Nonlinear Methods: Splines/GAM/MARS

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Contents

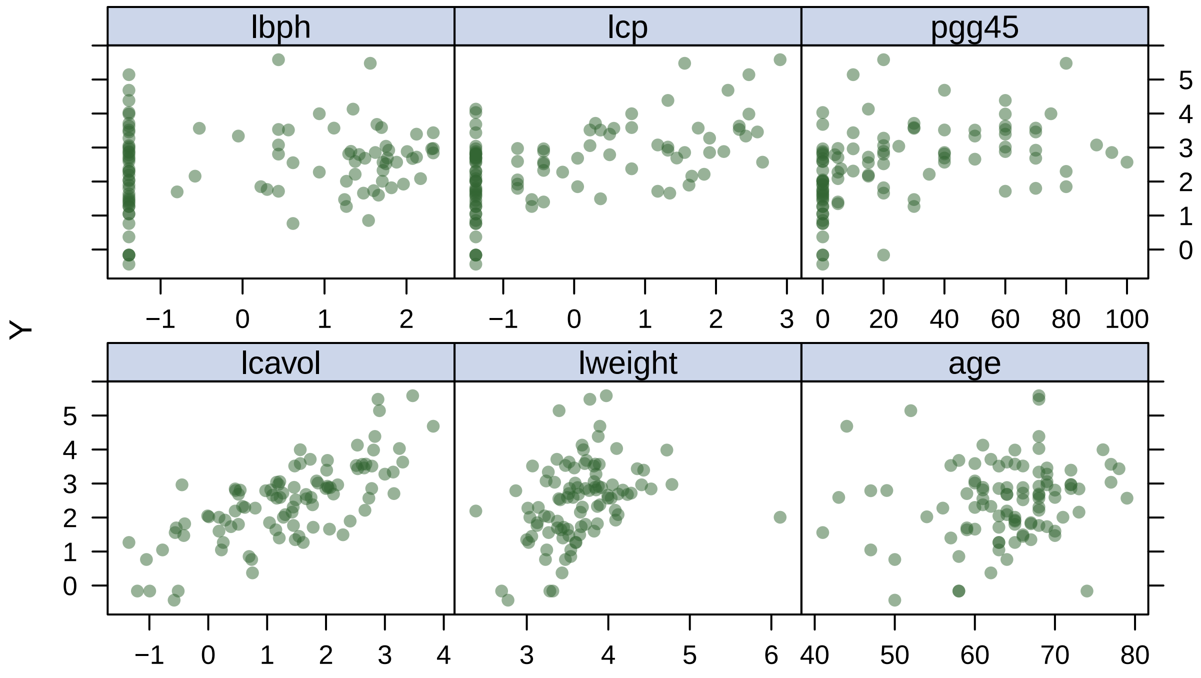
```r
library(caret)
library(splines)
library(mgcv) # for gam model
library(pdp) # for partial dependence plot
library(earth) # implement MARS
library(tidyverse)
library(ggplot2)
library(lasso2) # only for data
```

We will use a prostate cancer dataset for illustration. The data come from a study that examined the association between the level of prostate specific antigen (PSA) and a number of clinical measures in men who were about to receive a radical prostatectomy. The dataset can be found in the package `lasso2`. The response is the log PSA level (`lpsa`).

```r
data(Prostate)

# matrix of predictors
x <- model.matrix(lpsa~.,Prostate)[,-1]
# vector of response
y <- Prostate$lpsa
```

We use scatterplot to explore the relationship between the log PSA level and other variables. The variable percentage Gleason score 4/5 (`pgg45`) shows some potentially nonlinear trend.

```r
theme1 <- trellis.par.get()
theme1$plot.symbol$col <- rgb(.2, .4, .2, .5)
theme1$plot.symbol$pch <- 16
theme1$plot.line$col <- rgb(.8, .1, .1, 1)
theme1$plot.line$lwd <- 2
theme1$strip.background$col <- rgb(.0, .2, .6, .2)
trellis.par.set(theme1)

# svi and gleason were not included in the plot (they take discrete values)
featurePlot(x[,-c(5,7)], y, plot = "scatter", labels = c("","Y"),
            type = c("p"), layout = c(3, 2))
```



In what follows, we first fit univariate nonlinear models to investage the association between `lpsa` and `pgg45` for illustration. We then build multivariate prediction models for prediction.

Polynomial regression

The function `poly()` returns a matrix whose columns are a basis of orthogonal polynomials, which essentially means that each column is a linear combination of `pgg45`, `pgg45^2`, `pgg45^3`, and `pgg45^4`.

```
fit1 <- lm(lpsa~pgg45, data = Prostate)
fit2 <- lm(lpsa~poly(pgg45,2), data = Prostate)
fit3 <- lm(lpsa~poly(pgg45,3), data = Prostate)
fit4 <- lm(lpsa~poly(pgg45,4), data = Prostate)
fit5 <- lm(lpsa~poly(pgg45,5), data = Prostate)
# try corrplot::corrplot(cor(poly(Prostate$pgg45,5)))
```

Use `anova()` to test the null hypothesis that a simpler model is sufficient to explain the data against the alternative hypothesis that a more complex model is required. In order to use ANOVA, the models must be nested.

```
anova(fit1,fit2,fit3,fit4,fit5)
```

```
## Analysis of Variance Table
##
## Model 1: lpsa ~ pgg45
## Model 2: lpsa ~ poly(pgg45, 2)
## Model 3: lpsa ~ poly(pgg45, 3)
## Model 4: lpsa ~ poly(pgg45, 4)
## Model 5: lpsa ~ poly(pgg45, 5)
##   Res.Df     RSS Df Sum of Sq      F   Pr(>F)
## 1     95 105.103
## 2     94  96.807  1    8.2961 8.0535 0.005599 **
## 3     93  96.179  1    0.6280 0.6096 0.436967
## 4     92  94.711  1    1.4684 1.4255 0.235609
## 5     91  93.741  1    0.9701 0.9418 0.334394
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Step function

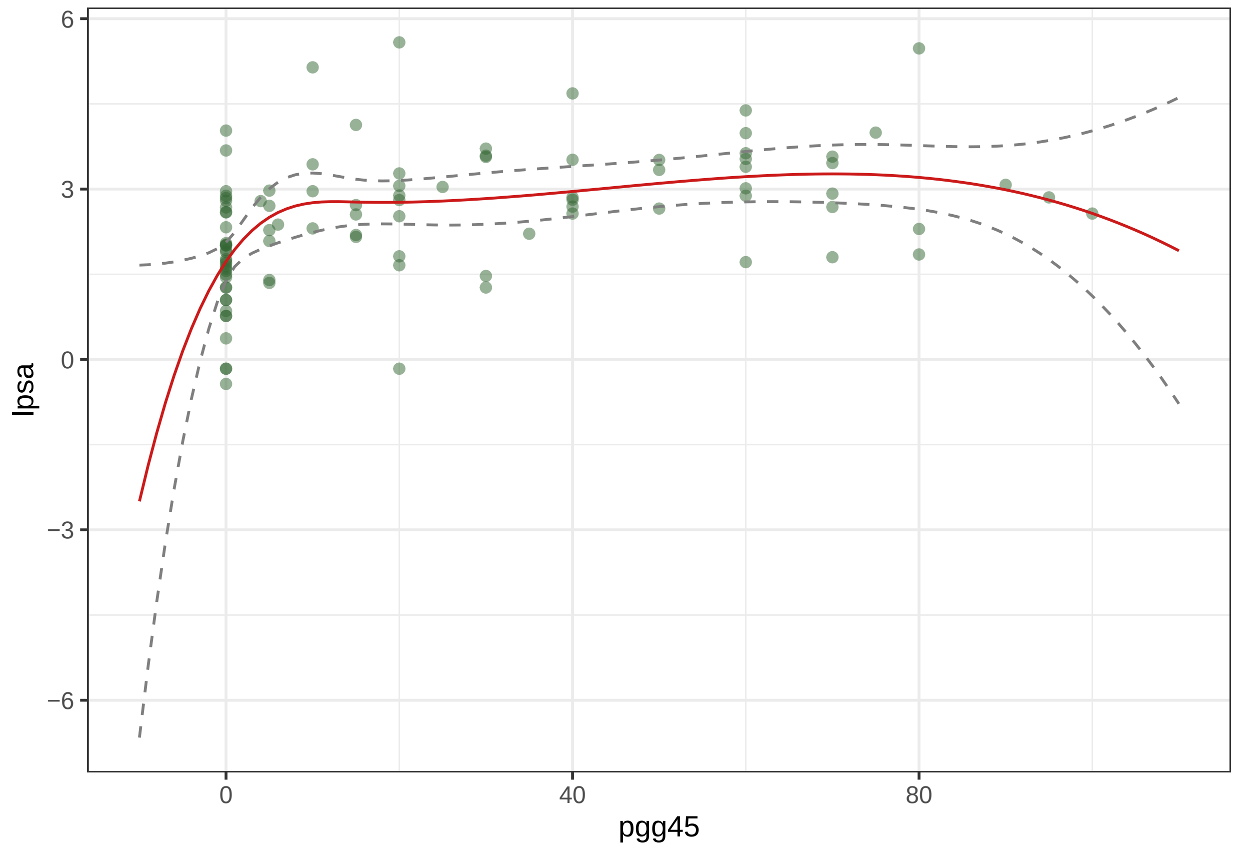
The function `cut()` can be used to create step function basis. The argument `breaks` can be used to specify the cutpoints.

```
fit.sf <- lm(lpsa~cut(pgg45, 4), data = Prostate) # cut variables into 4 equal spaces intervals
```

Cubic splines

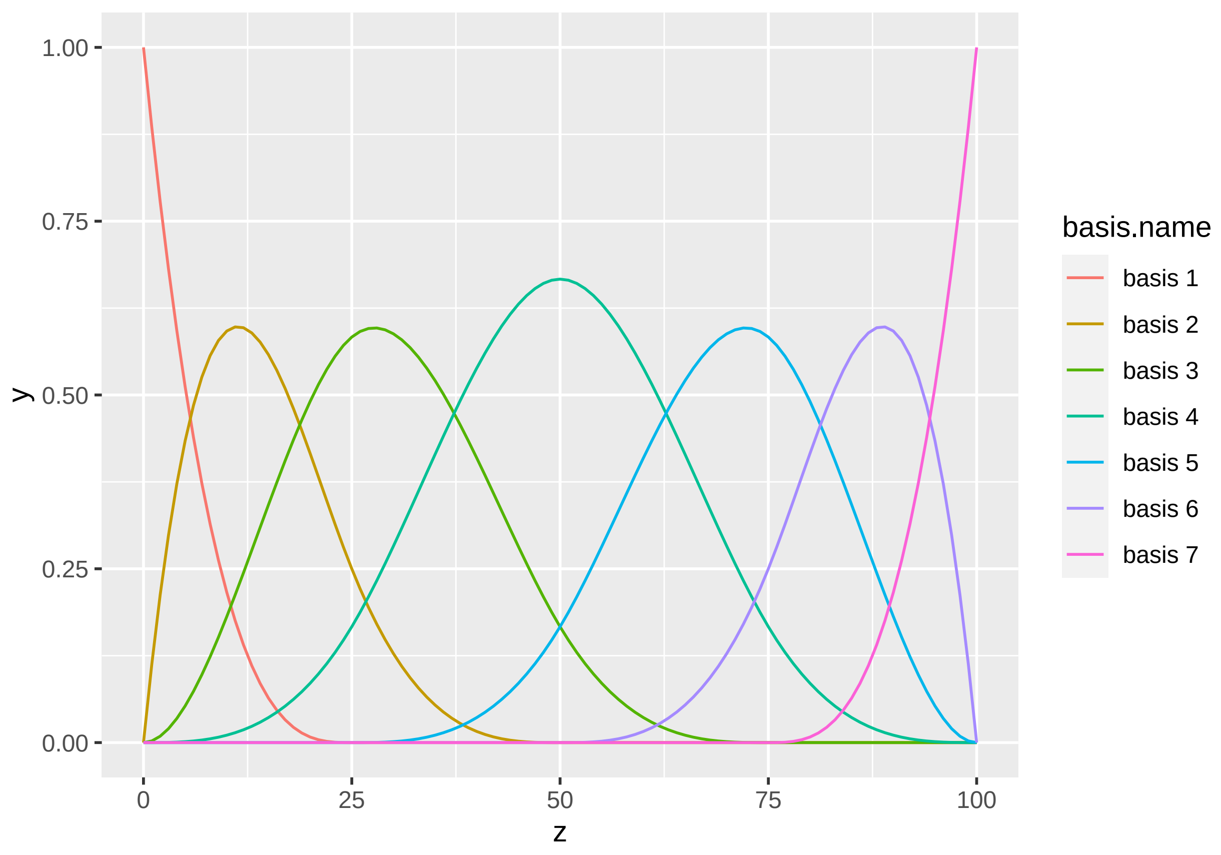
We fit a cubic spline model. Degree of freedom `df` (or knots `knots`) need to be specified. The argument `degree` denotes the degree of the piecewise polynomial; default is 3 for cubic splines.

```
fit.bs <- lm(lpsa~bs(pgg45, df = 4), data = Prostate) # quiet a lot filled wit zeros
# defalt intercept = FALSE , if set TRUE
# fit.bs <- lm(lpsa~bs(pgg45, knots = c(-0.1,20,40,60)), data = Prostate)
# 0 may be in pgg45 so add negative knots

# Note that the range of pgg45 is [0,100], and this is only for
# illustrating fitted curve beyond the boundary knots
pgg45.grid <- seq(from = -10, to = 110, by = 1)

pred.bs <- predict(fit.bs,
                   newdata = data.frame(pgg45=pgg45.grid),
                   se = TRUE)

pred.bs.df <- data.frame(pred = pred.bs$fit,
                         pgg45 = pgg45.grid,
                         upper = pred.bs$fit+2*pred.bs$se,
                         lower = pred.bs$fit-2*pred.bs$se)

p <- ggplot(data = Prostate, aes(x = pgg45, y = lpsa)) +
     geom_point(color = rgb(.2, .4, .2, .5))

p + geom_line(aes(x = pgg45, y = pred), data = pred.bs.df,
              color = rgb(.8, .1, .1, 1)) +
    geom_line(aes(x = pgg45, y = upper), data = pred.bs.df,
              linetype = 2, col = "grey50") +
    geom_line(aes(x = pgg45, y = lower), data = pred.bs.df,
              linetype = 2, col = "grey50") + theme_bw()
```



B-spline basis for cubic splines

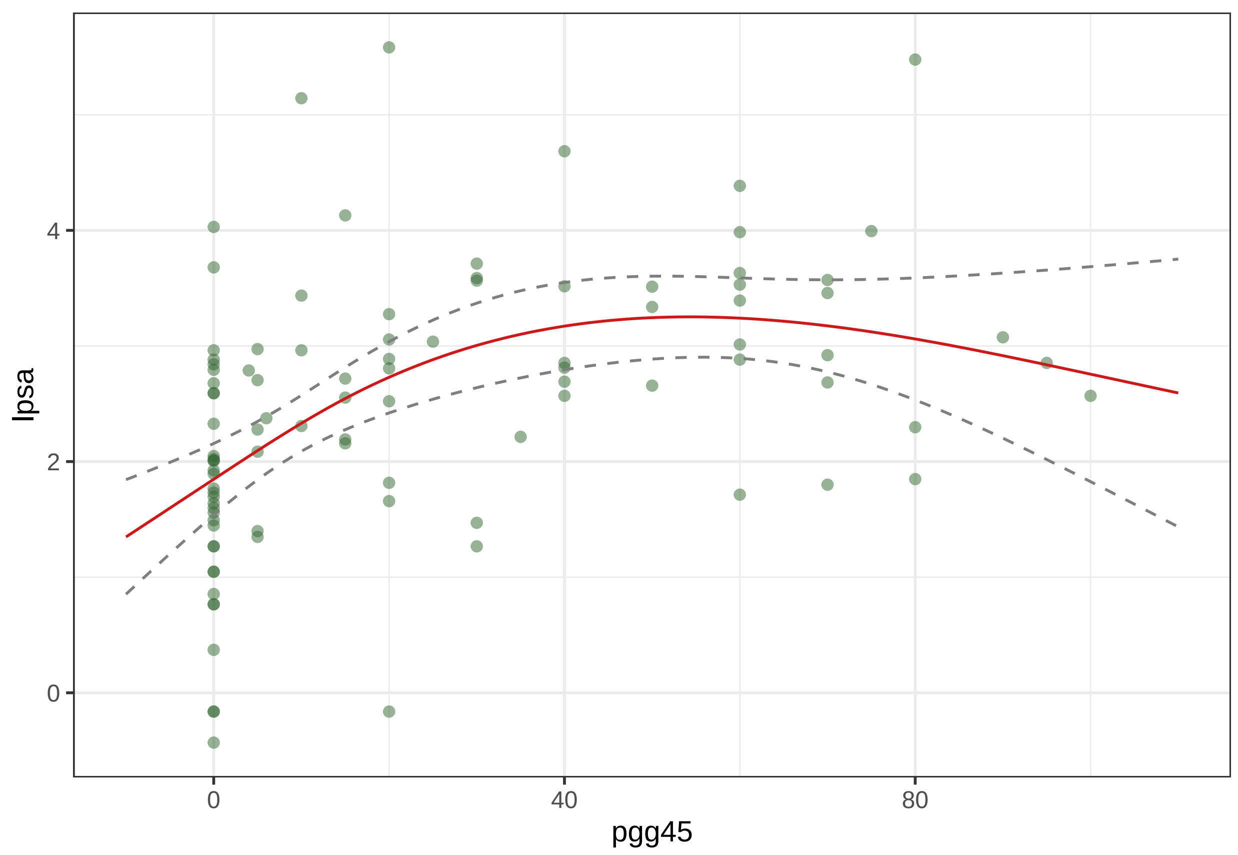
```
df.bs <- 7
z <- seq(from = 0, to = 100, by = 1)
bsz <- data.frame(bs(z, df = df.bs, intercept = TRUE))
names(bsz) <- paste("basis", 1:df.bs)
bsz$z <- z

bsz2 <- bsz %>%
  gather(paste("basis", 1:df.bs), key = basis.name, value='y')

ggplot(data = bsz2, aes(x=z, y=y)) +
  geom_line(aes(color=basis.name))
```



Natural cubic splines

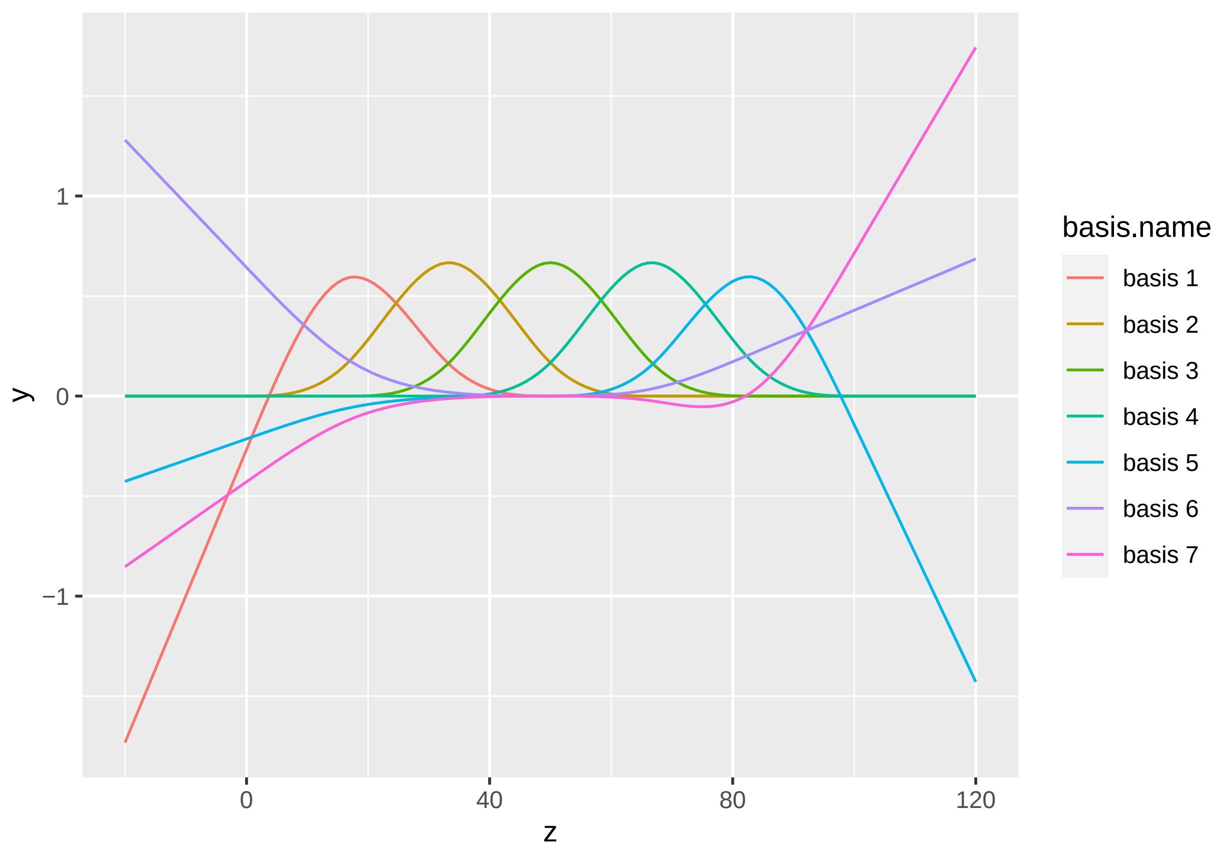
We then fit a natural cubic spline model that extrapolate linearly beyond the boundary knots.

```
fit.ns <- lm(lpsa~ns(pgg45, df = 2), data = Prostate)
# fit.ns <- lm(lpsa~ns(pgg45, knots = c(20,40,60)), data = Prostate)
#ns(Prostate$pgg45, df = 2) attr knots equals to 50%(15)
#bs(Prostate$pgg45,df=6) 6+1-4 = K+4 -> K=3
#always plus 1 intercept for total df
pred.ns <- predict(fit.ns,
                   newdata = data.frame(pgg45=pgg45.grid),
                   se=TRUE)

pred.ns.df <- data.frame(pred = pred.ns$fit,
                         pgg45 = pgg45.grid,
                         upper = pred.ns$fit+2*pred.ns$se,
                         lower = pred.ns$fit-2*pred.ns$se)


p + geom_line(aes(x = pgg45, y = pred), data = pred.ns.df,
              color = rgb(.8, .1, .1, 1)) +
    geom_line(aes(x = pgg45, y = upper), data = pred.ns.df,
              linetype = 2, col = "grey50") +
    geom_line(aes(x = pgg45, y = lower), data = pred.ns.df,
              linetype = 2, col = "grey50") + theme_bw()
```



B-spline basis for natural cubic splines

```
df.ns <- 7
z <- seq(from = -20, to = 120, by = 1)
nsz <- data.frame(ns(z, df = df.ns, Boundary.knots = c(0,100), intercept = TRUE))
# cubic splines boundary knots doesn't count
#ns(z, df = df.ns, Boundary.knots = c(0,100), intercept = TRUE)
# see the attr(,"knots")

names(nsz) <- paste("basis", 1:df.ns)
nsz$z <- z

nsz2 <- nsz %>%
  gather(paste("basis", 1:df.ns), key = basis.name, value='y')

ggplot(data = nsz2, aes(x=z, y=y)) +
  geom_line(aes(color=basis.name))
```



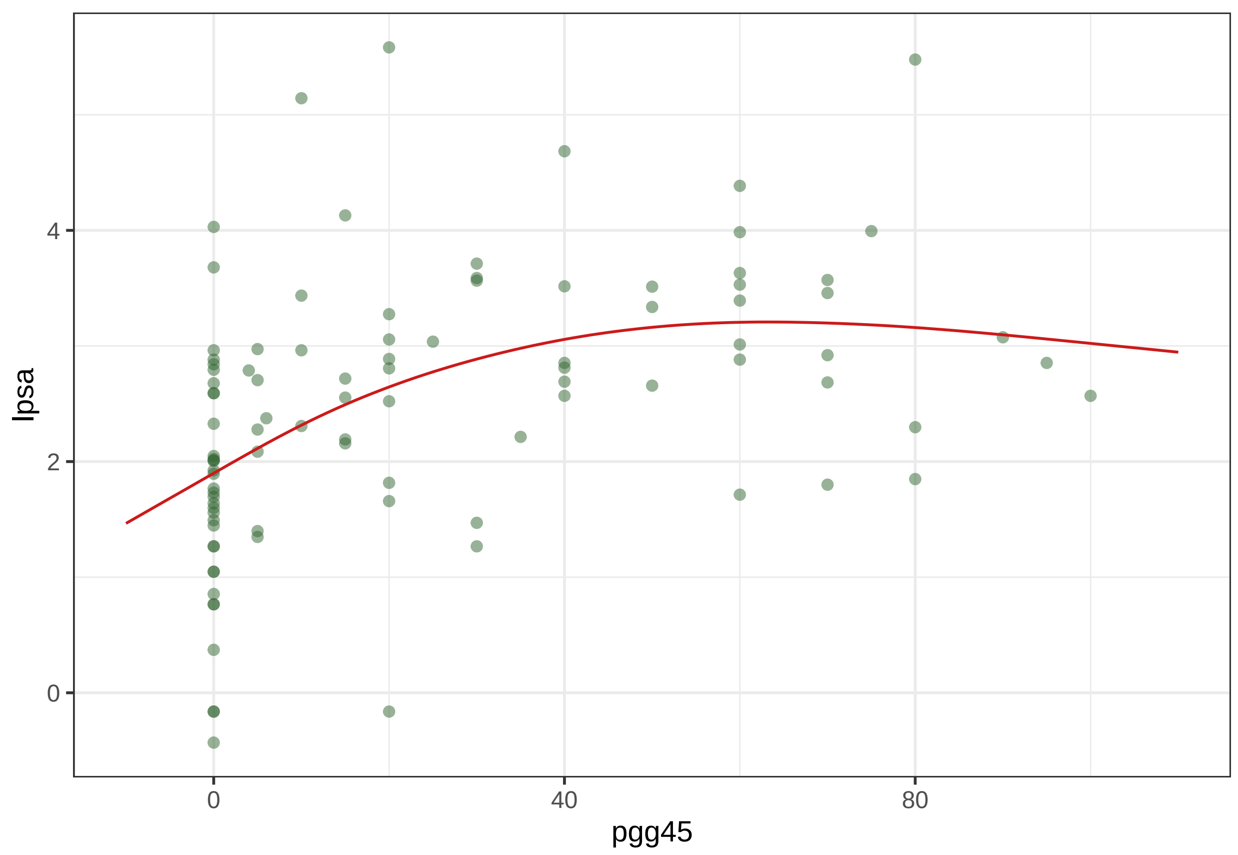
Smoothing splines

The function `smooth.spline()` can be used to fit smoothing spline models. Generalized cross-validation is used to select the degree of freedom (trace of the smoother matrix).

```
fit.ss <- smooth.spline(Prostate$pgg45, Prostate$lpsa)
#fit.ss <- smooth.spline(Prostate$pgg45, Prostate$lpsa, lambda = 1)
fit.ss$df
```

```
## [1] 3.24361
```

```
pred.ss <- predict(fit.ss,
                   x = pgg45.grid)

pred.ss.df <- data.frame(pred = pred.ss$y,
                         pgg45 = pgg45.grid)

p +
geom_line(aes(x = pgg45, y = pred), data = pred.ss.df,
          color = rgb(.8, .1, .1, 1)) + theme_bw()
```

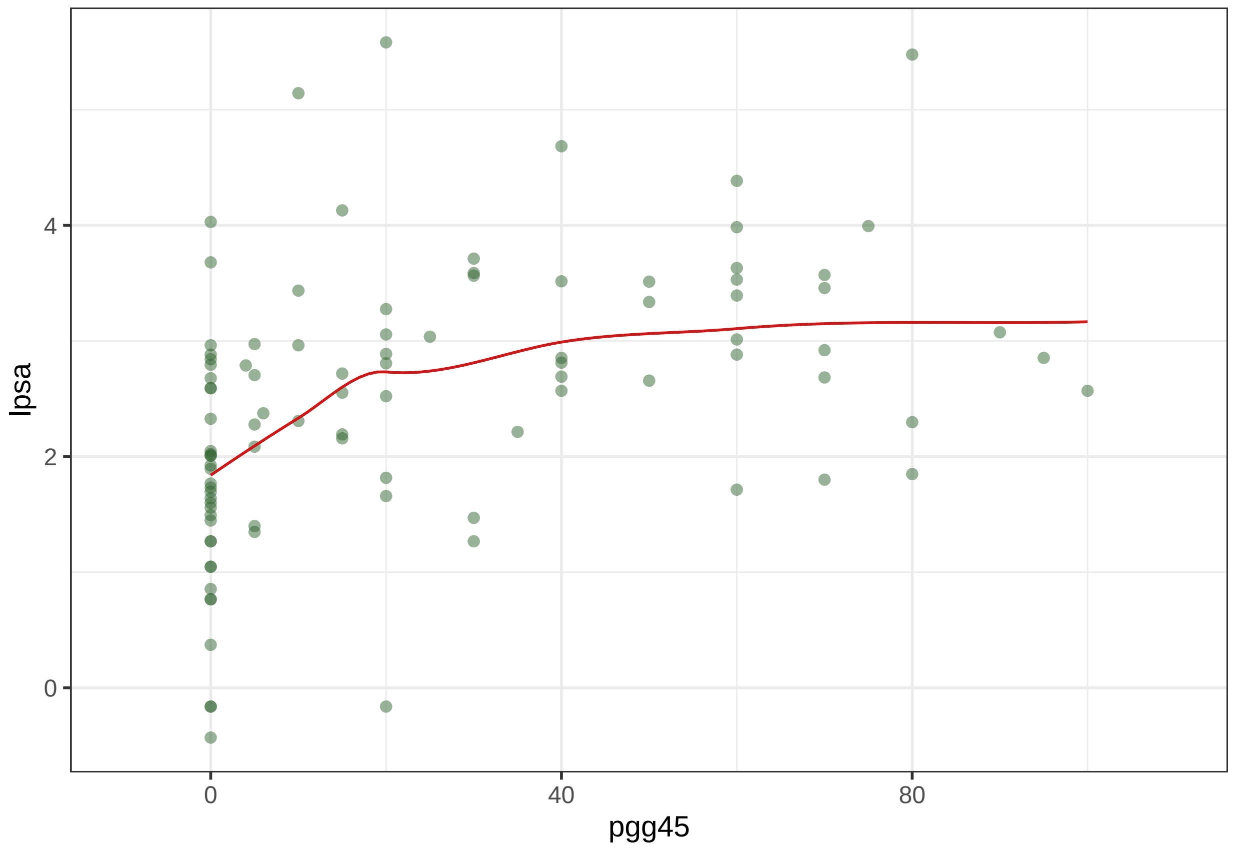


why only one line: smoothing spline is not using least square, is using a penalized least square, so it can't give a confidence interval.

Local regression

We perform a local polynomial regression using `loess()`.

```
fit.loess <- loess(lpsa~pgg45, data = Prostate, degree = 1, span = 0.75)
# loess(lpsa~pgg45, data = Prostate, degree = 1, span = 0.5)
pred.loess <- predict(fit.loess,
                      newdata = data.frame(pgg45 = pgg45.grid))

pred.loess.df <- data.frame(pred = pred.loess,
                            pgg45 = pgg45.grid)

p + geom_line(aes(x = pgg45, y = pred), data = pred.loess.df,
              color = rgb(.8, .1, .1, 1)) + theme_bw()
```



`degree = 1` means fit a local linear model, 0 for local constant, 2 for quadratic model. `loess()` got a parameter called `span` , the default is `0.75`

Generalized additive model (GAM)

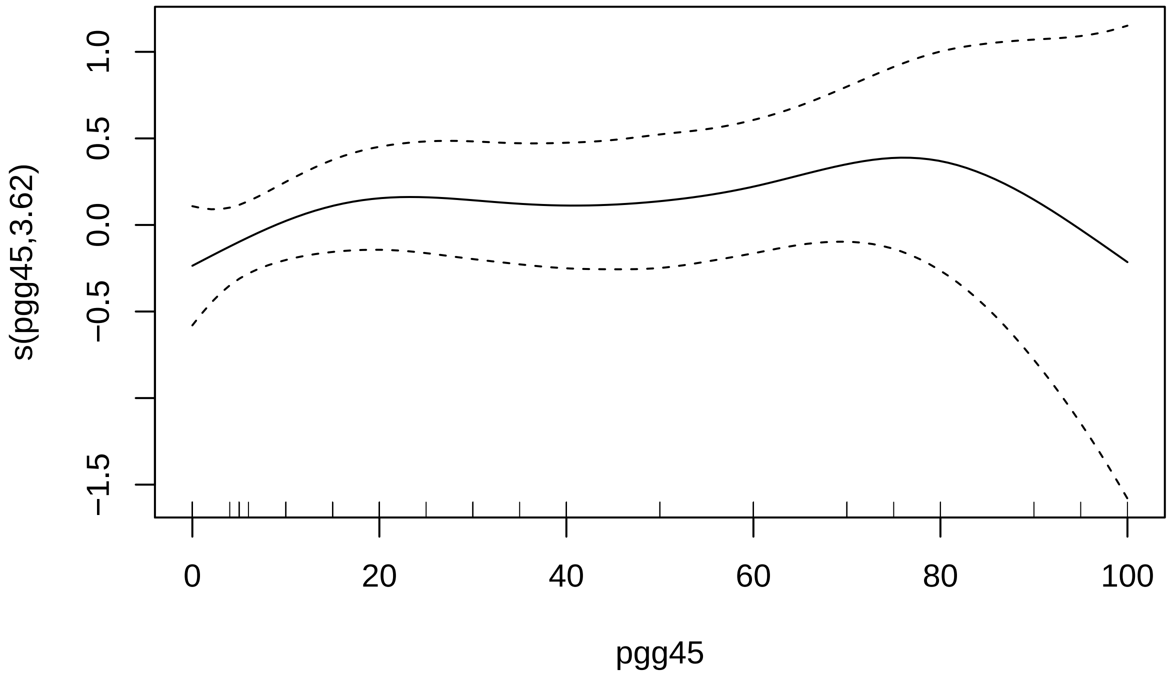
`gam()` fits a generalized additive model (GAM) to data, the term 'GAM' being taken to include any quadratically penalized GLM and a variety of other models estimated by a quadratically penalised likelihood type approach. In `gam()`, built-in nonparametric smoothing terms are indicated by `s` for smoothing splines. The package `gam` also provides a function `gam()`. GCV is used to select the degree of freedom. Confidence/credible intervals are readily available for any quantity predicted using a fitted model.

```
gam.m1 <- gam(lpsa~age+pgg45+lcavol+lweight+lbph+svi+lcp+gleason, data = Prostate)
gam.m2 <- gam(lpsa~age+s(pgg45)+lcavol+lweight+lbph+svi+lcp+gleason,
              data = Prostate, )
#gam(lpsa~age+s(pgg45)+s(lcavol)+lweight+lbph+svi+lcp+gleason, data = Prostate)
#plot shows that s(lcavol) returns a linear relation
gam.m3 <- gam(lpsa~age+s(pgg45)+te(lcavol,lweight)+lbph+svi+lcp+gleason,
              data = Prostate)

anova(gam.m1, gam.m2, gam.m3, test = "F")
```

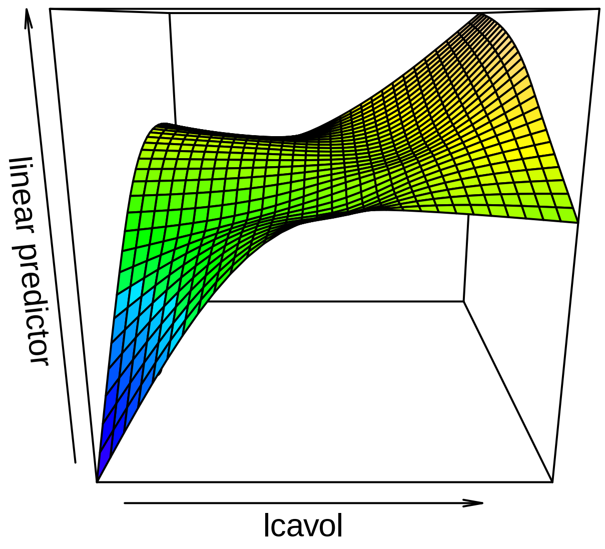
```
## Analysis of Deviance Table
##
## Model 1: lpsa ~ age + pgg45 + lcavol + lweight + lbph + svi + lcp + gleason
## Model 2: lpsa ~ age + s(pgg45) + lcavol + lweight + lbph + svi + lcp +
##     gleason
## Model 3: lpsa ~ age + s(pgg45) + te(lcavol, lweight) + lbph + svi + lcp +
##     gleason
##   Resid. Df Resid. Dev      Df Deviance      F  Pr(>F)
## 1    88.000     44.163
## 2    84.485     41.132  3.5154   3.0312 2.0734 0.10120
## 3    73.739     31.975 10.7461   9.1569 2.0489 0.03636 *
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

`te()`: `s()`:spline

```
plot(gam.m2) # y-label means the edf
```



```
vis.gam(gam.m3, view = c("lcavol","lweight"),
        color = "topo")
```



`plot(gam.m2)` also gives credible interval not confidence interval With the current support from `caret`, you may lose a significant amount of flexibility in `mgcv`.

```
ctrl1 <- trainControl(method = "cv", number = 10)
# you can try other options

set.seed(2)
gam.fit <- train(x, y,
                 method = "gam",
                 # tuneGrid = data.frame(method = "GCV.Cp", select = c(TRUE,FALSE)),
                 trControl = ctrl1) # based on the # of possible value of predictors to deside using sp


gam.fit$bestTune
```

```
##   select method
## 2   TRUE GCV.Cp
```

```
gam.fit$finalModel
```

```
##
## Family: gaussian
## Link function: identity
##
## Formula:
```

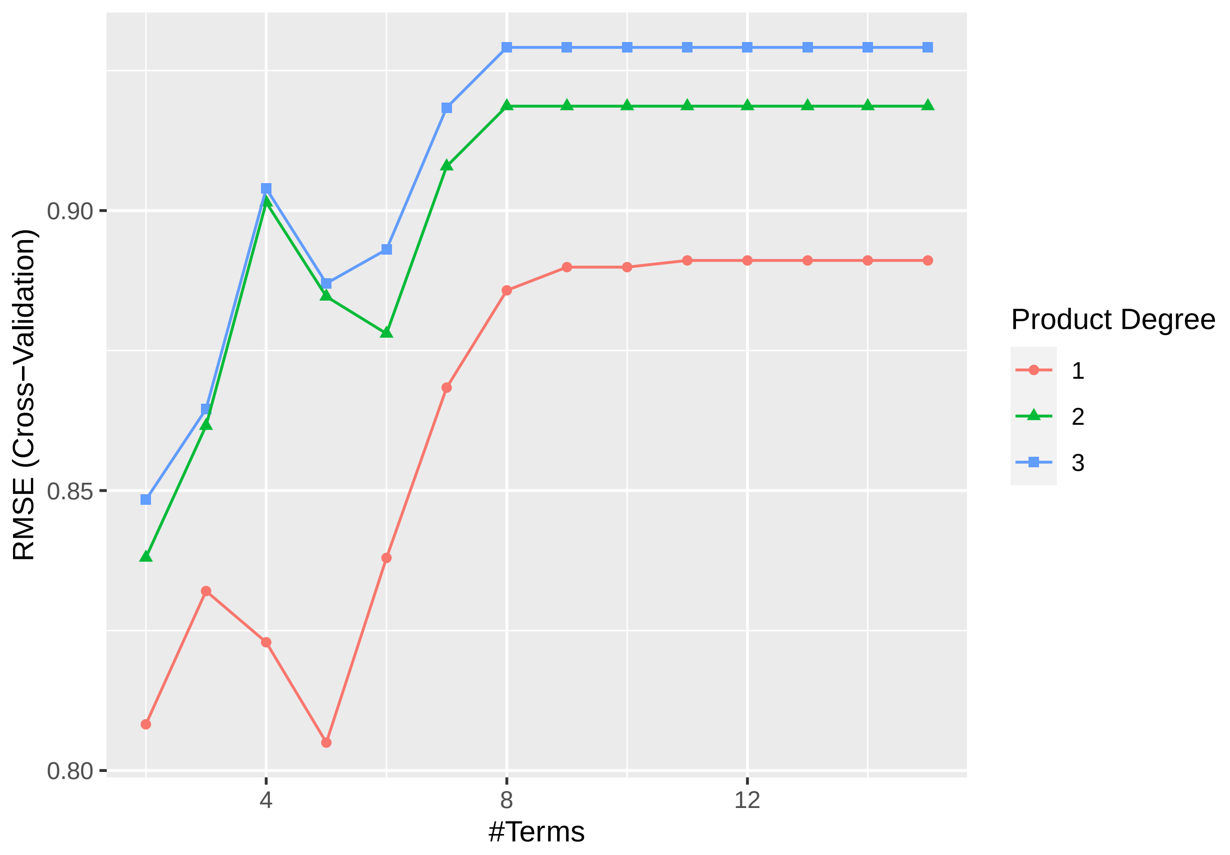
```
## .outcome ~ svi + gleason + s(pgg45) + s(lcp) + s(age) + s(lbph) +
##     s(lweight) + s(lcavol)
##
## Estimated degrees of freedom:
## 3.651 0.000 1.470 0.716 1.520 4.582  total = 14.94
##
## GCV score: 0.5357211
```

`gam.fit` shows that the second edf, which is the edf of `s(lcp)` is zero, which means it was not included in the model.

Multivariate Adaptive Regression Splines (MARS)

We next create a piecewise linear model using multivariate adaptive regression splines (MARS). Since there are two tuning parameters associated with the MARS model: the degree of interactions and the number of retained terms, we need to perform a grid search to identify the optimal combination of these hyperparameters that minimize prediction error

```
mars_grid <- expand.grid(degree = 1:3,
                         nprune = 2:15)

set.seed(2)
mars.fit <- train(x, y,
                  method = "earth",
                  tuneGrid = mars_grid,
                  trControl = ctrl1)

ggplot(mars.fit)
```



```
mars.fit$bestTune
```

```
##   nprune degree
## 4      5      1
```

```
coef(mars.fit$finalModel) # shows the terms(hinge functions) included in the final model
```

```
##         (Intercept)  h(lcavol-2.40964)  h(2.40964-lcavol) h(3.83622-lweight)
##          3.31668457         1.18965538        -0.43756141        -0.88094773
##         h(10-pgg45)
##         -0.04983056
```

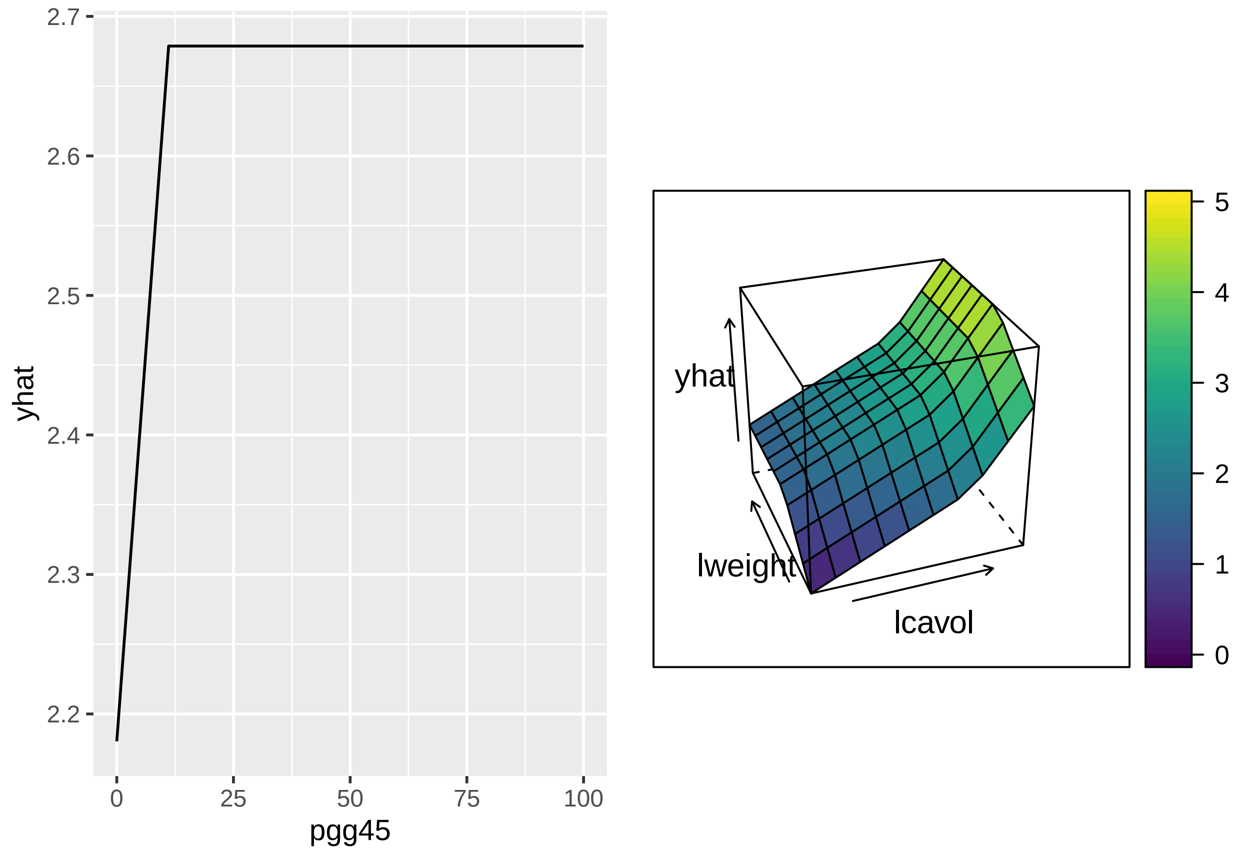
```
# check Prostate$pgg45 == 10
```

`ggplot(mars.fit)` shows that 1 product degree give the best rmse which means there is no product, and the # of term is 5

To better understand the relationship between these features and `lpsa`, we can create partial dependence plots (PDPs) for each feature individually and also an interaction PDP. This is used to examine the marginal effects of predictors.

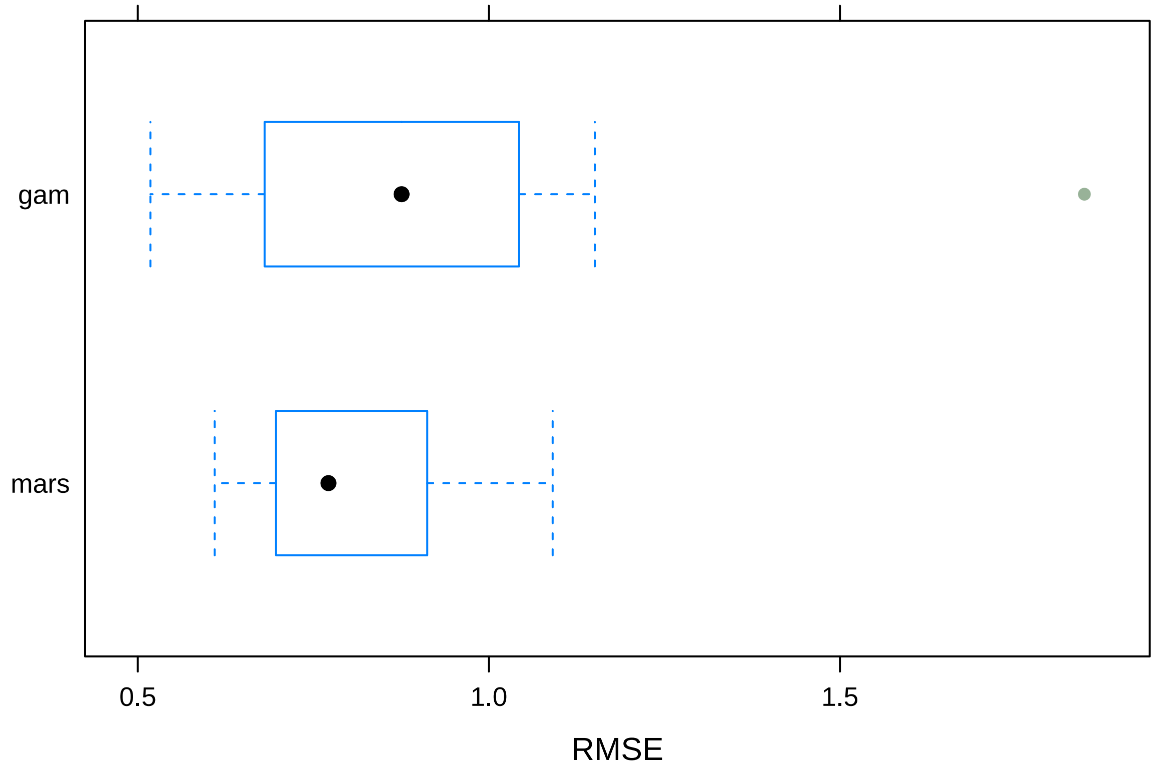
```
p1 <- pdp::partial(mars.fit, pred.var = c("pgg45"), grid.resolution = 10) %>% autoplot()
# use pdp::partial to avoid confusion
# a grid of ten values
```

```
p2 <- pdp::partial(mars.fit, pred.var = c("lcavol", "lweight"),
                   grid.resolution = 10) %>%
      pdp::plotPartial(levelplot = FALSE, zlab = "yhat", drape = TRUE,
                       screen = list(z = 20, x = -60))

grid.arrange(p1, p2, ncol = 2)
```



`p1` just gives us the hinge function of pgg45, run `coef(mars.fit$finalModel)` and check the terms

```
bwplot(resamples(list(mars = mars.fit,
               gam = gam.fit)), metric = "RMSE")
```



$f(x_1, \cdots, x_p)$, to provide some info of each pair of var affects the outcome.

$$Y vs. x_1$$

we can integral $x_2, \cdots, x_p$ to get the partial dependence plot the empirical marginal distribution of x_1

$$\frac{1}{n}\sum_{i=1}^{n}\hat{f}(x1, x_{i2}, x_{i3}, \cdots, x_{ip})$$

in linear regression

$$f(x) = \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3$$

$$\hat{f}(x) = \frac{1}{n}\sum_{i=1}^{n}(\hat{\beta}_1 x_1 + \hat{\beta}_2 x_{i2} + \hat{\beta}_3 x_{i3})$$

just $\hat{\beta}_1 x_1$

in GAM

$\hat{f}(x) = \hat{f}_1(x_1) + \hat{f}_2(x_2)$ $\hat{f}(x) = \frac{1}{n}\sum(\hat{f}_1(x_1) + \hat{f}_2(x_{i2})) = \hat{f}_1(x_1) + constant$

for the 2-D plot $\frac{1}{n}\sum_{i=1}^{n}\hat{f}(x_1, x_2, x_{i3}, \cdots, x_{ip})$

only give the trend on average, *interpret carefully*, never same to $f(x)$