6: Generalized Additive Models

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June 18, 2018

Ideas and issues illustrated by the graphs in this vignette

Generalized Additive Models (GAMs) extend linear and generalized linear models to include smooth functions of explanatory variables, where the smoothness may be determined automatically. The graphs shown here illustrate some of the possibilities.

Note: Figure 6.9 shows the results of simulations. The version of this figure that is shown in Section 2 is, in order to keep to a minimum the time taken to process the vignette, for 25 simulations only. This is useful mainly as a check that the code does what is expected of it. More realistically, specify 500 or 1000 (as in the text) simulations.

```
# 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

```
fig6.1 <- function(plotit=TRUE){
    matohms <- data.frame(model.matrix(with(fruitohms, ~ poly(juice, 4))))
    names(matohms) <- c("Intercept", paste("poly4",1:4, sep=""))
    form <- formula(paste(paste(names(matohms), collapse="+"), "~ juice"))
    matohms$juice <- fruitohms$juice
    gph1 <- xyplot(form, data=matohms, layout=c(1,5), scales=list(tck=0.5),
                   ylab="Basis terms",
                   strip=strip.custom(strip.names=TRUE,
                   var.name="",
                   sep=expression(""),
                   factor.levels=c("Constant","Linear","Quadratic",
```

```
                                "Cubic","Quartic")),
                panel=function(x,y,...){
                    llines(smooth.spline(x,y))},
                outer=TRUE,
                legend=list(top=list(fun=grid::textGrob,
                            args=list(label="A: Basis functions",
                            just="left", x=0))))
    b <- coef(lm(I(ohms/1000) ~ poly(juice,4), data=fruitohms))
    matohms <- sweep(model.matrix(with(fruitohms, ~ poly(juice, 4))),
                     2, b, "*")
    matohms <- data.frame(matohms)
    names(matohms) <- c("Intercept", paste("poly4",1:4, sep=""))
    form <- formula(paste(paste(names(matohms), collapse="+"), "~ juice"))
    matohms$juice <- fruitohms$juice
    matohms$Kohms <- fruitohms$ohms/1000
    nam <- lapply(1:5, function(x)substitute(A %*% B,
                                  list(A=round(b[x],2),
                                       B=c("Constant","Linear",
                                       "Quadratic","Cubic",
                                       "Quartic")[x])))
    gph2 <- xyplot(form, data=matohms, layout=c(1,5),, scales=list(tck=0.5),
                ylab="Add the contributions from these curves",
                strip=strip.custom(strip.names=TRUE,
                var.name="",
                sep=expression(""),
                factor.levels=as.expression(nam)),
                panel=function(x,y,...){
                    llines(smooth.spline(x,y))},
                outer=TRUE,
                legend=list(top=list(fun=grid::textGrob,
                      args=list(label="B: Contribution to fitted curve",
                                just="left", x=0))))
    if(plotit){
        print(gph1, position=c(0,0,.5,1))
        print(gph2, position=c(.5,0,1,1), newpage=FALSE)
}
    invisible(list(gph1, gph2))
}
```

```
fig6.2 <- function(){
    plot(ohms ~ juice, data=fruitohms, ylim=c(0, max(ohms)*1.02))
    ## 3 (=2+1) degrees of freedom natural spline
    fitns2 <- fitted(lm(ohms ~ splines::ns(juice, df=2), data=fruitohms))
    lines(fitns2 ~ juice, data=fruitohms, col="gray40")
```

```
    ## 4 (=3+1) degrees of freedom natural spline
    fitns3 <- fitted(lm(ohms ~ splines::ns(juice, df=3), data=fruitohms))
    lines(fitns3 ~ juice, data=fruitohms, lty=2, lwd=2, col="gray40")
    legend("topright", title="D.f. for cubic regression natural spline",
           legend=c("3  [ns(juice, 2)]",
           "4  [ns(juice, 3)]"),
           lty=c(1,2), lwd=c(1,2), cex=0.8)
    plot(ohms ~ juice, data=fruitohms, ylim=c(0, max(ohms)*1.02))
    ## 3 (=2+1) degrees of freedom natural spline
    fitns2 <- fitted(lm(ohms ~ splines::ns(juice, df=2), data=fruitohms))
    lines(fitns2 ~ juice, data=fruitohms, col="gray40")
    ## 4 (=3+1) degrees of freedom natural spline
    fitns3 <- fitted(lm(ohms ~ splines::ns(juice, df=3), data=fruitohms))
    lines(fitns3 ~ juice, data=fruitohms, lty=2, lwd=2, col="gray40")
    legend("topright", title="D.f. for cubic regression natural spline",
           legend=c("3  [ns(juice, 2)]",
           "4  [ns(juice, 3)]"),
           lty=c(1,2), lwd=c(1,2), cex=0.8)
}
```

```
fig6.3 <- function(){
    ohms.lm <- lm(ohms ~ ns(juice, df=3), data=fruitohms)
    termplot(ohms.lm, partial=TRUE, se=TRUE)
}
```

```
fig6.4 <- function(plotit=TRUE){
    matohms2 <- model.matrix(with(fruitohms, ~ splines::ns(juice, 2)))
    matohms3 <- model.matrix(with(fruitohms, ~ splines::ns(juice, 3)))
    m <- dim(matohms3)[1]
    longdf1 <- data.frame(juice=rep(fruitohms$juice,4),
                          basis2 = c(as.vector(matohms2),rep(NA,m)),
                          basis3 = as.vector(matohms3),
                          gp = factor(rep(c("Intercept",
                          paste("spline",1:3, sep="")),
                          rep(m,4))))
    gph1 <- xyplot(basis3 ~ juice | gp, data=longdf1, layout=c(1,4),
                   scales=list(tck=0.5),
                   ylab="Basis terms", strip=FALSE,
                   strip.left=strip.custom(strip.names=TRUE,
                   var.name="",
                   sep=expression(""),
                   factor.levels=c("Constant","Basis 1","Basis 2",
                   "Basis 3")),
```

```
                  par.settings=simpleTheme(lty=c(2,2,1,1)),
                  panel=function(x,y,subscripts){
                      llines(smooth.spline(x,y))
                      y2 <- longdf1$basis2[subscripts]
                      if(!any(is.na(y2))) llines(smooth.spline(x,y2),lty=1)},
                  outer=TRUE,
                  legend=list(top=list(fun=grid::textGrob,
                              args=list(label="A:Basis functions",
                              just="left", x=0))))
    b2 <- coef(lm(I(ohms/1000) ~ splines::ns(juice,2), data=fruitohms))
    b3 <- coef(lm(I(ohms/1000) ~ splines::ns(juice,3), data=fruitohms))
    spline2 <- as.vector(sweep(matohms2, 2, b2, "*"))
    spline3 <- as.vector(sweep(matohms3, 2, b3, "*"))
    longdf2 <- data.frame(juice=rep(fruitohms$juice,4),
                         spline2 = c(spline2, rep(NA,m)), spline3=spline3,
                         gp = factor(rep(c("Intercept",
                                     paste("spline",1:3, sep="")),
                         rep(m,4))))
    yran <- range(c(spline2, spline3))
    yran <- c(-6,8.5)
    gph2 <- xyplot(spline3 ~ juice | gp, data=longdf2, layout=c(1,4),
                  scales=list(tck=0.5, y=list(at=c(-4, 0, 4,8))), ylim=yran,
                  ylab="Add these contributions (ohms x 1000)", strip=FALSE,
                  strip.left=strip.custom(strip.names=TRUE,
                  var.name="",
                  sep=expression(""),
                  factor.levels=c("Const","Add 1","Add 2","Add 3")),
                  par.settings=simpleTheme(lty=c(2,2,1,1)),
                  panel=function(x,y,subscripts){
                      llines(smooth.spline(x,y))
                      y2 <- longdf2$spline2[subscripts]
                      if(!any(is.na(y2))) llines(smooth.spline(x,y2),lty=1)},
                  outer=TRUE,
                  legend=list(top=list(fun=grid::textGrob,
                              args=list(label="B: Contribution fo fitted curve",
                              just="left", x=0))))
    if(plotit){
        print(gph1, position=c(0,0,.5,1))
        print(gph2, position=c(.5,0,1,1), newpage=FALSE)
    }
    invisible(list(gph1, gph2))
}
```

```
fig6.5 <- function(){
    res <- resid(lm(log(Time) ~ log(Distance), data=worldRecords))
    wr.gam <- gam(res ~ s(log(Distance)), data=worldRecords)
    plot(wr.gam, residuals=TRUE, pch=1, las=1, ylab="Fitted smooth")
}
```

```
fig6.6 <-
function () {
    res <- resid(lm(log(Time) ~ log(Distance), data=worldRecords))
    wr.gam <- gam(res ~ s(log(Distance)), data=worldRecords)
    gam.check(wr.gam)
}
```

```
fig6.7 <-
function (mf=3,nf=2)
{
  opar <- par(mfrow=c(mf,nf), mar=c(0.25, 4.1, 0.25, 1.1))
    set.seed(29)         # Ensure exact result is reproducible
    res <- resid(lm(log(Time) ~ log(Distance), data=worldRecords))
    npanels <- mf*nf
    for(i in 1:npanels){
        permres <- sample(res)  # Random permutation
                                        # 0 for left-handers;  1 for right
        perm.gam <- gam(permres ~ s(log(Distance)), data=worldRecords)
        plot(perm.gam, las=1, rug=if(i<5) FALSE else TRUE, ylab="Fit")
    }
  par(opar)
}
```

```
fig6.8 <- function(){
    meuse.gam <- gam(log(lead) ~ s(elev) + s(dist) + ffreq + soil,
                            data=meuse)
    plot(meuse.gam, residuals=TRUE, se=TRUE, pch=1)
    termplot(meuse.gam, terms="ffreq", se=TRUE)
    termplot(meuse.gam, terms="soil", se=TRUE)
}
```

```
fig6.9 <- function(nsim=1000, caption=NULL){
  opar <- par(mfrow=c(1,2), oma=c(0,0,1.6,0.6))
  if(missing(caption))captCol <- "black" else captCol <- "blue"
  if(is.null(caption))caption <- paste("Graphs are from", nsim, "simulations")
```

```
    if(!exists("meuseML.gam"))
    meuseML.gam <- gam(log(lead) ~ s(elev) + s(dist) + ffreq + soil,
                       data=meuse, method="ML")
    if(!exists("meusexML.gam"))
    meusexML.gam <- gam(log(lead) ~ s(elev, dist) + ffreq + soil,
                        data=meuse, method="ML")
    ## Now simulate from meuseML.gam
    simY <- simulate(meuseML.gam, nsim=nsim)
    simResults <- matrix(0, nrow=nsim, ncol=3)
    colnames(simResults) <- c( "deltaDf", "fsim", "psim")
    for(i in 1:nsim){
        mML.gam <- gam(simY[,i] ~ s(elev) + s(dist) + ffreq + soil,
                       data=meuse, method="ML")
        mxML.gam <- gam(simY[,i] ~ s(elev, dist) + ffreq + soil,
                        data=meuse, method="ML")
        aovcomp <- anova(mML.gam, mxML.gam, test="F")
        simResults[i,] <- unlist(aovcomp[2, c("Df", "F", "Pr(>F)")])
    }
    ## Now plot the £p£-statistics and £F£-statistics
    ## against the change in degrees of freedom:
    colcode <- c("gray", "black")[1+(simResults[,"deltaDf"]>=1)]
    simResults <- as.data.frame(simResults)
    plot(psim ~ deltaDf, log="y", xlab="Change in degrees of freedom",
         ylab=expression(italic(p)*"-value"), col=colcode, data=simResults)
    abline(v=1, lty=2, col="gray")
    mtext("A", side=3, line=0.25, adj=0)
    mtext("1", side=1, at=1, line=0, cex=0.75)
    plot(fsim ~ deltaDf, log="y", xlab="Change in degrees of freedom",
         ylab=expression(italic(F)*"-statistic"),  col=colcode,
         data=simResults)
    abline(v=1, lty=2, col="gray")
    mtext("1", side=1, at=1, line=0, cex=0.75)
    mtext("B", side=3, line=0.25, adj=0)
  mtext(side=3, line=0.5, adj=0.052, outer=TRUE, caption, col=captCol)
    invisible(simResults)
  par(opar)
}
```

```
fig6.10A <- function(){
    if(!exists("meuseML.gam"))
    meuseML.gam <- gam(log(lead) ~ s(elev) + s(dist) + ffreq + soil,
                       data=meuse, method="ML")
    plot(meuseML.gam)
    termplot(meuseML.gam, terms="ffreq", se=TRUE)
```

```
    termplot(meuseML.gam, terms="soil", se=TRUE)
    mtext(side=3, line=0.65, "A: Add effects of dist and elev", outer=TRUE,
          cex=0.8, adj=0)
}
```

```
fig6.10B <- function(){
    if(!exists("meusexML.gam"))
    meusexML.gam <- gam(log(lead) ~ s(elev, dist) + ffreq + soil,
                        data=meuse, method="ML")
    plot(meusexML.gam)
    termplot(meusexML.gam, terms="ffreq", se=TRUE)
    termplot(meusexML.gam, terms="soil", se=TRUE)
    mtext(side=3, line=0.65, "B: Fit surface to dist and elev", outer=TRUE,
      cex=0.8, adj=0)
}
```

```
fig6.10 <- function()
print("Run fig6.10A() and fig6.10B() separately")
```

```
fig6.11 <- function(){
    hand <- with(cricketer, as.vector(as.vector(unclass(left)-1)))
                                    # 0 for left-handers
                                    # 1 for right
    hand.gam <- gam(hand ~ s(year), data=cricketer, family=binomial)
    plot(hand.gam, las=1, xlab="", ylab="Pr(left-handed)",
         trans=function(x)exp(x)/(1+exp(x)),
         shift=mean(predict(hand.gam)))
}
```

```
fig6.12 <- function(mf=3,nf=2){
    opar <- par(mfrow=c(mf,nf), mar=c(0.25, 4.1, 0.25, 1.1))
    npanel <- mf*nf
    for(i in 1:npanel){
        hand <- sample(c(0,1), size=nrow(cricketer), replace=TRUE,
                       prob=c(0.185, 0.815))
                                    # 0 for left-handers
                                    # 1 for right
        hand.gam <- gam(hand ~ s(year), data=cricketer, family=binomial)
        plot(hand.gam, las=1, xlab="",
             rug=if(i<4)FALSE else TRUE,
             trans=function(x)exp(x)/(1+exp(x)),
```

```
            shift=mean(predict(hand.gam)))
        }
        par(opar)
}
```

```
fig6.13 <- function(){
    rtlef <- data.frame(with(cricketer, as(table(year, left), "matrix")))
    rtlef <- within(rtlef, year <- as.numeric(rownames(rtlef)))
    right.gam <-  gam(right ~ s(year), data=rtlef, family=poisson)
    left.gam <-  gam(left ~ s(year), data=rtlef, family=poisson)
    rtlef <- within(rtlef,
                {fitright <- predict(right.gam, type="response")
                 fitleft <- predict(left.gam, type="response")})
    key.list <- list(text=expression("Right-handers", "Left-handers",
        "Left-handers "%*%" 4"),
                     corner=c(0,1), x=0, y=0.985,
                     points=FALSE, lines=TRUE)
    parset <- simpleTheme(col=c("blue", "purple", "purple"),
                          lty=c(1,1,2), lwd=c(2,2, 1))
    gph <- xyplot(fitright+fitleft+I(fitleft*4) ~ year, data=rtlef,
                  auto.key=key.list, par.settings=parset,tck=-0.05,
                  xlab="",
                  ylab="Number of cricketers\nborn in given year",
                  type="l", ylim=c(0,70))
    print(gph)
}
```

```
countAccs <- function(data=airAccs, dateCol="Date",
                      fromDate = as.Date("2006-01-01"),
                      by="1 day", prefix="num"){
  dfCount <- eventCounts(data, dateCol=dateCol,
                       from= fromDate, by=by,
                       prefix=prefix)
  dfCount[, "day"] <- julian(dfCount[,"Date"], origin=fromDate)
  dfCount
}
##
fig6.14 <- function()
    print("Run the separate functions fig6.14A() and fig6.14B()")
fig6.14A <- function(fromDate=as.Date("2006-01-01"), basis.df=50){
  if(!exists('dfDay06'))dfDay06 <- countAccs(fromDate=fromDate)
year <- seq(from=fromDate, to=max(dfDay06$Date), by="1 year")
atyear=julian(year, origin=fromDate)
```

```
dfDay06.gam <-
  gam(formula = num ~ s(day, k=basis.df), family = quasipoisson,
      data = dfDay06)
av <- mean(predict(dfDay06.gam))
plot(dfDay06.gam, xaxt="n", shift=av, trans=exp, rug=FALSE, xlab="",
     ylab="Estimated rate per day")
axis(1, at=atyear, labels=format(year, "%Y"))
mtext(side=3, line=0.75, "A: Events per day, vs date", adj=0)
}
fig6.14B <- function(fromDate=as.Date("2006-01-01"), basis.df=50){
  if(!exists('dfWeek06'))dfWeek06 <- countAccs(fromDate=fromDate,
                                               by="1 week")
dfWeek06.gam <- gam(num~s(day, k=basis.df), data=dfWeek06,
                    family=quasipoisson)
av <- mean(predict(dfWeek06.gam))
year <- seq(from=fromDate, to=max(dfWeek06$Date), by="1 year")
atyear=julian(year, origin=fromDate)
plot(dfWeek06.gam, xaxt="n", shift=av, trans=exp, rug=FALSE, xlab="",
      ylab="Estimated rate per week")
axis(1, at=atyear, labels=format(year, "%Y"))
mtext(side=3, line=0.75, "B: Events per week, vs date", adj=0)
}
```

2 Show the Figures

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

```
if(!exists("meuse")){
    msg <- "Cannot find package 'sp',"
        if(!require("sp"))
          return(paste(msg, "cannot do graph."))
    data("meuse", package="sp", envir = environment())
    }
```

```r
fig6.1()
```

```r
fig6.2()
```

```r
fig6.3()
```

```r
fig6.4()
```

```r
fig6.5()
```

```r
fig6.6()
```

```r
fig6.7()
```

```r
if(exists("meuse")) fig6.8() else
  print("Cannot locate data set 'meuse', hence cannot plot")
```

```r
{
caption <- paste("These are from 25 simulations.",
                 "More usefully, try, eg: fig6.9(nsim=500)")
if(exists("meuse")) fig6.9(nsim=25, caption=caption) else
  print("Cannot locate data set 'meuse', hence cannot plot")
}
```

```r
if(exists("meuse")) fig6.10A() else
  print("Cannot locate data set 'meuse', hence cannot plot")
```

```r
if(exists("meuse")) fig6.10B() else
  print("Cannot locate data set 'meuse', hence cannot plot")
```

```r
fig6.11()
```

```r
fig6.12()
```

```r
fig6.13()
```

```r
{
  fig6.14A(fromDate=as.Date("2010-01-01"), basis.df=50)
  fig6.14B(fromDate=as.Date("2010-01-01"), basis.df=50)
}
```