Nonlinear Methods: Splines/GAM/MARS

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Contents

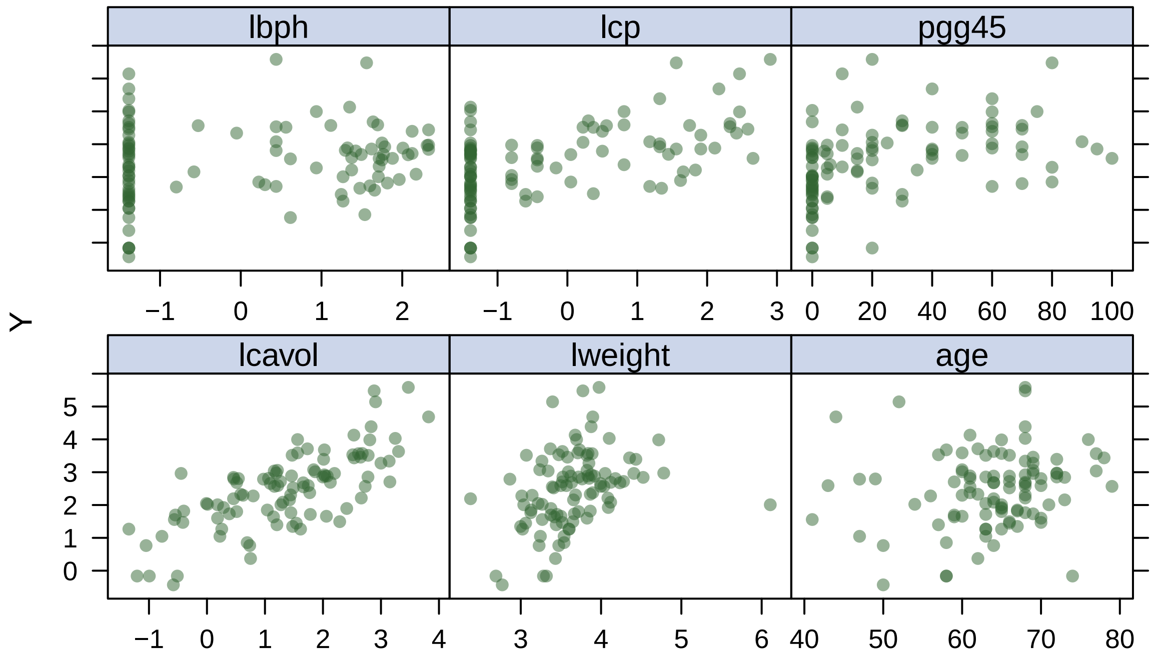
```r
library(caret)
library(tidymodels)
library(splines)
library(mgcv)
library(pdp)
library(earth)
library(tidyverse)
library(ggplot2)
library(bayesQR) # only for data
```

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 `bayesQR`. 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 potentially nonlinear trend.

```r
# Get the image parameters of the current trellis graph
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)
# Set the modified parameters as the global style for the trellis graph
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)
```

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

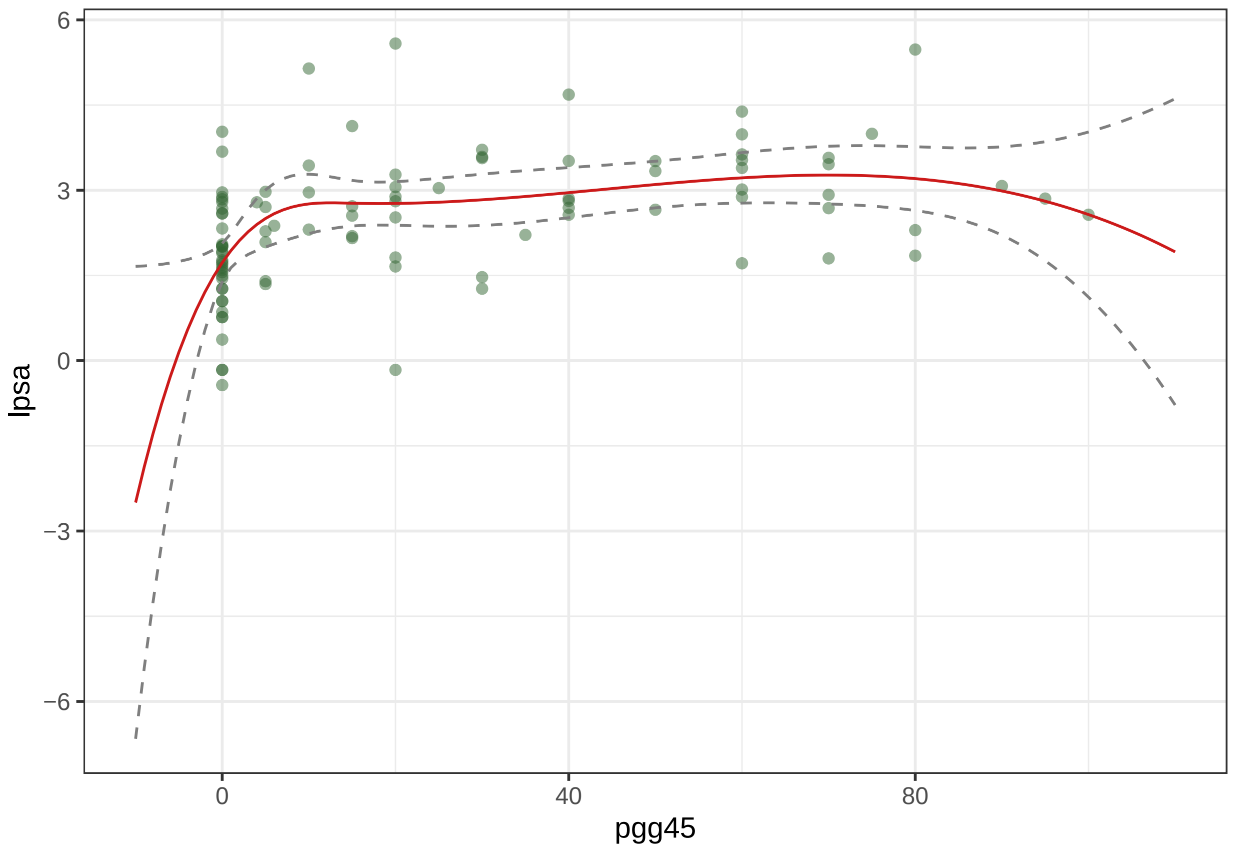
The function `cut()` can be used to create step function basis. The argument `breaks` can be used to specify the cutpoints.

```
fit.sf <- lm(lpsa ~ cut(pgg45, 4), data = Prostate)
```

Cubic splines

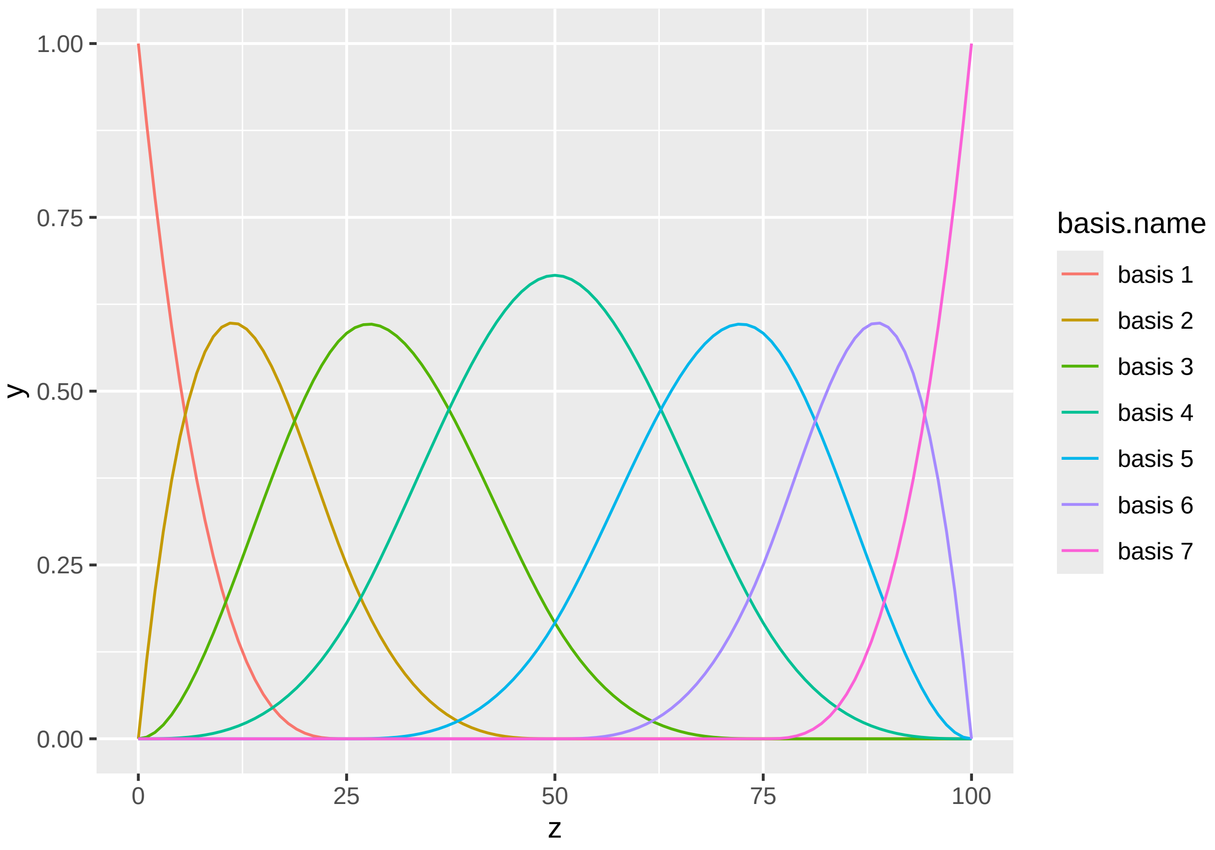
We fit a cubic spline model. The function `bs()` generates the B-spline basis matrix for polynomial splines. Degree of freedom `df` (or knots `knots`) need to be specified. The argument `degree` in `bs()` denotes the degree of the piecewise polynomial; default is 3 for cubic splines.

```
fit.bs <- lm(lpsa ~ bs(pgg45, df = 4), data = Prostate)
# fit.bs <- lm(lpsa~bs(pgg45, knots = c(20,40,60)), data = Prostate)

# 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

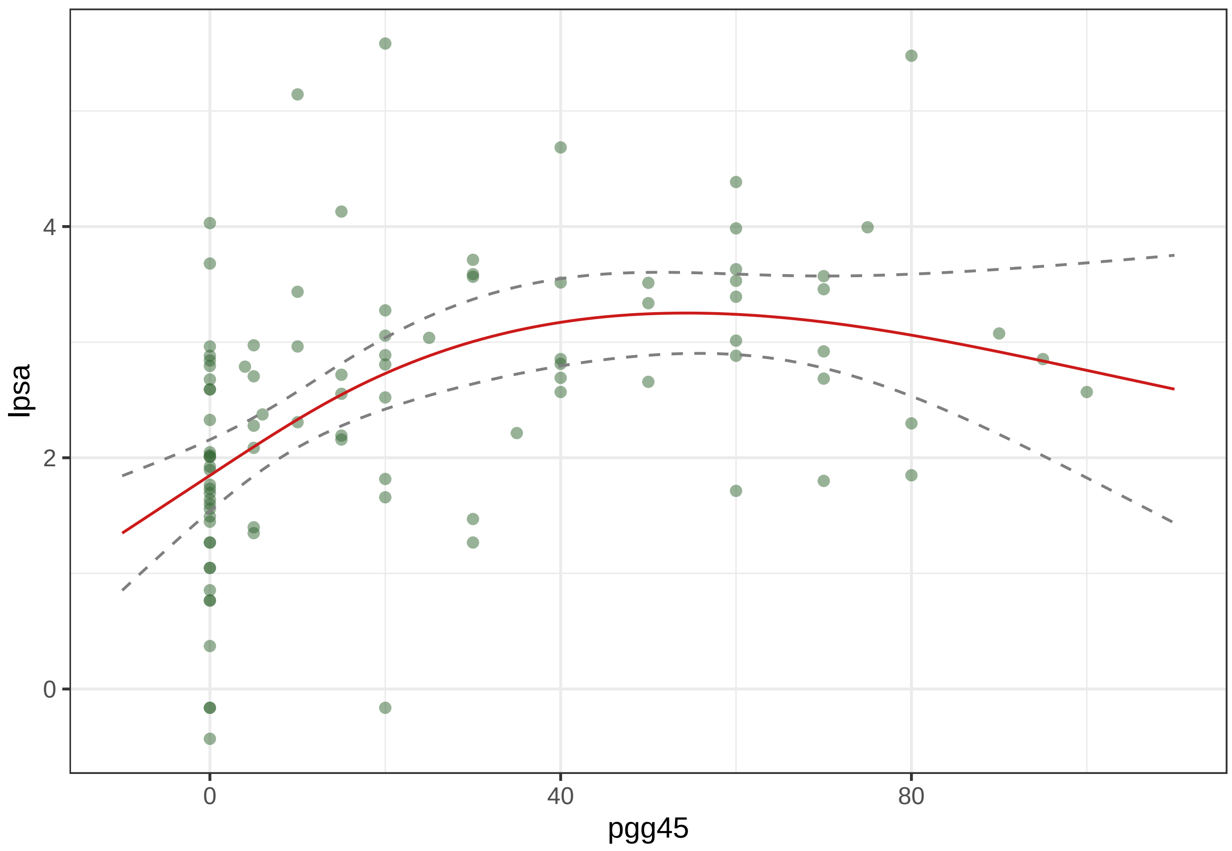
```
df.bs <- 7
z <- seq(from = 0, to = 100, by = 1)

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

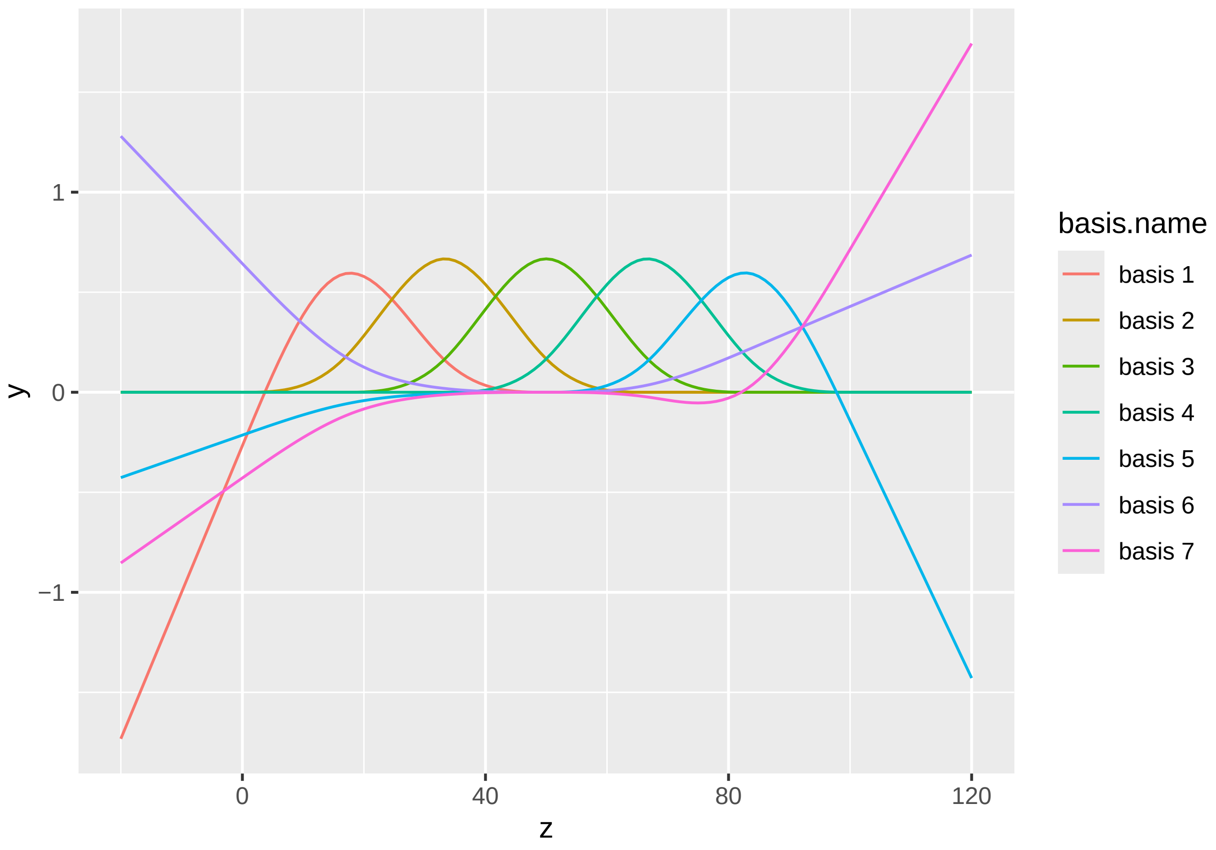
We then fit a natural cubic spline model that extrapolate linearly beyond the boundary knots. The function `ns()` generates the B-spline basis matrix for natural cubic splines.

```
fit.ns <- lm(lpsa~ns(pgg45, df = 2), data = Prostate)
# fit.ns <- lm(lpsa~ns(pgg45, knots = c(20,40,60)), data = Prostate)

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

```r
df.ns <- 7
z <- seq(from = -20, to = 120, by = 1)

# Boundary.knots: boundary points at which to impose the natural boundary conditions
# (default is the range of the data)
nsz <- data.frame(ns(z, df = df.ns, Boundary.knots = c(0, 100), intercept = TRUE))

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))
```



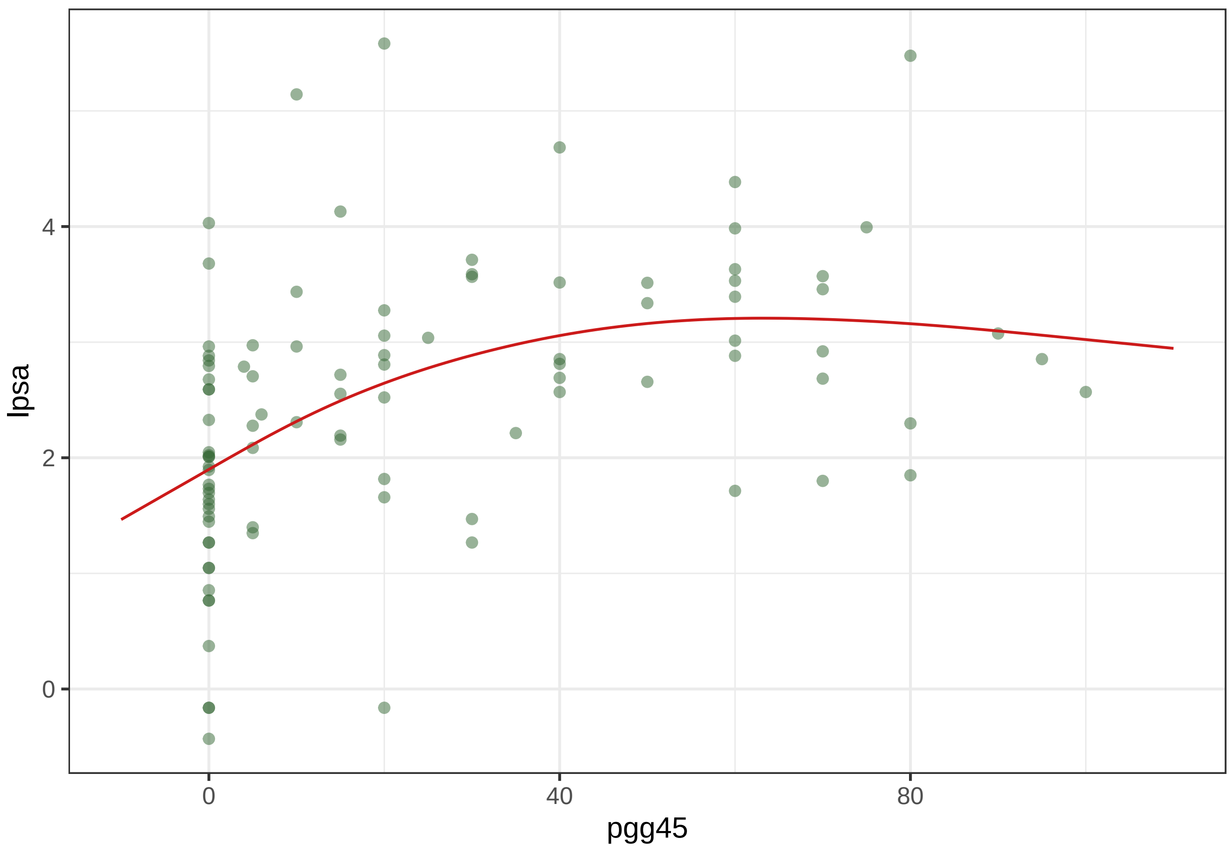
Smoothing splines

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$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()
```



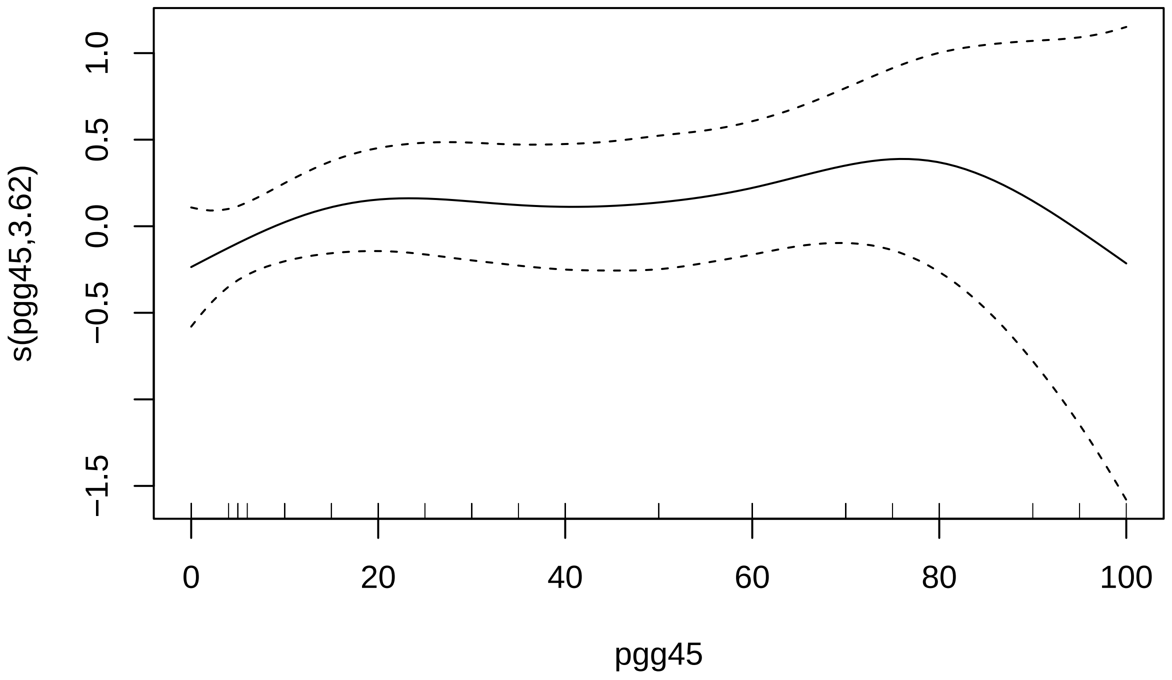
Generalized additive model (GAM)

`gam()` fits a generalized additive model (GAM) to data. 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. Credible intervals are readily available for any quantity predicted using a fitted model.

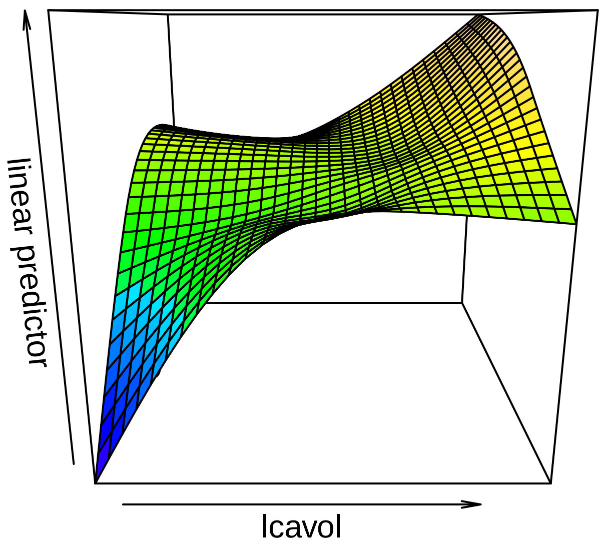
```r
gam.m1 <- gam(lpsa ~ age + pgg45 + lcavol + lweight + lbph + svi + lcp + gleason,
              data = Prostate)
gam.m2 <- gam(lpsa ~ age + s(pgg45) + lcavol + lweight + lbph + svi + lcp + gleason,
              data = Prostate)
gam.m3 <- gam(lpsa ~ age + s(pgg45) + te(lcavol,lweight) + lbph + svi + 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
```

```
plot(gam.m2)
```



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



With the current support from `caret`, you may lose a significant amount of flexibility in `mgcv`.

```
ctrl1 <- trainControl(method = "cv", number = 10)

set.seed(2)
gam.fit <- train(x, y,
                 method = "gam",
                 # tuneGrid = data.frame(method = "GCV.Cp", select = c(TRUE,FALSE)),
                 trControl = ctrl1)
```

```r
gam.fit$bestTune
```

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

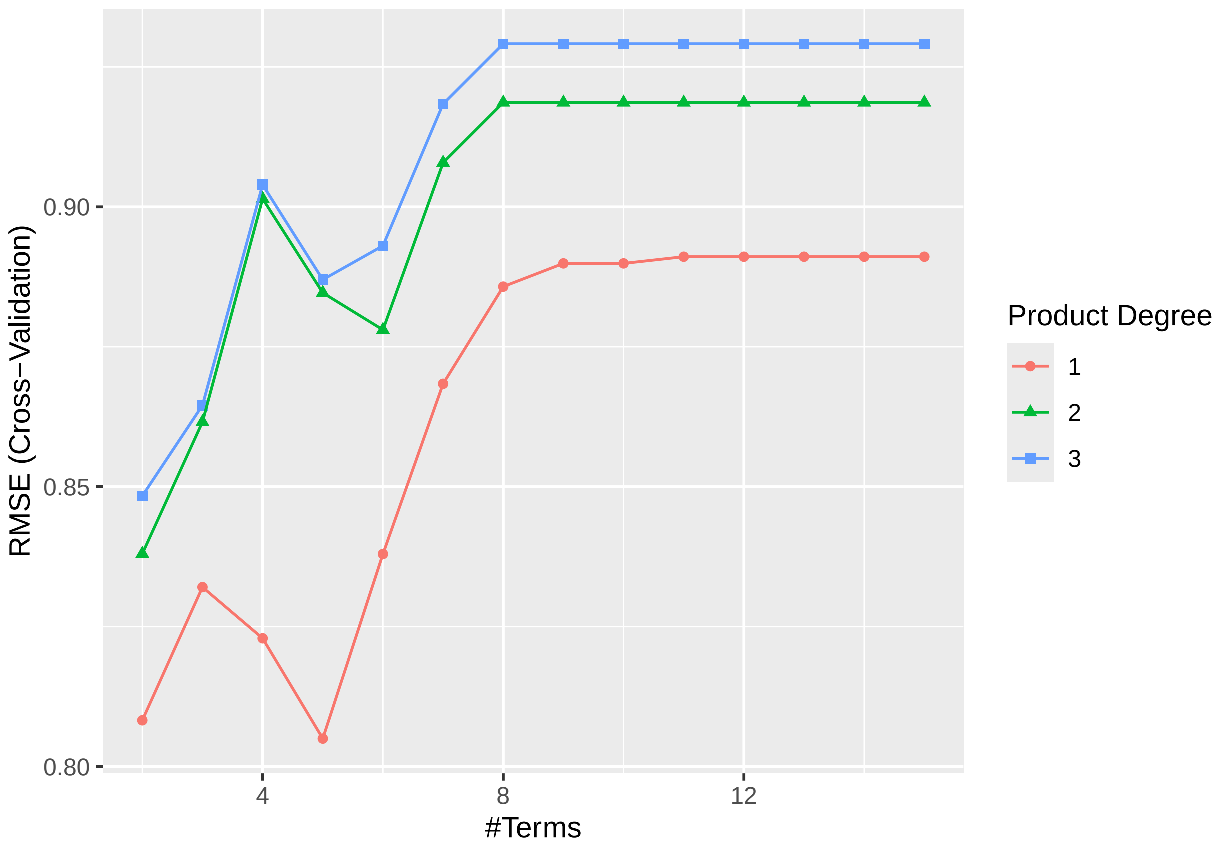
```r
gam.fit$finalModel
```

```
##
## 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
```

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

```r
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)
```



```r
mars.fit$bestTune
```

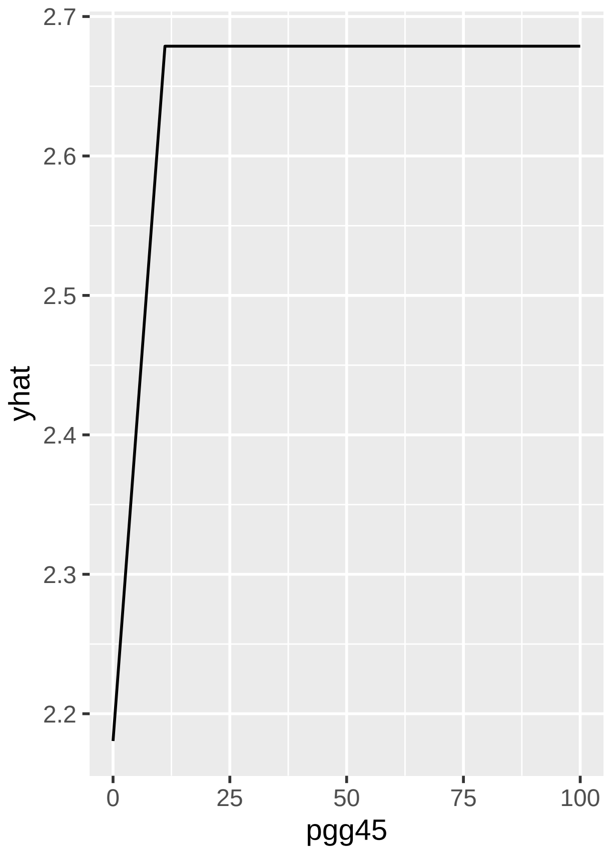
```
##   nprune degree
## 4      5      1
```

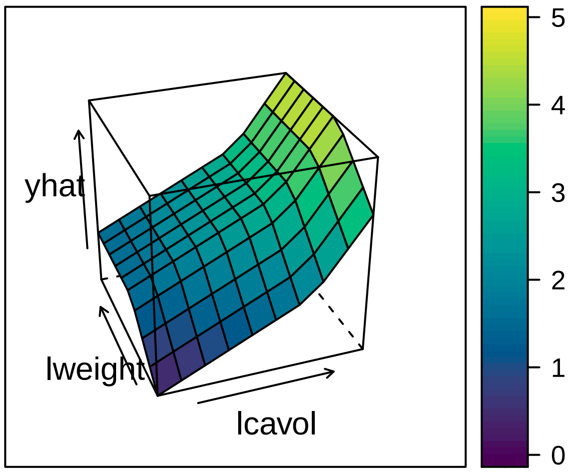
```r
coef(mars.fit$finalModel)
```

```
##        (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
```

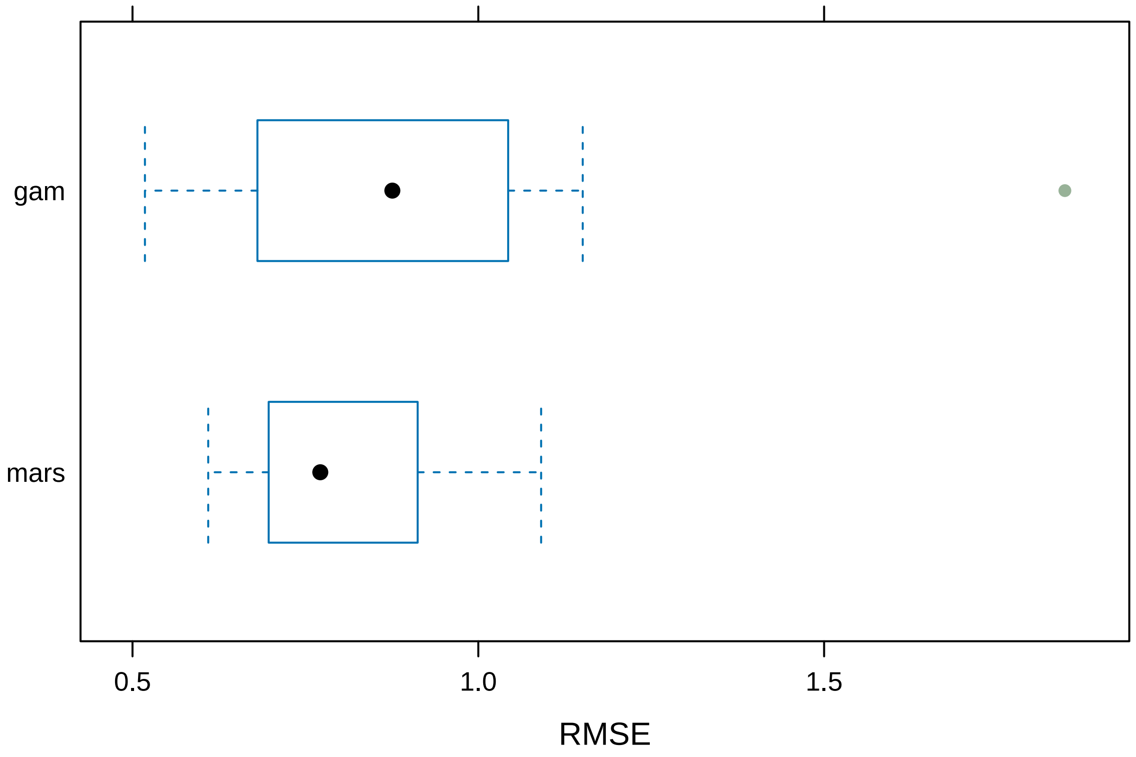
To better understand the relationship between these features and `lpsa`, we can create partial dependence plots (PDPs) for each feature individually and also an interaction PDP. This is used to examine the marginal effects of predictors.

```r
p1 <- pdp::partial(mars.fit, pred.var = c("pgg45"), grid.resolution = 10) |> autoplot()

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))

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





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



Using tidymodels (optional)

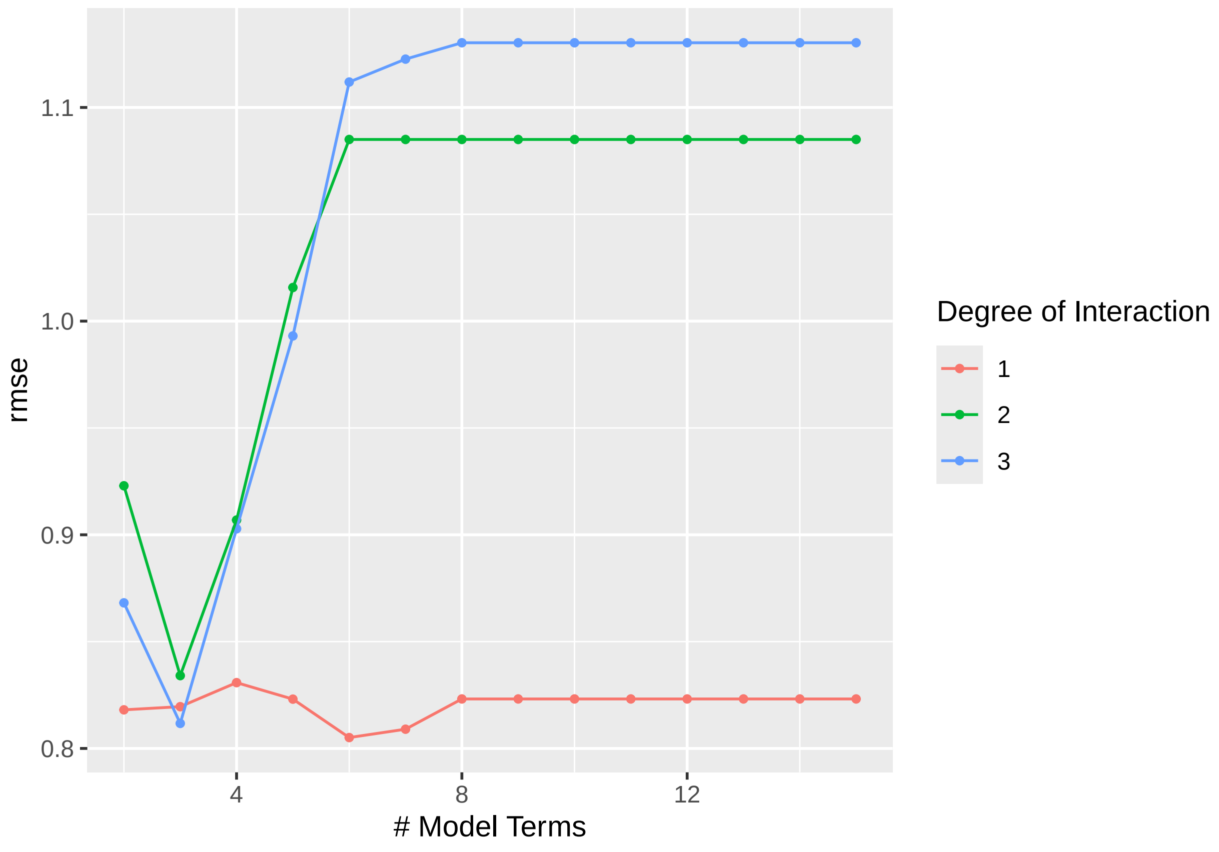
```
# GAM model
set.seed(2)
cv_folds <- vfold_cv(Prostate, v = 10) # you can try other options

# Model specification for GAM
gam_spec <- gen_additive_mod(select_features = tune()) |>
  set_engine("mgcv") |>
  set_mode("regression")


# Set up the workflow
gam_workflow <- workflow() |>
  add_model(gam_spec,
            formula = lpsa ~ s(lcavol) + s(lweight) + s(age) + s(lbph) +
                             svi + s(lcp) + gleason + s(pgg45)) |>
  add_formula(lpsa ~ lcavol + lweight + age + lbph + svi + lcp + gleason + pgg45)

# choose the tuning parameter
gam_res <-
  gam_workflow |> tune_grid(resamples = cv_folds)

show_best(gam_res, metric = "rmse")
```

```
## # A tibble: 2 x 7
##   select_features .metric .estimator  mean     n std_err .config
##   <lgl>           <chr>   <chr>      <dbl> <int>   <dbl> <chr>
## 1 TRUE            rmse    standard   0.861    10  0.0461 Preprocessor1_Model2
## 2 FALSE           rmse    standard   0.933    10  0.0894 Preprocessor1_Model1
```

```
# Update the model spec
final_gam_spec <- gam_spec |>
  update(select_features = "TRUE")

gam_fit <- fit(final_gam_spec,
               formula = lpsa ~ s(lcavol) + s(lweight) + s(age) + s(lbph) +
                         svi + s(lcp) + gleason + s(pgg45),
               data = Prostate)

gam_model <- extract_fit_engine(gam_fit)
gam_model
```

```
##
## Family: gaussian
## Link function: identity
##
## Formula:
## lpsa ~ s(lcavol) + s(lweight) + s(age) + s(lbph) + svi + s(lcp) +
##     gleason + s(pgg45)
##
## Estimated degrees of freedom:
## 4.582 1.520 1.470 0.716 0.000 3.651  total = 14.94
##
## GCV score: 0.5357211
```

```r
# Model Specification for MARS
mars_spec <- mars(num_terms = tune(),
                  prod_degree = tune()) |>
  set_engine("earth") |>
  set_mode("regression")

# mars_spec |> extract_parameter_dials("num_terms")
# mars_spec |> extract_parameter_dials("prod_degree")

# Tuning Grid
mars_grid_set <- parameters(num_terms(range = c(2, 15)),
                            prod_degree(range = c(1, 3)))
mars_grid <- grid_regular(mars_grid_set, levels = c(14, 3))

# Set up the workflow
mars_workflow <- workflow() |>
  add_model(mars_spec) |>
  add_formula(lpsa ~ .)

mars_tune <- tune_grid(
  mars_workflow,
  resamples = cv_folds,
  grid = mars_grid
)


autoplot(mars_tune, metric = "rmse")
```



```r
# Select the best combination of parameters based on the RMSE metric
mars_best <- select_best(mars_tune, metric = "rmse")

# Update the model spec
final_mars_spec <- mars_spec |>
  update(num_terms = mars_best$num_terms,
         prod_degree = mars_best$prod_degree)

mars_fit <- fit(final_mars_spec, formula = lpsa ~ ., data = Prostate)

mars_model <- extract_fit_engine(mars_fit)
coef(mars_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
```