Smoothing splines in R

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1 Smoothing splines in R

In this video, we will learn how to fit smoothing splines in R. In particular, we will simulate data, and learn to fit smoothing splines in R by fixing a spar/λ value, and by computing a cross validation estimate of spar/λ.

Let's start with a simulation. We'll create a data frame, with a predictor, x, as realizations from a $U(0, \pi/2)$, and let $Y = \sin(\pi x) + \varepsilon$, where $\varepsilon \overset{iid}{\sim} N(0, 0.5^2)$.

[1]:
```
set.seed(88888)

n = 150
x = runif(n, 0, pi/2)
y = sin(pi*x) + rnorm(n, 0, 0.5) + 4

df = data.frame(x = x, y = y)
head(df)
```

A data.frame: 6 × 2

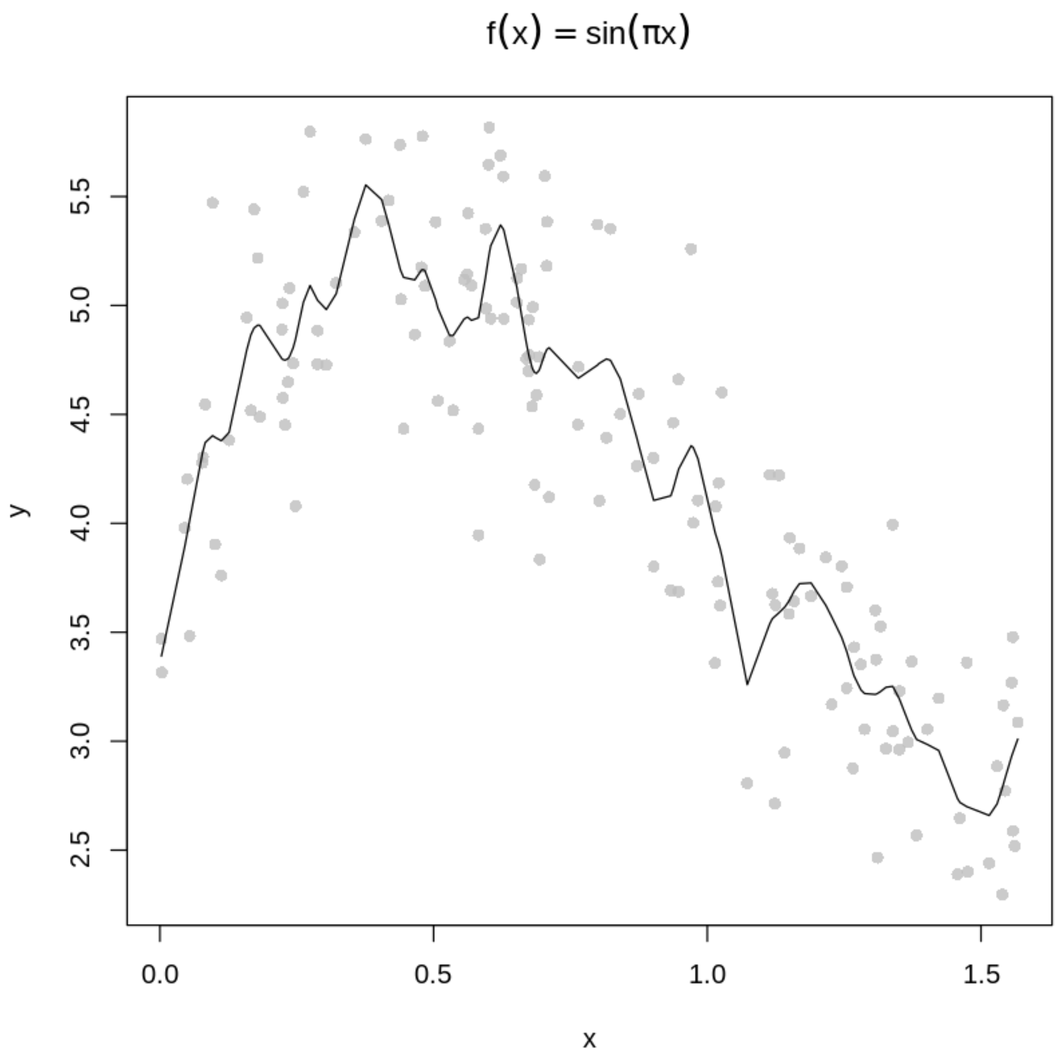
	x <dbl>	y <dbl>
1	0.3760199	5.763870
2	0.9016790	4.300436
3	1.2164907	3.843510
4	1.3107582	2.465646
5	0.4385922	5.737440
6	1.0267308	4.600813

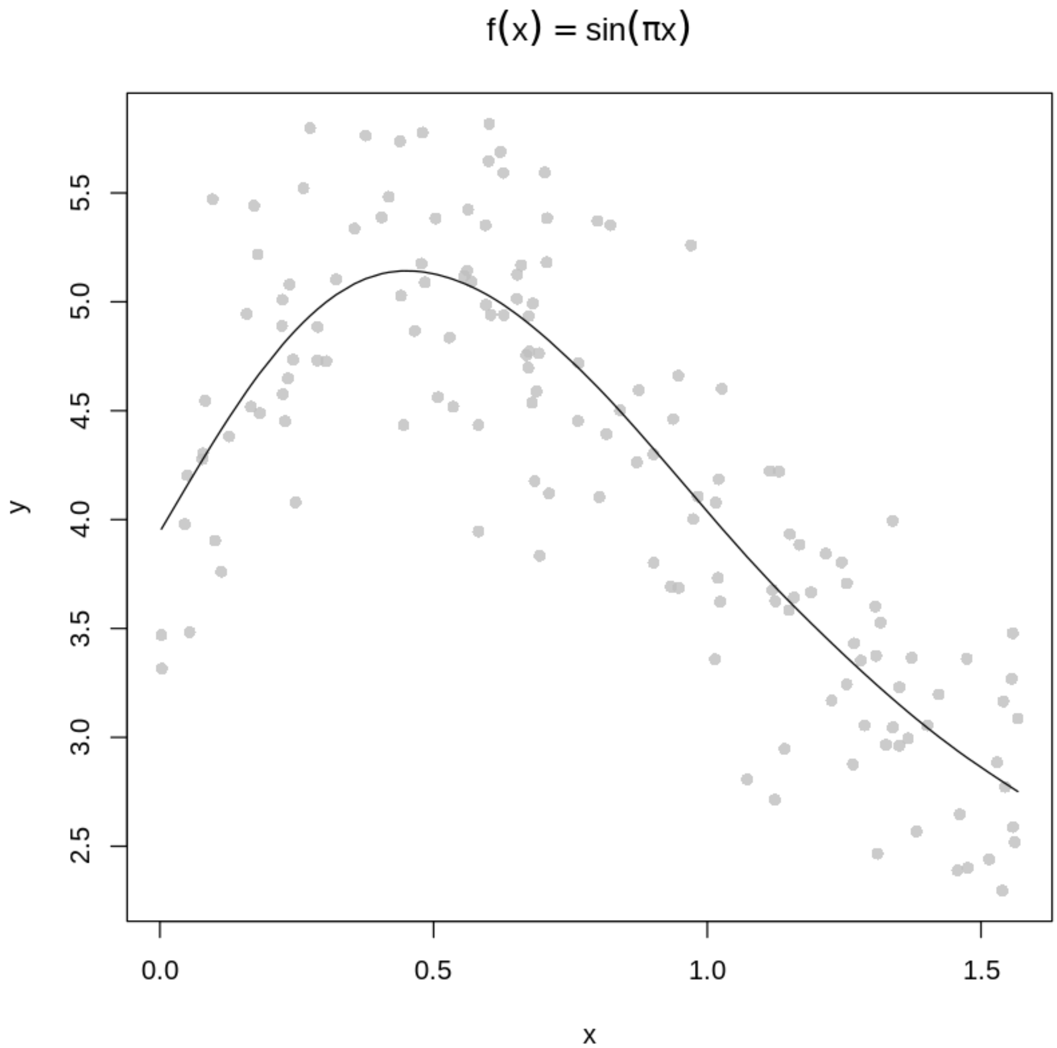
The function `smooth.spline()` can easily compute a smoothing spline estimate, $\widehat{f}(x)$, of the true function $f(x) = \sin(\pi x)$. We'll specify the `x` and `y` coordinates, and the `spar`. Recall again that `spar` is monotone function of the smoothing parameter λ. Experimenting with different values of `spar` can help find a suitable smooth. Also, by leaving `spar` unspecified, R will choose a smoothing parameter value using a cross validation procedure.

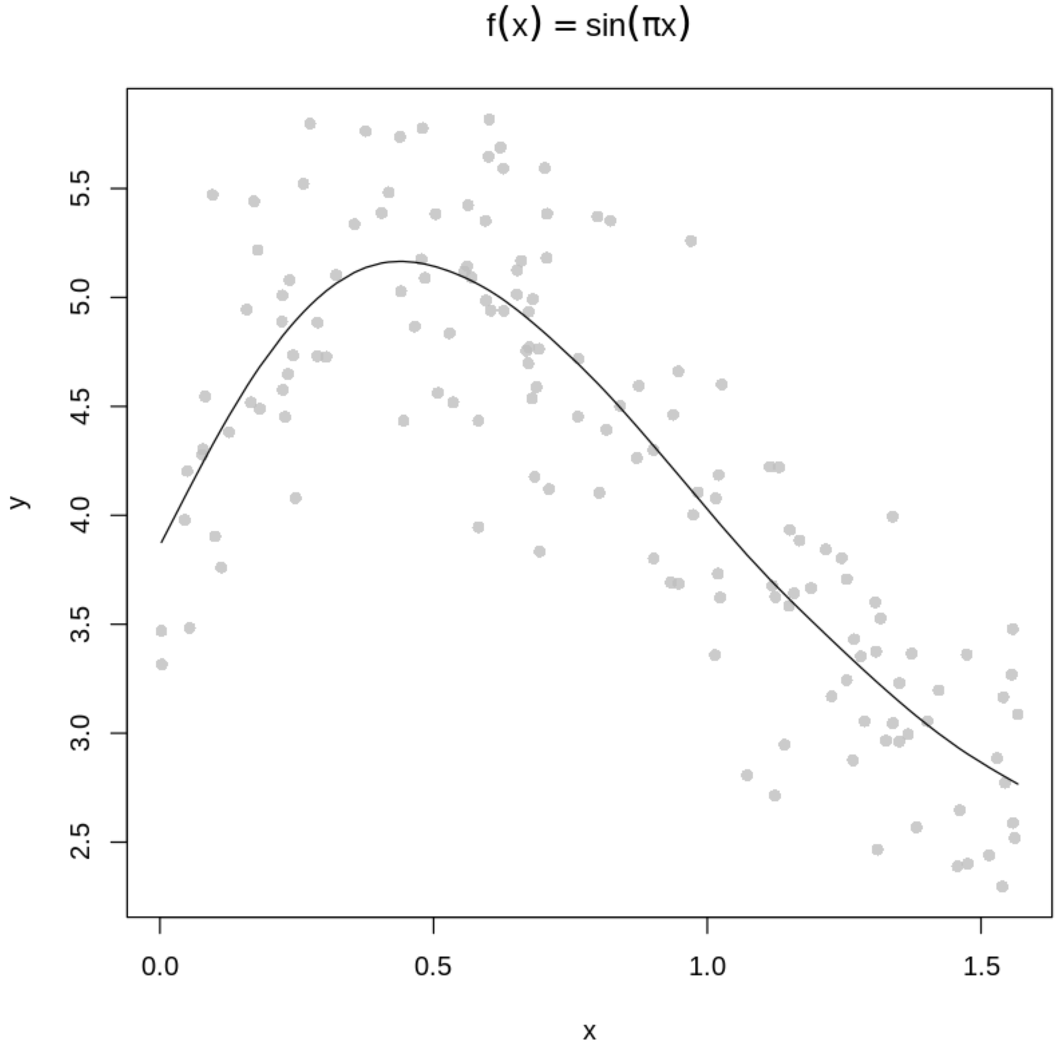
For visualization purposes, we'll make a scatter plot of the data, and overlay the smoothing spline using the `lines()` function. We'll do this with a low value and a high value for spar/λ, along with an automatically chosen spar/λ.

[2]:
```
library(ggplot2)
```

```
plot(y ~ x, main = expression(f(x) == sin(pi*x)), pch = 16, col = alpha("grey",␣
 ↪0.8))
lines(smooth.spline(x, y, spar = 0.5))

plot(y ~ x, main = expression(f(x) == sin(pi*x)), pch = 16, col = alpha("grey",␣
 ↪0.8))
lines(smooth.spline(x,y, spar = 1))

plot(y ~ x, main = expression(f(x) == sin(pi*x)), pch = 16, col = alpha("grey",␣
 ↪0.8))
lines(smooth.spline(x,y))
```




f(x) = sin(πx)
y
x
0.0
0.5
1.0
1.5
2.5
3.0
3.5
4.0
4.5
5.0
5.5



Note that the first fit appears to be too rough, which indicates that λ is too small. The second fit appears to be much better, capturing trends without modeling noise in the data. The last fit, which automatically chooses λ based on a cross validation procedure. One variant of cross validation is as follows.

Choose a grid of λ values (or, since the `smooth.spline()` function is in terms of `spar`, below we'll choose a grid of spar values). For each spar/λ_j:

1. For $i = 1, .., n$, split the data into a training set of all data points *except* the i^{th} point. The i^{th} point serves as the testing set, on which we'll calculate the cross validation error.
2. Fit the smoothing spline model on the training set. For $i = 1, .., n$ compute $\left(y_i - \widehat{f}_{\lambda_j(i)}(x_i)\right)^2$, where $\widehat{f}_{\lambda_j(i)}(\cdot)$ is the predicted smooth fit on the training set (the notation (i) suggests that we are leaving the i^{th} point out of the fit), using λ_j (or corresponding spar value). Note that

the pair (x_i, y_i) is the point that was *left out* of the training set, i.e., it is our test set.

3. For each spar/λ_j, compute

$$CV(\lambda_j) = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - \widehat{f}_{\lambda_j(i)}(x_i)\right)^2. \tag{1}$$

4. Choose the value of λ that with the smallest $CV(\lambda)$.

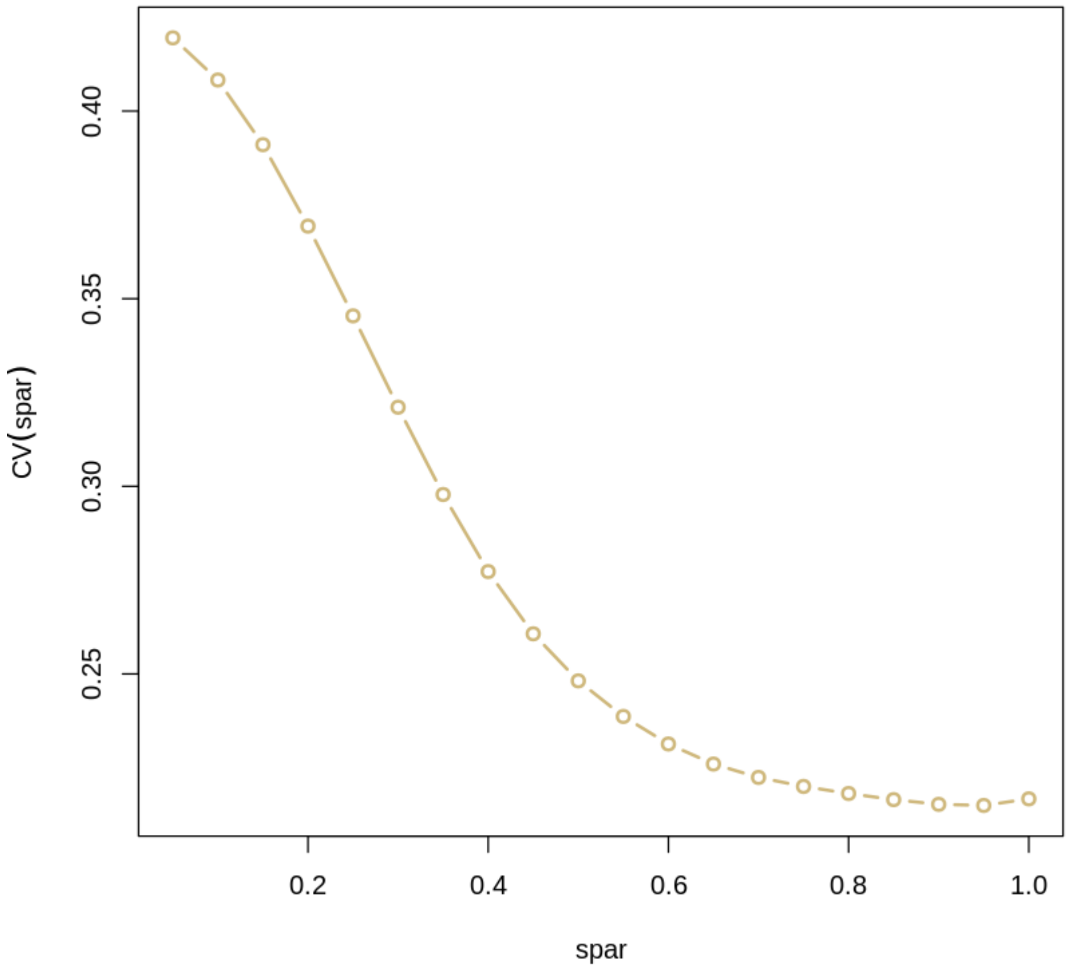
Let's implement this procedure in R.

[3]:
```
spar_seq = seq(from=0.05,to=1, by=0.05) # grid of spar values
CV_err_spar = rep(NA,length(spar_seq))

for(j in 1:length(spar_seq)){
    spar_using = spar_seq[j]
    CV_err = rep(NA, n) #recall that n is the sample size, as defined above
    for(i in 1:n){
        x_test = x[i] #leave one x value out for CV
        y_test = y[i] #leave one y value out for CV

        x_tr = x[-i] #make the remaining x values the x values for the training␣
 ↪set
        y_tr = y[-i] #make the remaining y values the y values for the training␣
 ↪set

    y_test_predict = predict(smooth.spline(x = x_tr,y = y_tr, spar =␣
 ↪spar_using), x_test) #predicted value in test set
    CV_err[i] = (y_test - y_test_predict$y)^2 # squared error
    }

CV_err_spar[j] = mean(CV_err) #CV: mean of the squared errors

}

s = spar_seq[which.min(CV_err_spar)] #the "best" spar value, as measured by␣
 ↪leave-one-out CV

cat("The cross validation procedure chooses spar = ", s, ".")
```

```
The cross validation procedure chooses spar =  0.95 .
```

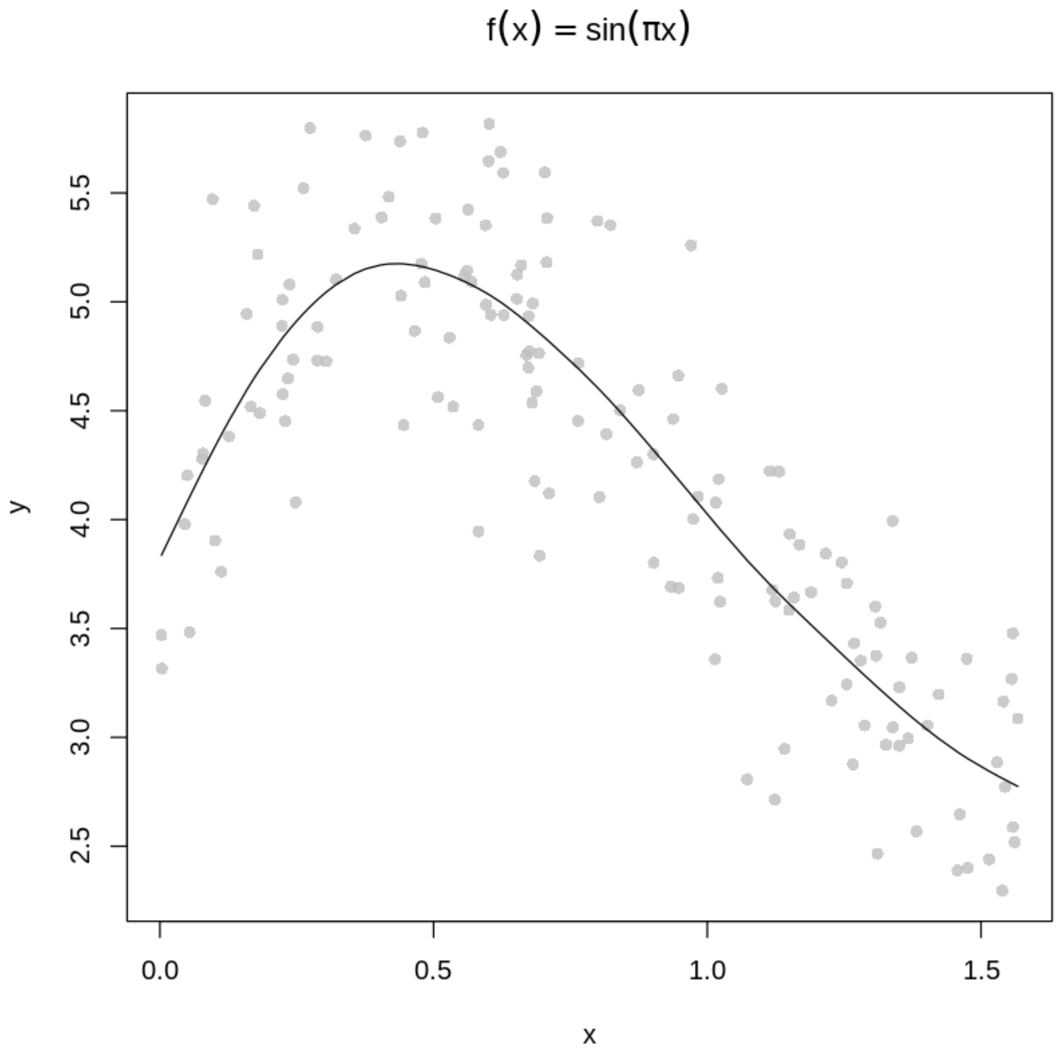
We can plot the "leave one out cross validation error" $CV(spar)$ as a function of spar to visualize the minimum.

[4]:
```
plot(x=spar_seq, y=CV_err_spar, type="b", lwd=2, col="#CFB87C",
     xlab="spar", ylab= expression(CV(spar)))
```



And, we can plot the simulated data and fitted smoothing spline fit using the spar of 0.95...

[5]:
```
plot(y ~ x, main = expression(f(x) == sin(pi*x)), pch = 16, col = alpha("grey",␣
↪0.8))
lines(smooth.spline(x,y, spar = s))
```



f(x) = sin(πx)
y
x
5.5
5.0
4.5
4.0
3.5
3.0
2.5
0.0
0.5
1.0
1.5


```
[ ]:
```