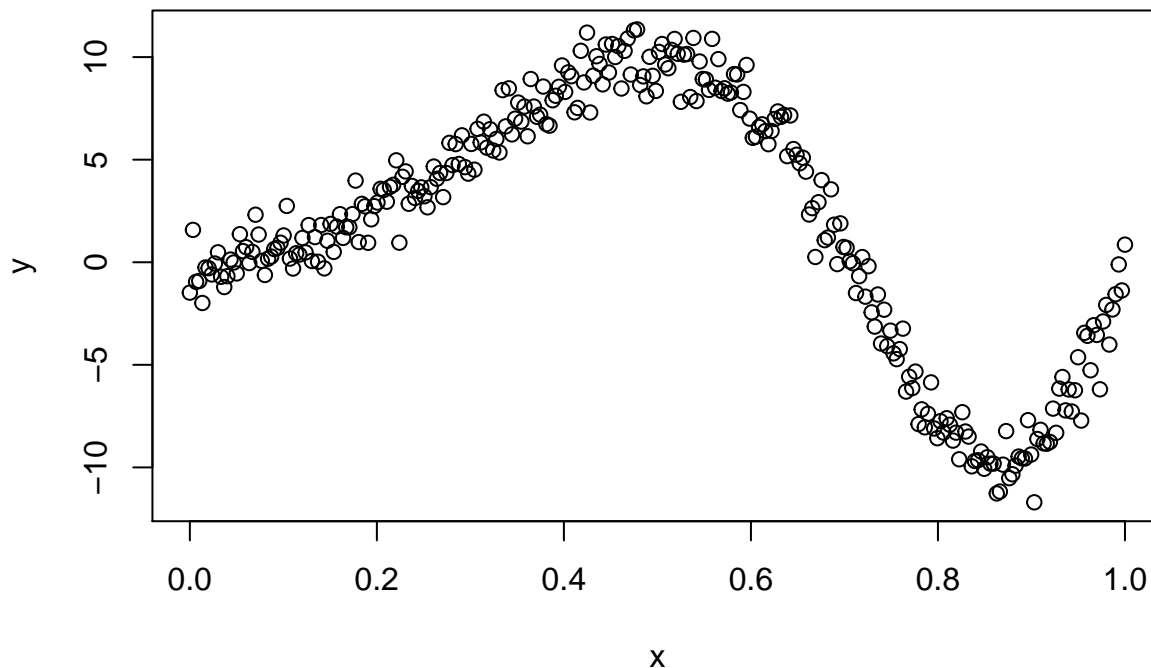


Introduction to Splines

Andy Shen, Devin Francom

Let's say you want to fit a model using some wiggly data. Maybe

```
set.seed(12)
n<-300
x<-seq(0,1,length.out=n)
y<-sin(2*pi*x^2)*10+rnorm(n)
plot(x,y)
```



One way to fit a model to data like this is to come up with a linear basis and fit a linear model using the basis as the X matrix (which we will call B). People often use splines as a basis. The simplest set of spline basis functions would be to make the i th basis function (i.e., the i th column of B) look like

$$B_{ij} = [s_i(x_j - t_i)]_+$$

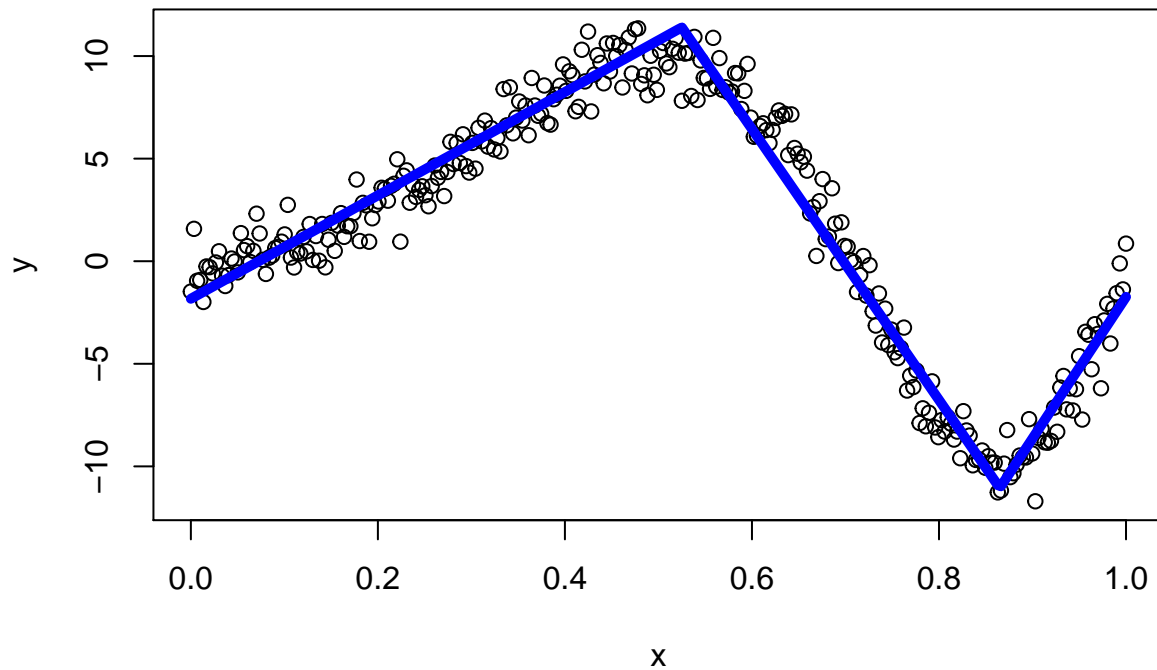
where $s \in \{-1, 1\}$, which we'll call the sign, and t is a value in the domain of x , which we will call a knot. Also, $[a]_+ = \max(0, a)$.

Try some combinations of s and t to see what your basis functions look like, and what the corresponding linear model fit looks like (using the `lm` function or your Bayesian linear model code). Try with different numbers of basis functions, also.

1 Manual Frequentist Spline Function

```
generate_spline <- function(tvec, y, x, nknot = length(tvec)) {  
  s <- sample(c(1), nknot, replace = TRUE)  
  Bmat <- matrix(NA, nknot, length(x))  
  hs <- Bmat  
  
  for(i in 1:nknot) {  
    for(j in 1:length(x)) {  
      Bmat[i,j] <- max(s[i] * (x[j] - tvec[i]), 0)  
    } #creating basis functions  
  }  
  
  mBmat <- t(Bmat)  
  mod <- lm(y ~ mBmat) #use gibbs to sample coefs in bayes  
  pred <- predict(mod)  
  
  sq <- x  
  for(ii in 1:nknot) {  
    if(s[ii] == 1) {  
      hs[ii,] <- sq - tvec[ii]  
      hs[ii,][sq < tvec[ii]] <- 0  
    }  
    else {  
      hs[ii,] <- -1*(sq - tvec[ii])  
      hs[ii,][sq < tvec[ii]] <- 0  
    }  
  } #setting x values  
  
  plot(x,y, main = "Manual Basis Spline")  
  lines(x, pred, type = "l", lwd = 5, col="blue1")  
  summary(mod)  
}  
  
tv <- c(0, 0.525, 0.865) #vector of t-values  
generate_spline(tv, y = y, x = x)
```

Manual Basis Spline



```
##
## Call:
## lm(formula = y ~ mBmat)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -3.5715 -0.8087 -0.0387  0.7499  3.4953
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  -1.8306     0.1817  -10.08  <2e-16 ***
## mBmat1         25.1946     0.5270   47.81  <2e-16 ***
## mBmat2        -91.2259     1.1975  -76.18  <2e-16 ***
## mBmat3        135.0260     3.6954   36.54  <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1.208 on 296 degrees of freedom
## Multiple R-squared:  0.963, Adjusted R-squared:  0.9626
## F-statistic: 2566 on 3 and 296 DF, p-value: < 2.2e-16
```

2 Bayesian Spline

```
library(mvtnorm)
bayes_spline <- function(tvec, y, x, nknot = length(tvec)) {
  s <- sample(c(1), nknot, replace = TRUE)
  Bmat <- matrix(NA, nknot, length(x))
  hs <- Bmat

  for(i in 1:nknot) {
    for(j in 1:length(x)) {
      Bmat[i,j] <- max(s[i] * (x[j] - tvec[i]), 0)
    } #creating basis
  } #X Matrix

  X <- t(Bmat)
  X <- cbind(1, X)

  p_sig <- function(a = 0, b = 0, n = nrow(X), beta) {
    a_term <- a + (n/2)
    b_term <- 0.5 * (2*b + (t(y - (X %%% beta)) %%% (y - (X %%% beta)))) #y, X defined above
    1 / rgamma(1, shape = a_term, rate = b_term)
  }

  p_beta <- function(sig_sq, tau_sq = 100, p = ncol(X)-1) {
    sig <- solve( (1/sig_sq) * (t(X) %%% X) + (1/tau_sq) * diag(p+1) )
    mu <- (1/sig_sq) * sig %%% t(X) %%% y
    rmvnorm(1, mean = mu, sigma = sig)
  }

  gibbs <- function(its) {
    mat_beta <- matrix(NA, its, ncol(X))
    mat_sig <- rep(NA, its)
    mat_sig[1] <- 0.01
    mat_beta[1,] <- rep(0, ncol(X))
    for(it in 2:its) {
      mat_beta[it,] <- p_beta(sig_sq = mat_sig[it-1])
      mat_sig[it] <- p_sig(beta = mat_beta[it,])
    }
    list(mat_beta, mat_sig)
  }

  its <- 3000
  a <- gibbs(its = its)
  mat_beta <- a[[1]] #beta values
  mat_sig <- a[[2]] #sig^2 values

  sq <- x
  for(ii in 1:nknot) {
    if(s[i] == 1) {
      hs[ii,] <- sq - tvec[ii]
      hs[ii,][sq < tvec[ii]] <- 0
    }
    else {

```

```

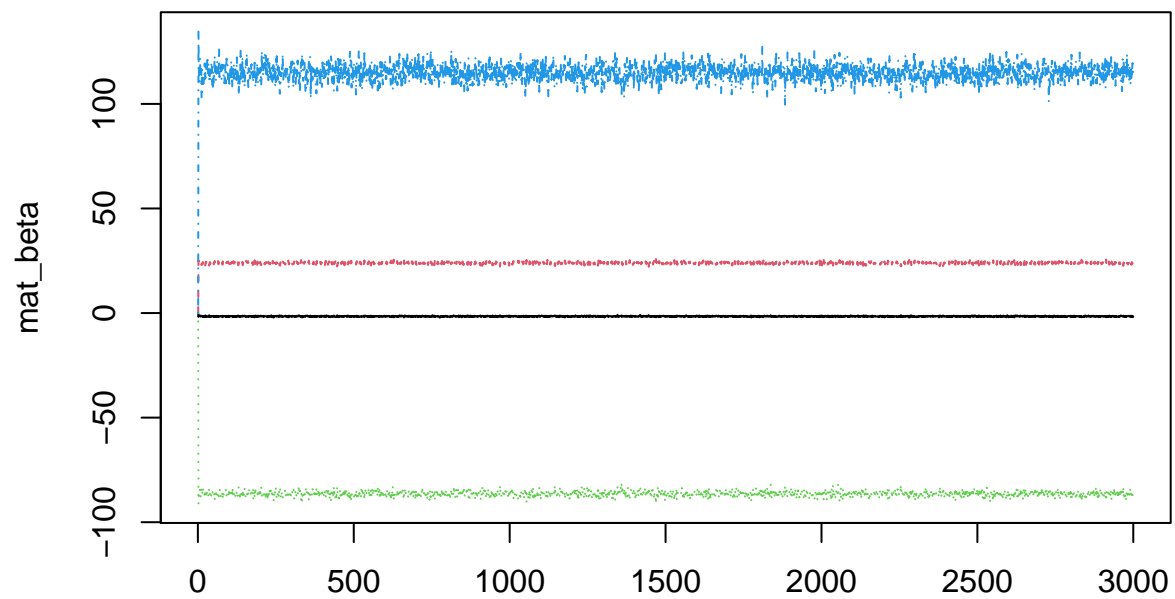
    hs[ii,] <- -1*(sq - tvec[ii])
    hs[ii,][sq > tvec[ii]] <- 0
  }
} #setting x values

list(mat_beta, mat_sig)
}
mat_beta <- bayes_spline(c(0, 0.525, 0.865), y = y, x = x)[[1]]
mat_sig <- bayes_spline(c(0, 0.525, 0.865), y = y, x = x)[[2]]

matplot(mat_beta, type = "l", main = "Sampled Model Coefficients")

```

Sampled Model Coefficients

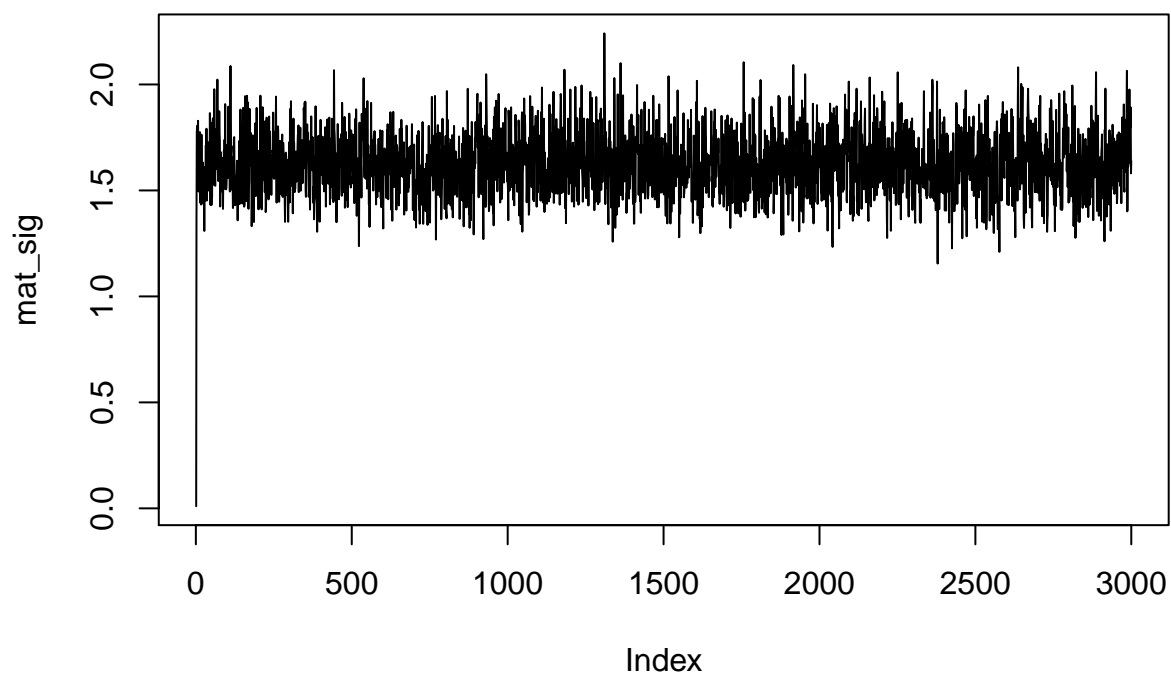


```

plot(mat_sig, type = "l", main = "Sampled sigma^2 values")

```

Sampled σ^2 values



```
burn <- 1:15  
colMeans(mat_beta[-burn,]) #target: -1.83, 25.19, -91.23, 135.03
```

```
## [1] -1.576187 23.966745 -86.398181 114.966455
```

```
mean(mat_sig[-burn]) #target: 1.46
```

```
## [1] 1.62259
```

Trying things out

```
t1 <- 0.5 #knot at 0.5
s <- 1
B1 <- rep(NA, length(x))

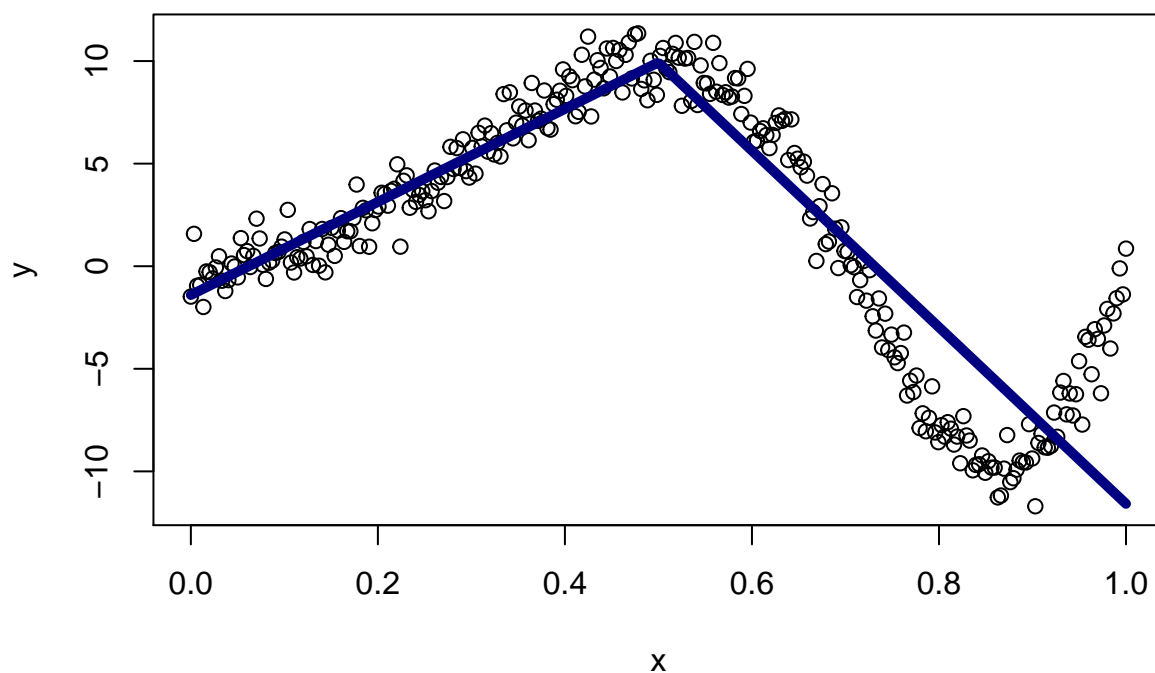
for(i in 1:length(x)) {
  B1[i] <- max(s * (x[i] - t1), 0)
}
mod <- lm(y ~ x + B1)
summary(mod)

##
## Call:
## lm(formula = y ~ x + B1)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -5.8060 -1.0370  0.0118  1.3000 12.4394
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  -1.4034     0.4206  -3.336 0.000957 ***
## x             22.6785     1.2327  18.398 < 2e-16 ***
## B1           -65.7131     2.2051 -29.801 < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 2.766 on 297 degrees of freedom
## Multiple R-squared:  0.8054, Adjusted R-squared:  0.8041
## F-statistic: 614.5 on 2 and 297 DF,  p-value: < 2.2e-16

cf <- mod$coefficients
sq <- x
hs <- sq - t1
hs[sq < t1] <- 0
yfit <- cf[1] + cf[2]*x + cf[3]*hs

plot(x,y, main = "Manual Basis Spline")
lines(x, yfit, type = "l", lwd = 5, col="navy")
```

Manual Basis Spline



Add another knot

```
t1 <- 0.525
t2 <- 0.865
s <- 1
B1 <- rep(NA, length(x))
B2 <- B1

for(i in 1:length(x)) {
  B1[i] <- max(s * (x[i] - t1), 0)
  B2[i] <- max(s * (x[i] - t2), 0)
}
mod <- lm(y ~ B1 + B2)

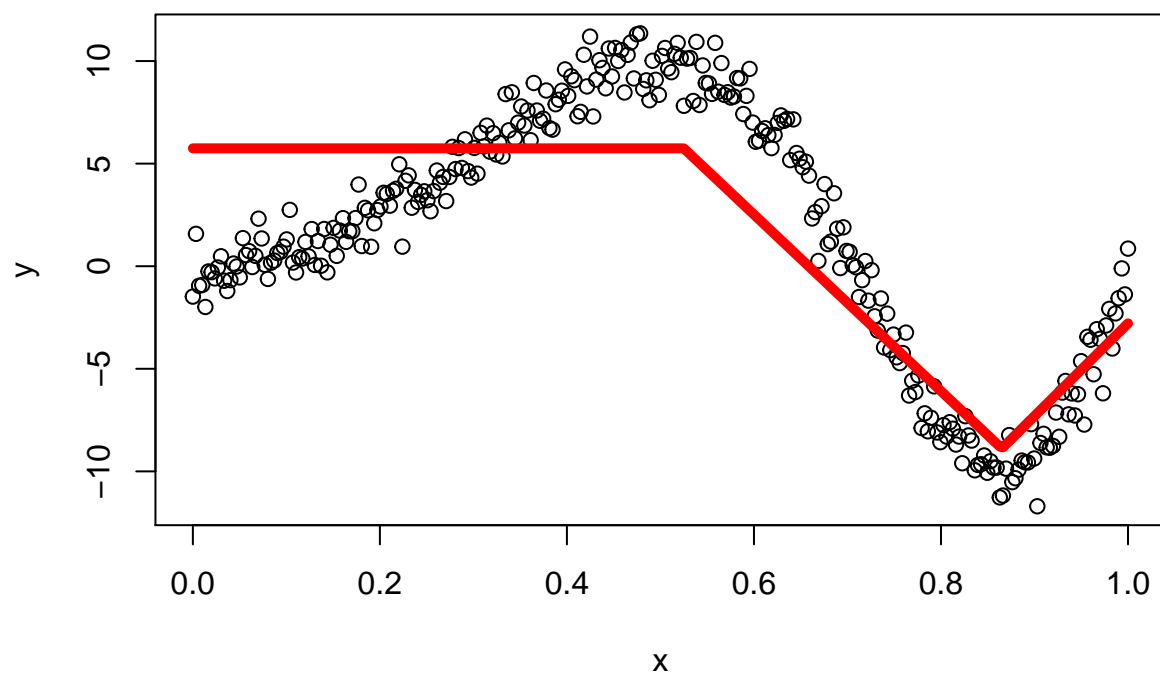
cf <- mod$coefficients
sq <- x
hs1 <- sq - t1
hs1[sq < t1] <- 0

hs2 <- sq - t2
hs2[sq < t2] <- 0

yfit <- cf[1] + cf[2]*x + cf[3]*hs1 + cf[4]*hs2
yfit2 <- predict(mod) #same thing

plot(x,y, main = "Manual Basis Spline")
lines(x, yfit2, type = "l", lwd = 5, col="red")
```


Manual Basis Spline



Add another knot (expected)

```
t1 <- 0 #knot at 0.5
t2 <- 0.525 #another knot at 0.85
t3 <- 0.865
s <- 1
B1 <- rep(NA, length(x))
B3 <- B2 <- B1

for(i in 1:length(x)) {
  B1[i] <- max(s * (x[i] - t1), 0)
  B2[i] <- max(s * (x[i] - t2), 0)
  B3[i] <- max(s * (x[i] - t3), 0)
}
mod <- lm(y ~ B1 + B2 + B3)
summary(mod)

##
## Call:
## lm(formula = y ~ B1 + B2 + B3)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -3.5715 -0.8087 -0.0387  0.7499  3.4953
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  -1.8306     0.1817  -10.08  <2e-16 ***
## B1             25.1946     0.5270   47.81  <2e-16 ***
## B2            -91.2259     1.1975  -76.18  <2e-16 ***
## B3            135.0260     3.6954   36.54  <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1.208 on 296 degrees of freedom
## Multiple R-squared:  0.963, Adjusted R-squared:  0.9626
## F-statistic: 2566 on 3 and 296 DF, p-value: < 2.2e-16

cf <- mod$coefficients
sq <- x

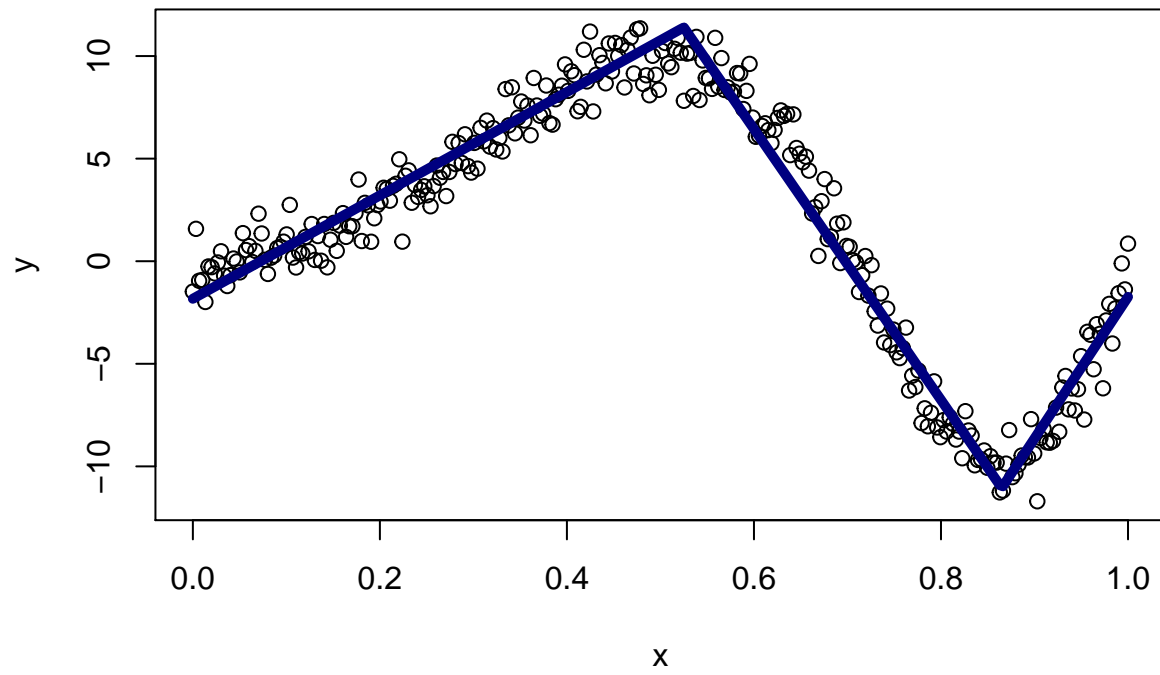
hs1 <- sq - t1
hs1[sq < t1] <- 0

hs2 <- sq - t2
hs2[sq < t2] <- 0

hs3 <- sq - t3
hs3[sq < t3] <- 0

yfit2 <- cf[1] + cf[2]*x + cf[3]*hs1 + cf[4]*hs2 + cf[5]*hs3
yfit <- predict(mod)
plot(x,y, main = "Manual Basis Spline")
lines(x, yfit, type = "l", lwd = 5, col="navy")
```

Manual Basis Spline

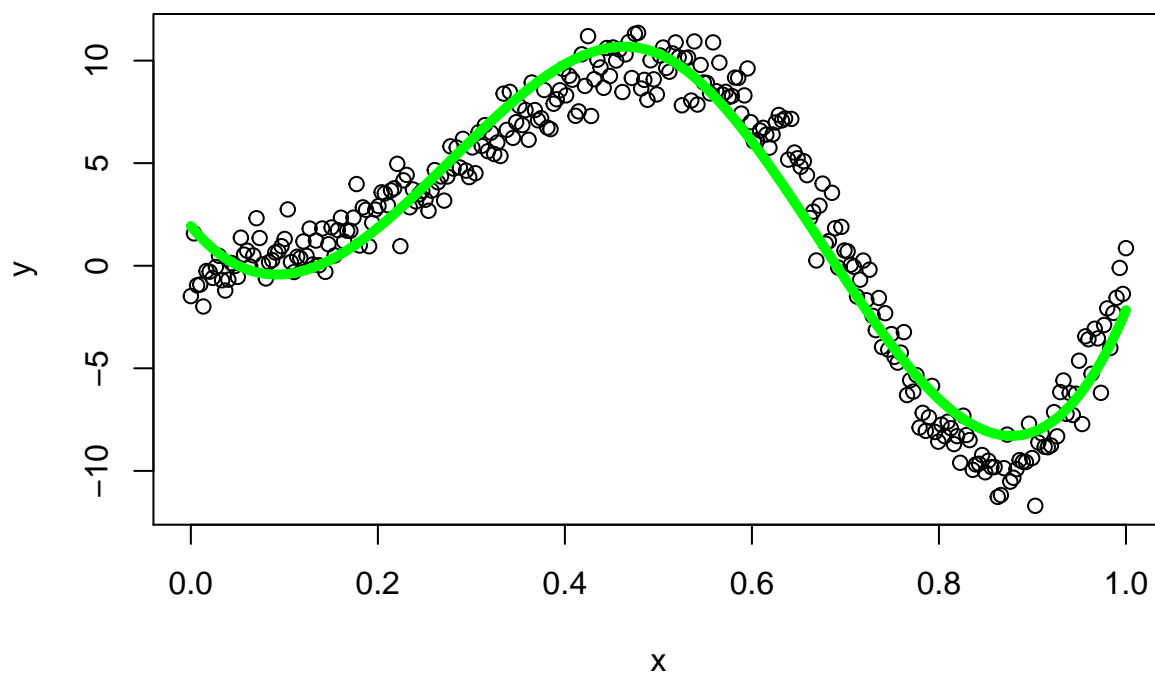


Using the bs() Function

1 Knot

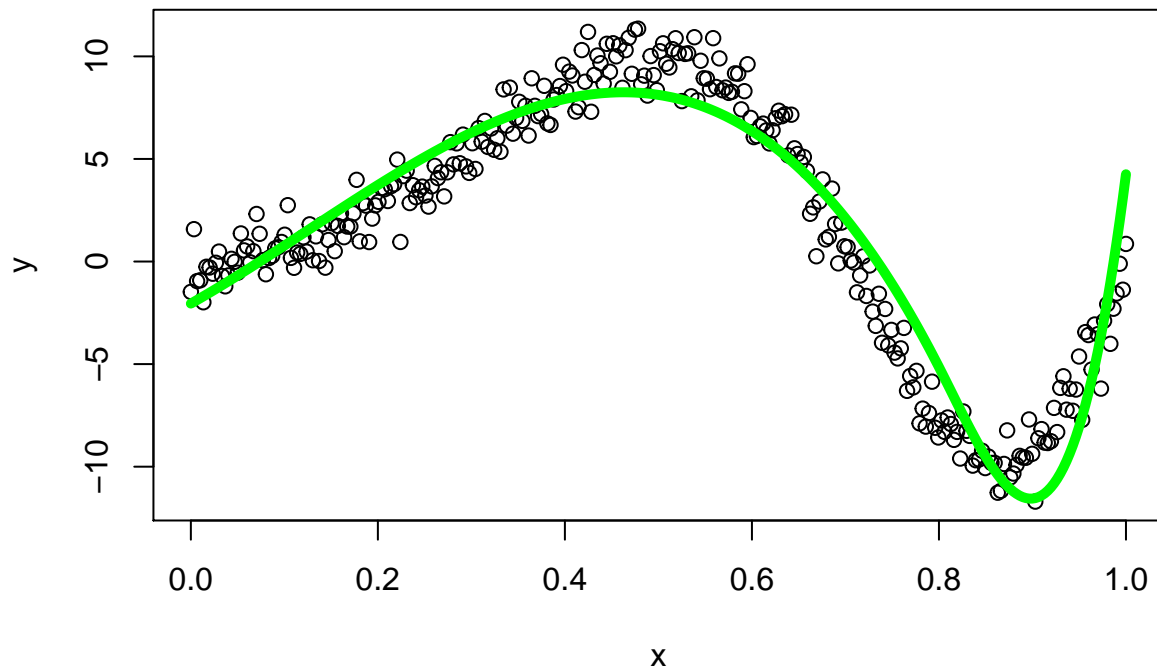
```
library(splines)
df <- data.frame(y, x)
m2 <- lm(y ~ bs(x, knots = 0.5), data = df)
pred <- predict(m2)

plot(x,y)
lines(x, pred, lwd = 5, col = "green")
```



```
m2 <- lm(y ~ bs(x, knots = 0.8), data = df)
pred <- predict(m2)

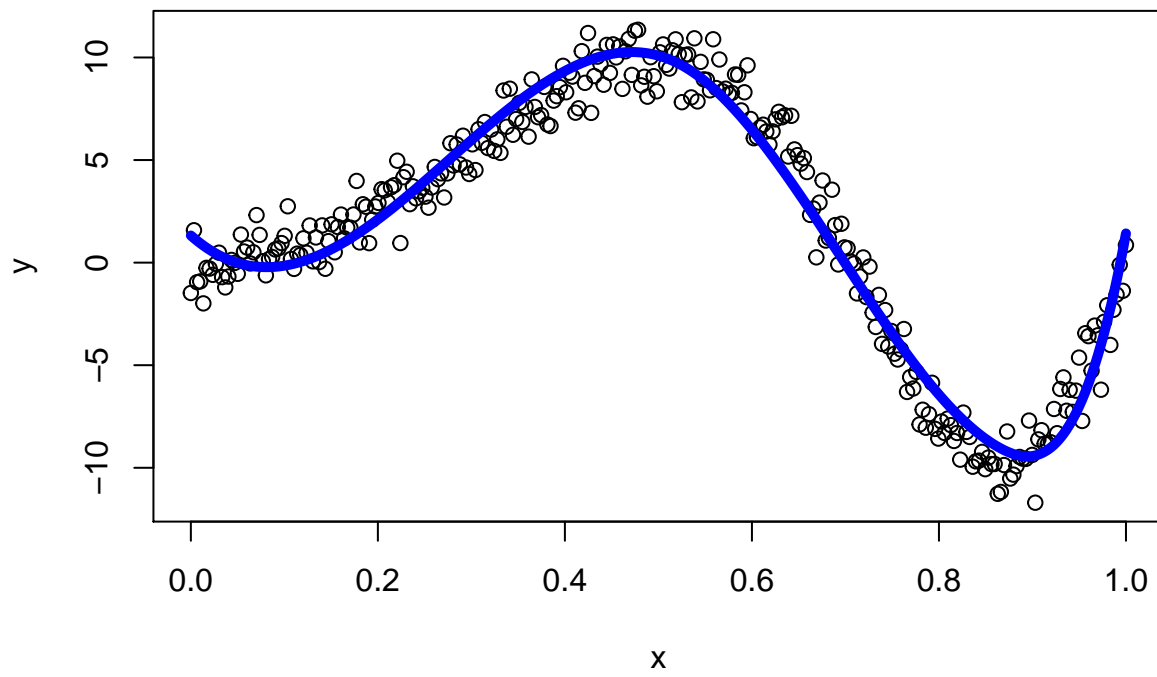
plot(x,y)
lines(x, pred, lwd = 5, col = "green")
```



2 Knots (Expected)

```
m1 <- lm(y ~ bs(x, knots = c(0.525, 0.865)), data = df)
pred <- predict(m1)

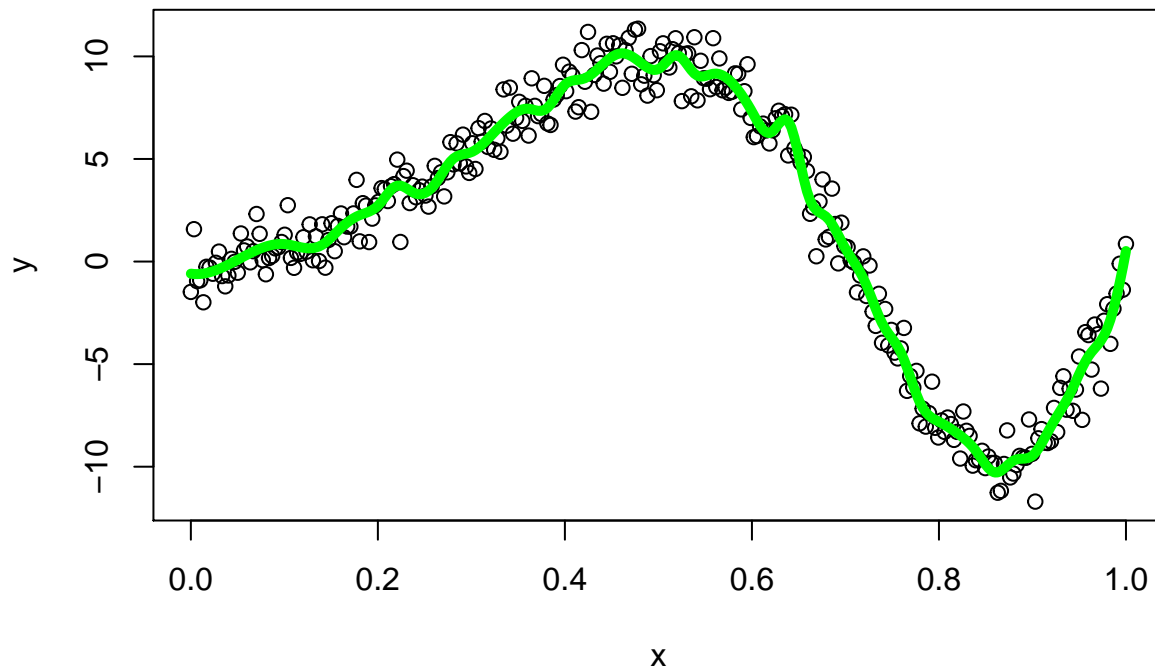
plot(x,y)
lines(x, pred, lwd = 5, col = "blue")
```



Too Many Knots

```
m2 <- lm(y ~ bs(x, knots = seq(0.1,1,by=0.02)), data = df)
pred <- predict(m2)

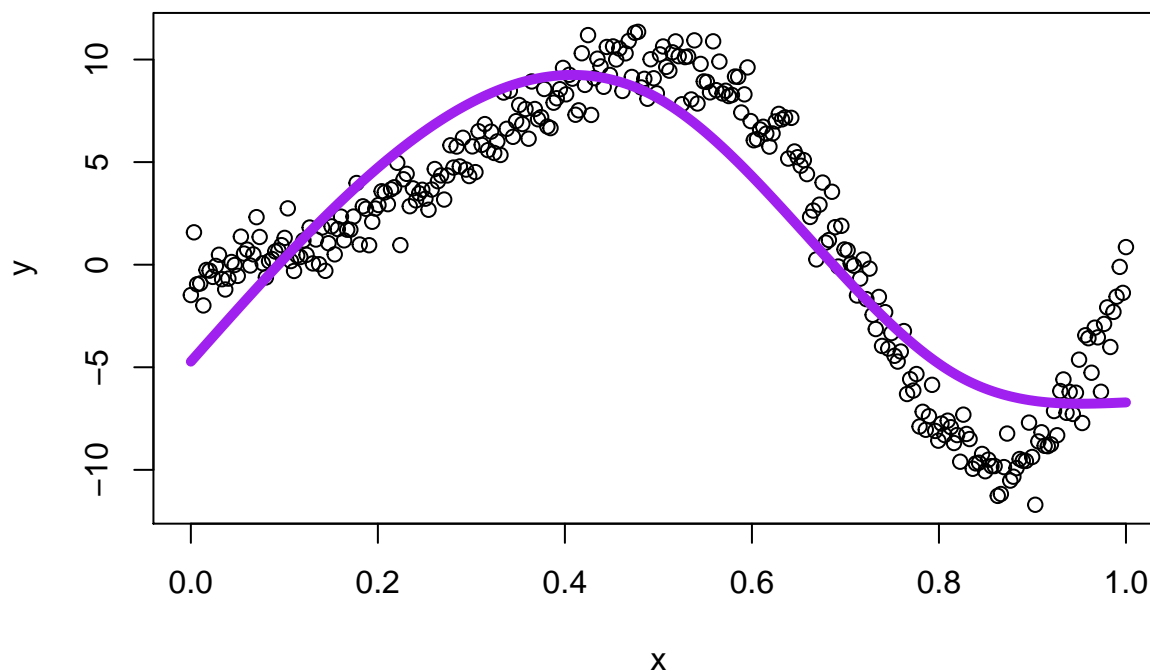
plot(x,y)
lines(x, pred, lwd = 5, col = "green")
```



Natural Splines

```
m3 <- lm(y ~ ns(x, knots = c(0.5, 0.82)), data = df)
pred <- predict(m3)
```

```
plot(x,y)
lines(x, pred, lwd = 5, col = "purple")
```



```
summary(m1)
```

```
##
## Call:
## lm(formula = y ~ bs(x, knots = c(0.525, 0.865)), data = df)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -2.8195 -0.9079  0.0429  0.8680  3.2511
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)      1.3218    0.3451   3.830 0.000157 ***
## bs(x, knots = c(0.525, 0.865))1  -7.0653    0.7472  -9.455 < 2e-16 ***
## bs(x, knots = c(0.525, 0.865))2   25.4800    0.5165  49.333 < 2e-16 ***
## bs(x, knots = c(0.525, 0.865))3  -12.6591    0.6171 -20.514 < 2e-16 ***
## bs(x, knots = c(0.525, 0.865))4  -11.0100    0.5118 -21.512 < 2e-16 ***
## bs(x, knots = c(0.525, 0.865))5    0.1012    0.6752   0.150 0.880987
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1.269 on 294 degrees of freedom
## Multiple R-squared:  0.9594, Adjusted R-squared:  0.9587
## F-statistic: 1390 on 5 and 294 DF, p-value: < 2.2e-16
```