Splines vs. polynomes for fitting non-linear relationships

Brice Ozenne

July 1, 2017

Contents

1 Simulate data 2

2 Prepare data with non linear transformations of X 2

3 Fit models 3

4 Extract the fitted values 3

5 Display fit 3

Note: this is document is inspired from `http://stackoverflow.com/questions/15837763/b-spline-confusion`

1 Simulate data

```
library(splines)
library(data.table)
library(ggplot2)
library(mgcv)

set.seed(1)
n <- 400

x <- 0:(n-1)/(n-1)
dt <- data.table(X = x,
         Ytrue =  0.2*x^11*(10*(1-x))^6+10*(10*x)^3*(1-x)^10)
dt[,Y := Ytrue + rnorm(n, 0, sd = 0.5)]
```

2 Prepare data with non linear transformations of X

```
dt[,X2 := X^2]
dt[,X3 := X^3]
dt[,X4 := X^4]
dt[,X5 := X^5]
dt[,X6 := X^6]

Xknots <- c(0.2, 0.5, 0.7)
SplineTempo <- bs(dt$X, knots = Xknots)
dt <- cbind(dt, setNames(as.data.frame(SplineTempo), paste0("S",1:ncol(SplineTempo))))
```

3 Fit models

```
lmPoly <- lm(Y ~ X + X2 + X3 + X4 + X5 + X6, data = dt)

lmSpline <- lm(Y ~ bs(x, knots = c(0.2, 0.5, 0.7)), data = dt)

lmSplineI <- lm(Y ~ S1 + S2 + S3 + S4 + S5 + S6, data = dt)
range(coef(lmSpline)-coef(lmSplineI)) # same as lmSpline

autoSpline <- gam(Y ~ s(X), data = dt)
```

```
[1] 0 0
```

Residual degree of freedom:

```
c(df.residual(lmPoly),df.residual(lmSpline), df.residual(autoSpline))
```

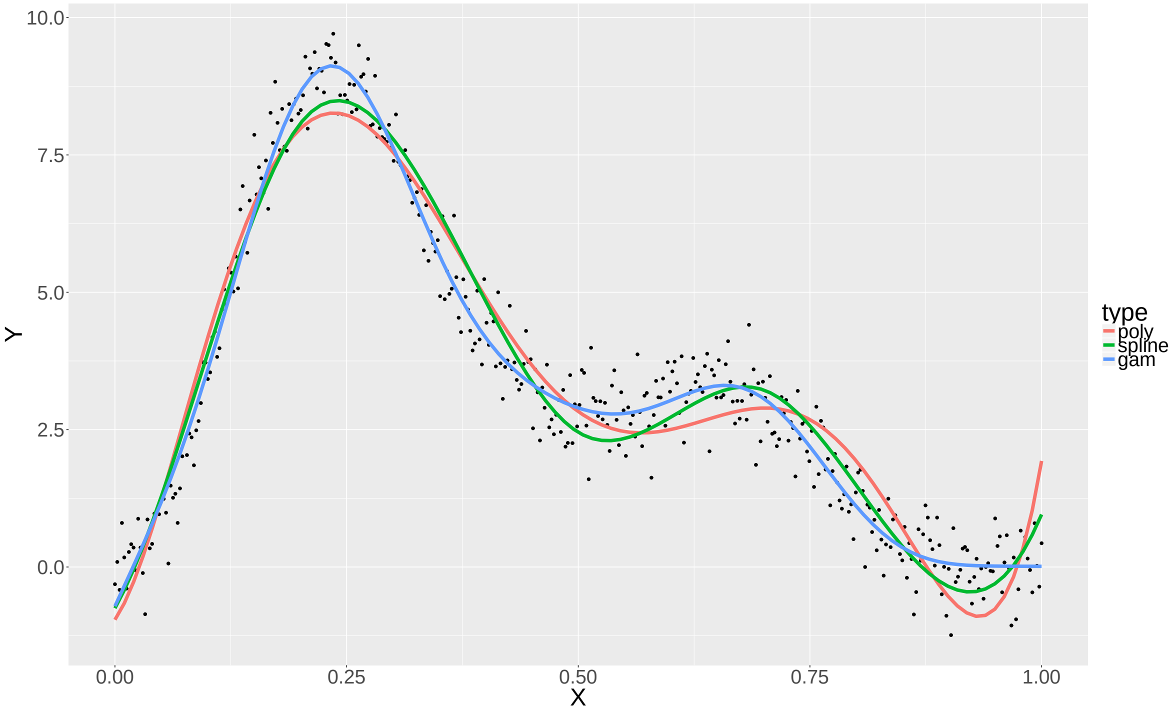
```
[1] 393.0000 393.0000 390.0559
```

4 Extract the fitted values

```
seqX <- seq(min(dt$X), max(dt$X), length = 100)

dt2 <- data.table(Y = dt$Y, X = dt$X, type = "observed")

predPoly <- predict(lmPoly, newdata = data.frame(X = seqX, X2 = seqX^2, X3 = seqX^3, X4 =
    seqX^4, X5 = seqX^5, X6 = seqX^6))
dt2 <- rbind(dt2, data.frame(Y = predPoly, X = seqX, type = "poly"))

predSpline <- predict(lmSpline, newdata = data.frame(x = seqX))
dt2 <- rbind(dt2, data.frame(Y = predSpline, X = seqX, type = "spline"))

predGam <- predict(autoSpline, newdata = data.frame(X = seqX))
dt2 <- rbind(dt2, data.frame(Y = predGam, X = seqX, type = "gam"))
```

5 Display fit

```
ggbase <- ggplot(dt2[dt2$type == "observed",], aes(x = X, y = Y)) + geom_point()
ggbase <- ggbase + geom_line(data = dt2[dt2$type != "observed",],
                 aes(x = X, y = Y, group = type, color = type),
                 size = 2)
 ggbase <- ggbase + theme(text = element_text(size=30))
```



Splines give a better fit compared to a 3rd order polynomial when the knots are correctly placed