- predict(train.rf, newdata=spam01, type="class")
    testClass <- predict(train.rf, newdata=test, type="class")
    rnprop <- prop.table(table(train[, outcome]))
    rfRates <- c(OOBerr=train.rf$err.rate[train.rf$ntree, "OOB"],
             trainerr=1-confusion(train$type, trainClass,
                                  printit=FALSE)$overall,
             testerr=1-confusion(spam2$type, testClass, printit=FALSE,
                                 prior=rnprop)$overall)
    rfRates
}
```

```r
fig9.11 <- function(){
if(!exists("Vowel"))
  return("Dataset 'Vowel' (from mlbench) is not available")
form <- paste("~", paste(paste("V", 2:10, sep= ""),
                         collapse="+"))
gph <- bwplot(formula(paste("Class", form)),
              scales=list(x="free"),
              data=Vowel, outer=TRUE, layout=c(3,3))
gph
}
```

2 Show the Figures

```r
pkgs <- c("DAAG","rpart","randomForest","MASS","mgcv","kernlab","mlbench")
z <- sapply(pkgs, require, character.only=TRUE, warn.conflicts=FALSE)
if(any(!z)){
  notAvail <- paste(names(z)[!z], collapse=", ")
  print(paste("The following packages need to be installed:", notAvail))
}
```

```r
fig9.1()
```

```r
    if(!exists('cuckoos.lda')){
        cuckoos <- within(cuckoos,
                          levels(species) <- abbreviate(levels(species), 8))
        cuckoos.lda <- lda(species ~ length + breadth, data=cuckoos)
        cuckoos.qda <- qda(species ~ length + breadth,
                                   data=cuckoos)
    }
```

```r
fig9.2()
```

```r
fig9.3()
```

```r
fig9.4()
```

```r
fig9.5()
```

```r
fig9.6()
```

```r
fig9.7()
```

```r
set.seed(31)
fig9.8()
```

```r
if(!exists("spam")){
  if(require("kernlab")) data("spam", package="kernlab") else
    print("Dataset 'spam' is not available")
}
if(exists("spam")){
nr <- sample(1:nrow(spam))
spam0 <- spam[nr[1:2601],]      ## Training
spam1 <- spam[nr[2602:3601],]   ## Holdout
spam01 <- spam[nr[1:3601],]     ## Use for training,
                                ## if holdout not needed
spam2 <- spam[nr[3602:4601],]   ## Test
spam01.lda <- lda(type~., data=spam01)
ldaError <- ldaErr()
set.seed(29)     ## Make results precisely reproducible
spam01.rp <- rpart(type~., data=spam01, cp=0.0001)
rpartError <- rpartErr()
set.seed(29)
spam01.rf <- randomForest(type ~ ., data=spam01)
rfError <- rfErr()
}
```

```
if(!exists('ticShown') | !exists('ticHeld')){
        cat("Will try to load dataset 'ticdata' from package 'kernlab'")
        if(require("kernlab"))
          data("ticdata", package="kernlab") else
          print("Dataset 'ticdata' is not available; get from kernlab")
if(exists('ticdata')){
          ## Use first 5822 observations for prediction
          ticShown <- ticdata[1:5822, ]
          ticHeld <- ticdata[-(1:5822), ]
      }
}
```

```
Will try to load dataset 'ticdata' from package 'kernlab'
```

```
if(!exists('tictrain') | !exists('tictest')){
tictrain <- ticShown[1:3822, ]
tictest <- ticShown[-(1:3822), ]
}
```

```
## Generated with seed=29
testLong <-
structure(list(test = c(61, 63, 65, 66, 65, 65, 67, 67, 63, 62,
62, 63, 65, 62, 65, 64, 63, 67, 67, 62, 59, 66, 68, 65, 62, 66,
66, 64, 65, 63, 59, 63, 65, 64, 66, 62, 65, 67, 65, 64, 64, 65,
63, 67, 63, 64, 68, 66, 68, 63), n0 = c(3596, 900, 600, 400,
270, 180, 120, 90, 60, 40, 3596, 900, 600, 400, 270, 180, 120,
90, 60, 40, 3596, 900, 600, 400, 270, 180, 120, 90, 60, 40, 3596,
900, 600, 400, 270, 180, 120, 90, 60, 40, 3596, 900, 600, 400,
270, 180, 120, 90, 60, 40), gp = c(1L, 1L, 1L, 1L, 1L, 1L, 1L,
1L, 1L, 1L, 2L, 2L, 2L, 2L, 2L, 2L, 2L, 2L, 2L, 2L, 3L, 3L, 3L,
3L, 3L, 3L, 3L, 3L, 3L, 3L, 4L, 4L, 4L, 4L, 4L, 4L, 4L, 4L, 4L,
4L, 5L, 5L, 5L, 5L, 5L, 5L, 5L, 5L, 5L, 5L)), .Names = c("test",
"n0", "gp"), row.names = c(NA, -50L), class = "data.frame")
```

```
opar <- par(mar=c(4.6,4.6,2.6, 0.6))
note <- paste("This plots stored results (seed=29), plus one further data point.",
              "\nType 'fig9.9(seed=31)' for graph shown in the text.")
oneExtra <- fig9.9(nn0 = 1800, repeats=1, plotit=FALSE)
df <- rbind(testLong, oneExtra)
nn0 <- unique(df$n0)
ndistinct <- length(unique(nn0))
test.gam <- gam(test ~ s(log(n0), k=min(ndistinct,3)), data=df)
plot(test.gam, se=T, residuals=T, pch=1, xaxt="n",
     xlab="n0, in 'sampsize=c(n0, 226)'",
```

```r
     ylab="# insurances, best 400 test",
     shift=mean(fitted(test.gam)))
axis(1, at=log(nn0), labels=paste(nn0), las=3)
mtext(side=3, line=0.5, note, col="blue")
par(opar)
```

```r
## Generated with seed=43
heldLong <-
structure(list(insure = c(108, 114, 120, 119, 121, 116, 114,
114, 110, 103, 110, 114, 116, 117, 117, 116, 110, 112, 110, 110,
110, 112, 118, 119, 119, 117, 113, 116, 110, 106, 108, 113, 115,
117, 114, 116, 116, 111, 109, 105, 108, 117, 117, 117, 116, 116,
115, 114, 111, 104), n0 = c(3596, 900, 600, 400, 270, 180, 120,
90, 60, 40, 3596, 900, 600, 400, 270, 180, 120, 90, 60, 40, 3596,
900, 600, 400, 270, 180, 120, 90, 60, 40, 3596, 900, 600, 400,
270, 180, 120, 90, 60, 40, 3596, 900, 600, 400, 270, 180, 120,
90, 60, 40), gp = c(1L, 1L, 1L, 1L, 1L, 1L, 1L, 1L, 1L, 1L, 2L,
2L, 2L, 2L, 2L, 2L, 2L, 2L, 2L, 2L, 3L, 3L, 3L, 3L, 3L, 3L, 3L,
3L, 3L, 3L, 4L, 4L, 4L, 4L, 4L, 4L, 4L, 4L, 4L, 4L, 5L, 5L, 5L,
5L, 5L, 5L, 5L, 5L, 5L, 5L)), .Names = c("insure", "n0", "gp"
), row.names = c(NA, -50L), class = "data.frame")
```

```r
opar <- par(mar=c(4.6,4.6,2.6, 0.6))
note <- paste("This plots stored results (seed=43), plus one further data point.",
              "\nType 'fig9.10(seed=47)' for graph shown in the text.")
oneExtra <- fig9.10(nn0 = 1800, repeats=1, plotit=FALSE)
df <- rbind(heldLong, oneExtra)
nn0 <- unique(df$n0)
ndistinct <- length(unique(nn0))
held.gam <- gam(insure ~ s(log(n0), k=min(ndistinct,3)), data=df)
plot(held.gam, se=T, residuals=T, pch=1, xaxt="n",
     xlab="n0, in 'sampsize=c(n0, 226)'",
     ylab="# insurances, best 400 held",
     shift=mean(fitted(held.gam)))
axis(1, at=log(nn0), labels=paste(nn0), las=3)
mtext(side=3, line=0.5, note, col="blue")
par(opar)
```

```r
    if(!exists('Vowel')){
        cat("Will try to load dataset 'Vowel' from package 'mlbench'")
        if(!requireNamespace("mlbench"))
          print("Package 'mlbench' is not installed") else
```

```
            data("Vowel", package="mlbench", envir=environment())
    }
```

```
Will try to load dataset 'Vowel' from package 'mlbench'

Loading required namespace:  mlbench
```

```
fig9.11()
```