36-617: Applied Linear Models

Nonparametric Regression I

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Announcements

- Work that is due:
  - Midterm solutions are (or will be) out today
  - The "Quiz" (Quiz 05) today will be a for-credit class survey
  - HW05 due Weds at 1159pm
- Midterm grades:
  - HW01-04, Quiz01-05, Participation, Take-home Midterm
- Over the fall break:
  - No hw assigned or due
  - No quiz on Mon after break
- Reading:
  - This week: Sheather Appx; ISLR Ch 7
  - Next week: Gelman & Hill Ch 9 & 10 (copies in week07 folder)
    - (read to get a sense rather than to get every detail)

Outline

- Two meanings of "Linear" model / linear smoother
  - $y = \beta_0 + \beta_1 x + \varepsilon,$ vs. $\hat{Y} = HY$
  - $df = tr(H)$
- Polynomial Regression
- Fixing Collinearity: Orthogonal basis for X
- Ridge Regression as a wiggliness/roughness penalty
  - Effective $df = tr(H_\lambda)$
- Cubic Regression Splines
- Variations
  - Natural Splines
  - Specifying the number of knots instead of the locations
- Smoothing Splines

Two meanings of “Linear” models

- Informally, we say a “linear” model involves a linear relationship (plus error) between x and y:

$$y_i = \beta_o + \beta_1 x_i + \varepsilon_i \tag{1}$$

- A more precise and generalizable definition is that the vector $\hat{y}$ is a linear function of the vector y:

$$\hat{y} = Hy \tag{2}$$

where $H = X\left(X^T X\right)^{-1} X^T$. Recall that

$$tr(H) = tr\left((X^T X)\left(X^T X\right)^{-1}\right) = p + 1 = df$$

- We will consider *linear models* and *linear smoothers* that generalize “linear” in the sense of (1) but preserve “linear” in the sense of (2)!

Polynomial Regression

- We already know about polynomial regression

$$y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \cdots + \beta_p x_i^p + \varepsilon_i$$

- This is just multiple regression where the columns of the X matrix are powers of x: $1, x, x^2, \dots, x^p$

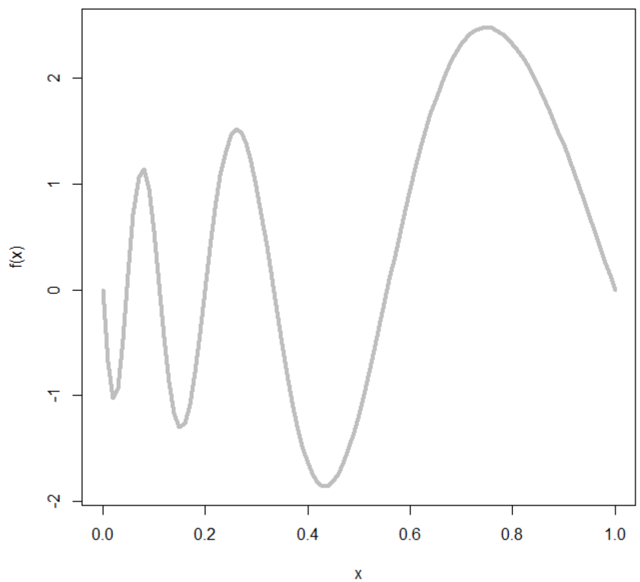
$$X = \begin{bmatrix} 1 & \cdots & x_1^p \\ \vdots & \ddots & \vdots \\ 1 & \cdots & x_n^p \end{bmatrix}$$

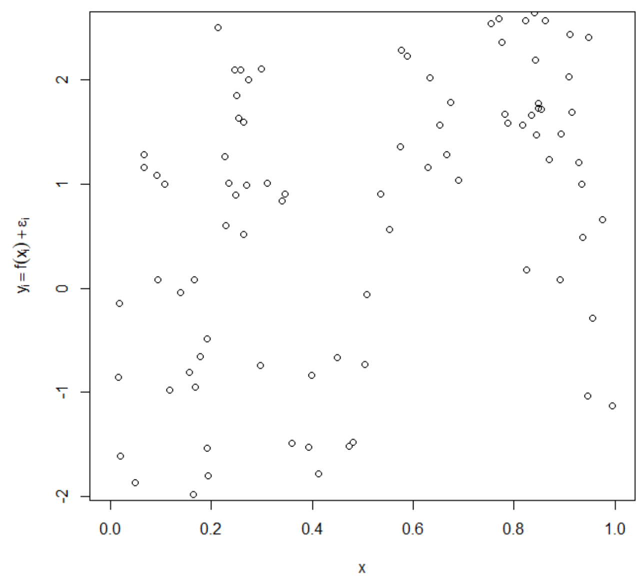
  and $df = tr(H) = p + 1$

- Good for estimating some nonlinear functions; but
  - Vif's tend to be large
  - Can be overly "wiggly" or "rough"

A Running Example…

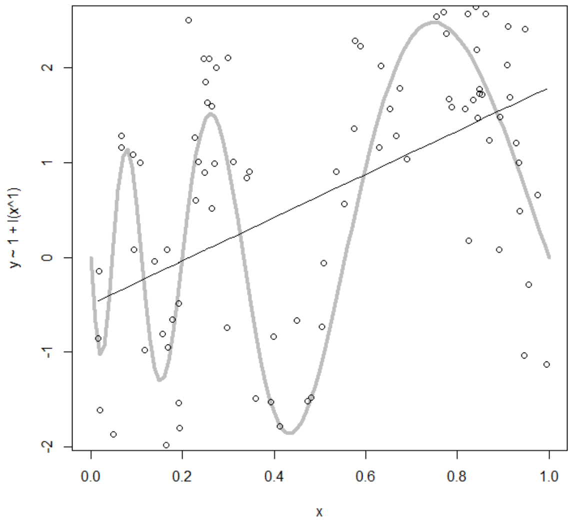
- For most of this lecture we will try to estimate $f(x)$ from the data $y_i = f(x_i) + \varepsilon_i$ where
  - $f(x) = (1 + 2x)\sin\left(\frac{2\pi}{0.25+0.75x}\right), x \in (0,1)$
  - $\varepsilon_i \sim N(0, \sigma^2), i = 1 \ldots 100 \qquad (\sigma^2 = 1)$

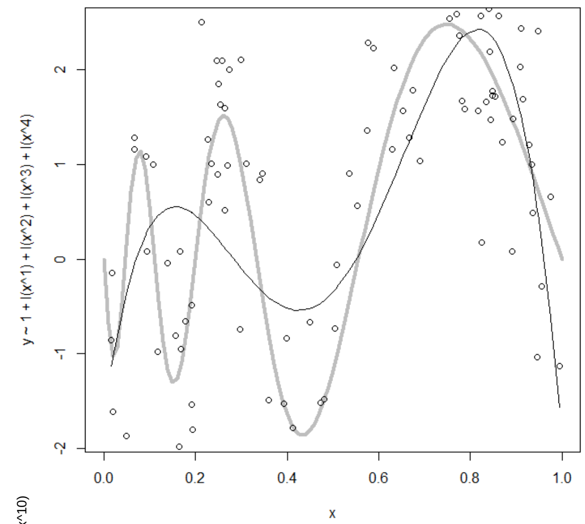


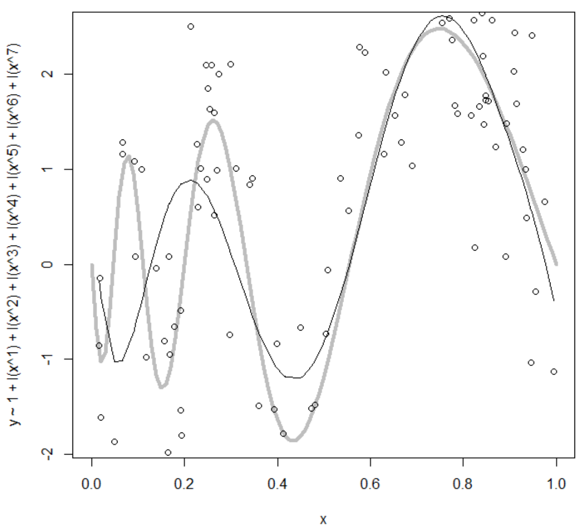


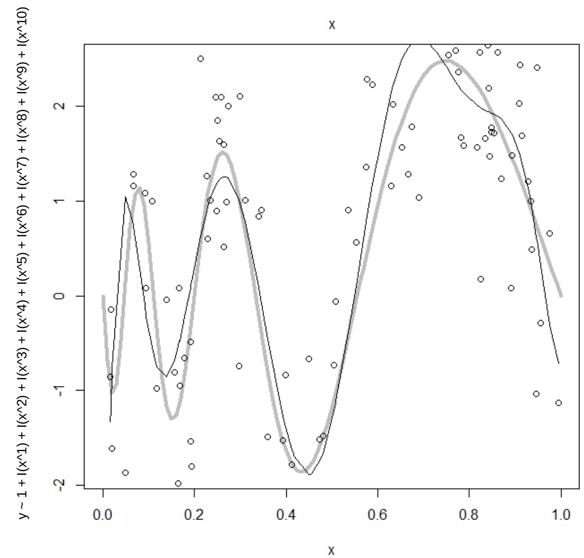
See the r file for this lecture for all sorts of computational details…

Polynomial regression of order 1,4,7,10









Powers of x have a lot of collinearity

```
> ## lmfit fits the 10th degree polynomial
> X <- model.matrix(lmfit)
> tr <- function(m) sum(diag(m))
> tr(X%*%solve(t(X)%*%X)%*%t(X))
[1] 10.9998      ## = 11, up to floating point error

> round(summary(lmfit)$coef,2)
              Estimate Std. Error t value Pr(>|t|)
(Intercept)      -5.93       1.90   -3.12     0.00
I(x^1)          379.17     128.10    2.96     0.00
I(x^2)        -7315.39    2696.74   -2.71     0.01
I(x^3)        63240.23   26773.03    2.36     0.02
I(x^4)      -290224.39  148518.47   -1.95     0.05
I(x^5)       771227.11  499693.74    1.54     0.13
I(x^6)     -1233102.85 1058658.55   -1.16     0.25
I(x^7)      1183276.84 1419406.84    0.83     0.41
I(x^8)      -645684.02 1167866.53   -0.55     0.58
I(x^9)       171639.32  537883.43    0.32     0.75
I(x^10)      -13430.82  106143.90   -0.13     0.90

> vif(lmfit)
      I(x^1)       I(x^2)       I(x^3)       I(x^4)
1.466822e+05 7.209028e+07 6.345761e+09 1.680260e+11
      I(x^5)       I(x^6)       I(x^7)       I(x^8)
1.634700e+12 6.343098e+12 1.000800e+13 5.972944e+12
      I(x^9)      I(x^10)
1.130705e+12 3.958930e+10
```

- The degrees of freedom are p+1 = 11, as expected
- The $\hat{\beta}$'s and their SE's are huge
- The vif's are enormous!

Fixing collinearity: Orthogonal basis for X

- The columns of X form a basis for a p+1 dimensional subspace S of $\Re^n$: $S = \{v \in \Re^n \ st \ v = X\beta \ for \ some \ \beta\}$.
- If we *replace the columns of X with orthogonal columns* that form a basis for the same space S* and use them to make a model matrix Z,
  - Fit, prediction, etc. for the model $y = Z\beta_z + \varepsilon$ will be the same
  - The vif's should all be 1's
  - The β_z's, $\widehat{\beta_z}$'s, and $SE(\beta_z)$'s will be different, but who cares?
- The columns of Z are called "*orthogonal polynomials over x*"
- The R function `poly(x,p)` provides a set of orthogonal polynomials for us.

*One way (among many) to do this is "Gram-Schmidt orthogonalization"

Let's try it...

10th degree polynomial with orthogonal columns

df = 11

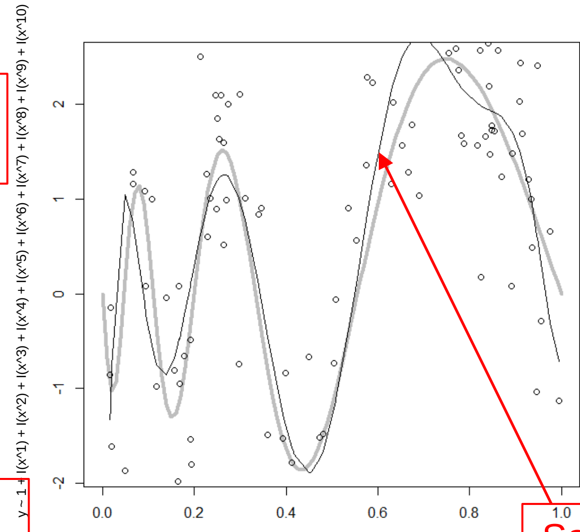
Columns of Z

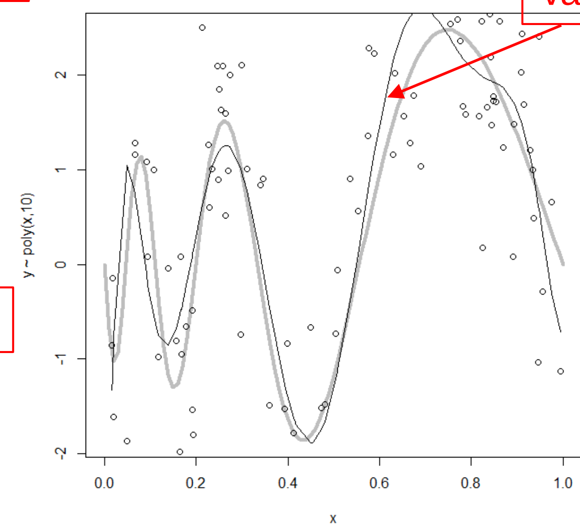
Different, well behaved $\widehat{\beta_z}$'s

vif's all 1's

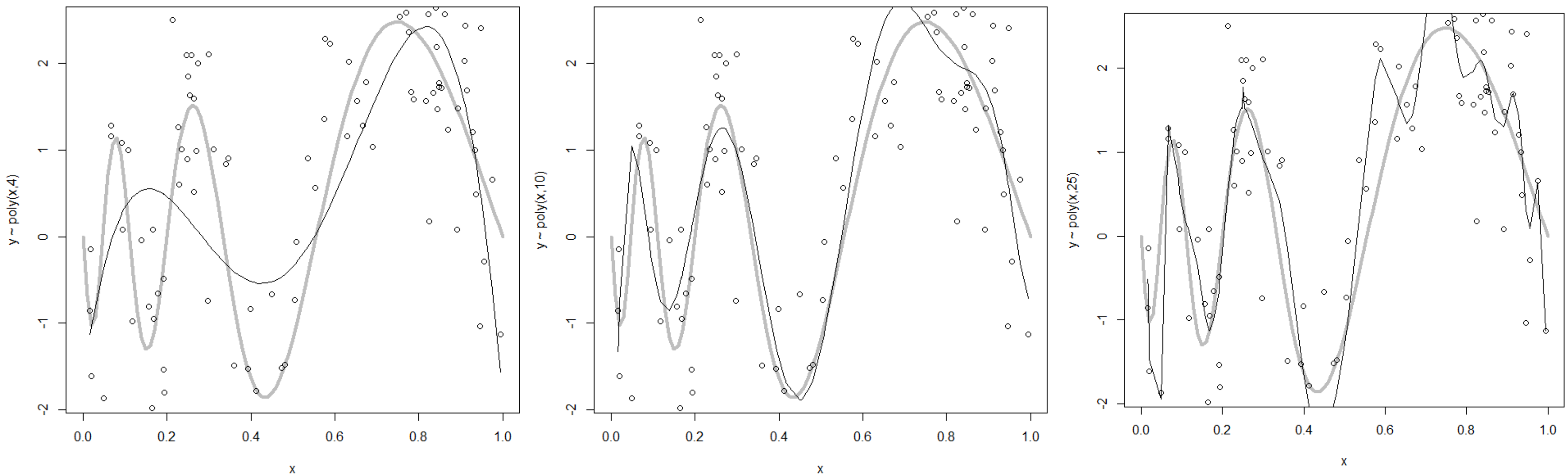
Same fitted values

```
> Polyfit <- lm(y ~ poly(x,10))
> Z <- model.matrix(polyfit)
> tr <- function(m) sum(diag(m))
> tr(Z%*%solve(t(Z)%*%Z)%*%t(Z))
[1] 11

> round(summary(polyfit)$coef,2)
             Estimate Std. Error t value Pr(>|t|)
(Intercept)      0.70       0.10    7.02     0.00
poly(x, 10)1     6.80       0.99    6.84     0.00
poly(x, 10)2     0.52       0.99    0.52     0.60
poly(x, 10)3    -3.78       0.99   -3.81     0.00
poly(x, 10)4    -7.43       0.99   -7.47     0.00
poly(x, 10)5     1.22       0.99    1.23     0.22
poly(x, 10)6     4.27       0.99    4.30     0.00
poly(x, 10)7    -2.28       0.99   -2.29     0.02
poly(x, 10)8    -4.56       0.99   -4.59     0.00
poly(x, 10)9     4.22       0.99    4.25     0.00
poly(x, 10)10   -0.13       0.99   -0.13     0.90

> vif(polyfit)
 poly(x, 10)1  poly(x, 10)2  poly(x, 10)3  poly(x, 10)4
 1             1             1             1
 poly(x, 10)5  poly(x, 10)6  poly(x, 10)7  poly(x, 10)8
 1             1             1             1
 poly(x, 10)9  poly(x, 10)10
 1             1
```





Polynomials tend to get too wiggly as the degree increases…



- A polynomial with enough flexibility to track the more complex parts of $f(x)$ starts to interpolate $f(x) + \varepsilon$, and becomes too wiggly for the less complex parts of $f(x)$.

Digression: Review of Ridge Regression

- Recall that in Ridge Regression we are minimizing the penalized RSS

$$\sum_{i=1}^{n}(y_i - X_i\beta)^2 + \lambda\sum_{i=1}^{n}\beta^2 = (Y - X\beta)^T(Y - X\beta) + \lambda\beta^T\beta$$

- Setting the derivative w.r.t. β equal to 0,

$$-2X^T(Y - X\beta) + 2\lambda\beta = 0$$

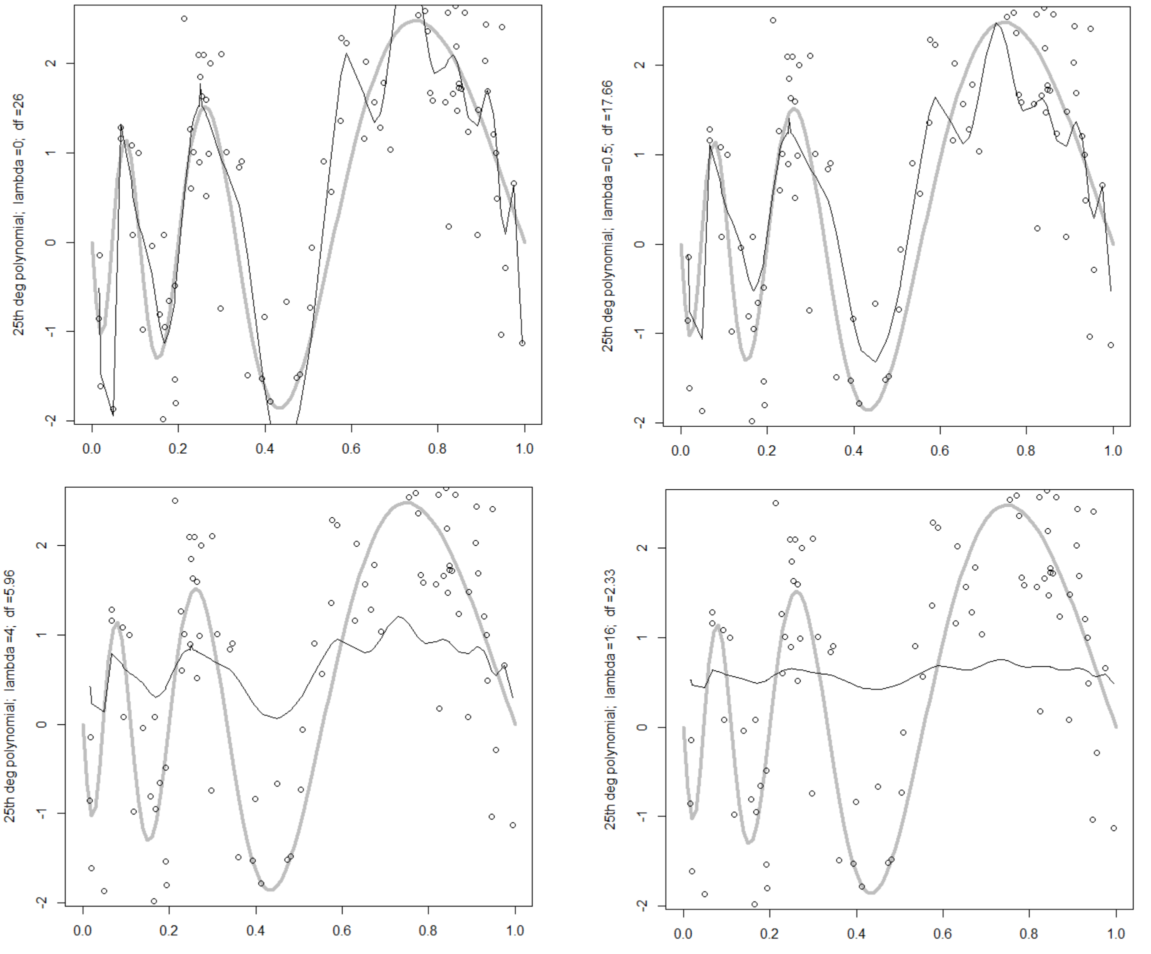
$$X^TY = \left(X^TX + \lambda I\right)\beta$$

$$\widehat{\beta_\lambda} = \left(X^TX + \lambda I\right)^{-1}X^TY$$

- *We are effectively dividing by a function of λ , and so $\widehat{\beta_\lambda}$ shrinks toward zero.*
- The hat matrix is $H_\lambda = X\left(X^TX + \lambda I\right)^{-1}X^T$, and we ***define*** $(effective)\ df = tr(H_\lambda)$

In the r file for this lecture I show how you can fit a ridge regression with nothing more than the lm() function in R.

Try to use ridge regression to control wiggliness/roughness of polynomial…

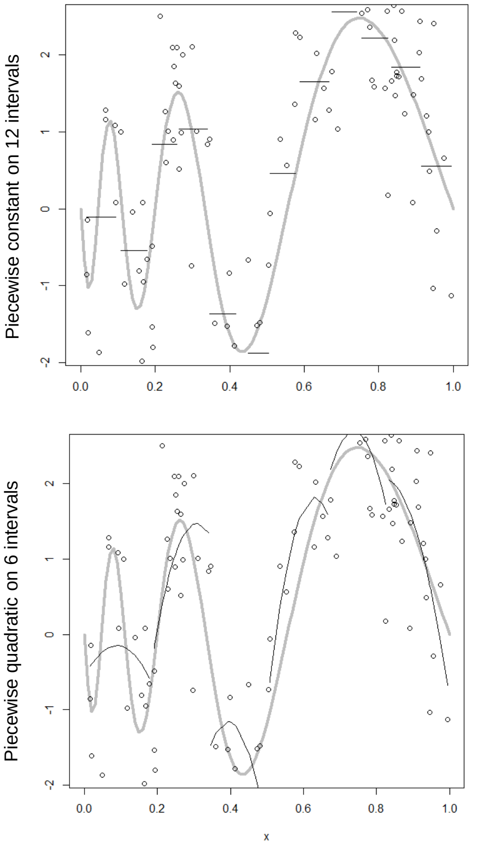


- $\lambda = 0$ corresponds to the least-squares fit (no shrinkage)
- For small positive λ, we reduce the scale of the wiggliness at the expense of some bias
- For larger values of λ, the curve is clearly shrinking towards a constant (the intercept, ≈ 0.70)
- Note how the (effective) df decreases as λ increases.

We *increase* df by increasing the polynomial degree; we *decrease* df by increasing λ.

A more “local” approach…

- Instead of fitting one curve to all the data, fit different curves to different sections of the data
  - Piecewise constant not very satisfying…
  - Piecewise polynomial still suffers from discontinuities…
  - →Impose continuity and smoothness constraints



We increase df either by increasing the number of intervals, or by increasing the polynomial degree

Cubic Regression Splines*

- Divide x up into m+1 intervals

$$(t_0 = -\infty, t_1], (t_1, t_2], \dots, (t_{m-1}, t_m], (t_m, t_{m+1} = \infty)$$

according to the <u>*knots*</u> $t_1, t_2, \dots, t_m$ and consider the regression

$$y = \sum_{k=1}^{m+1} 1_{\{x \in (t_{k-1}, t_k]\}} \left(a_k + b_k x + c_k x^2 + d_k x^3\right) + \varepsilon$$

$$= \sum_{k=1}^{m+1} 1_{\{x \in (t_{k-1}, t_k]\}} \, p_k(x) + \varepsilon$$

subject to the constraints

- $p_k(t_k) = p_{k+1}(t_k)$ for all $k = 1 \dots m$
- $p'_k(t_k) = p'_{k+1}(t_k)$ for all $k = 1 \dots m$
- $p''_k(t_k) = p''_{k+1}(t_k)$ for all $k = 1 \dots m$

*Cubic $p_k(x)$ are most popular, but obviously we could do something similar polynomials $p_k(x)$ of any degree

What are the degrees of freedom?

- Let $\beta = (a_1, b_1, c_1, d_1, \ldots, d_{m+1})^T$ and let X be the matrix of functions of x, so that $y = X\beta + \varepsilon$
- There are $m + 1$ $p_k(x)$'s with 4 parameters each
  - $+4(m+1)$ columns in the X matrix
- There are 3 linear constraints on the parameters at each of the m knots.
  - $-3m$ linear constraints on the columns of X
- So we can replace the columns of X with a basis for the same subspace with only

$$4(m+1) - 3m = m + 4$$

columns: *the df for the spline on m knots is m+4*.

What should the columns of the reduced X matrix be?

- After a little calculus*, one can show that the $m + 4$ columns of the reduced X can be written as $1, x, x^2, x^3, (x - t_1)_+^3, \ldots, (x - t_m)_+^3$, where

$$(x - t)_+ = \begin{cases} x - t, x \geq t \\ 0, x < t \end{cases}$$

- This "basis" for X suffers from collinearity problems, and an almost-orthogonal basis of "B-splines" is usually used instead.

*See exercise #1 on pp. 321ff of Ch 7 of James et al.'s *ISLR* book.

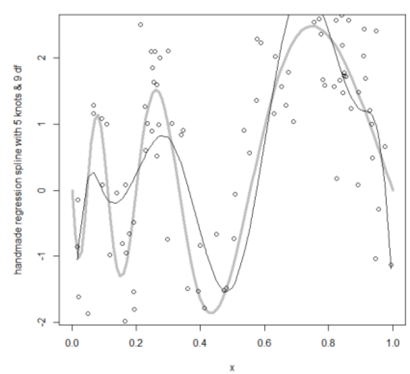
Our running example with cubic regression splines…

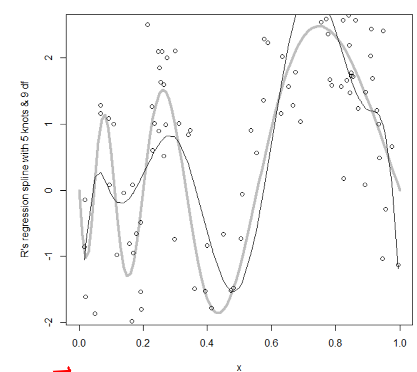
```
> library(splines)   ## for B-spline function bs()

> knots <- seq(.1,.9,by=.2) ; m <- length(knots)

> pos.part <- function(x) (x+abs(x))/2

> B <- data.frame(x=x,x2=x^2,x3=x^3) ## R supplies the intercept...
> for (k in knots) { B <- cbind(B,pos.part(x-k)^3) } ; B <- as.matrix(B)

> bjfit0 <- lm(y ~ B)
> X <- model.matrix(bjfit0)
> df <- round(sum(diag(X%*%solve(t(X)%*%X)%*%t(X))),2)
> ## setup() on the next line plots f(x) and the data...
> setup(paste("handmade regression spline with",
+ length(knots), "knots &",df,"df"))
> lines(x,predict(bjfit0))

> bsfit0 <- lm(y ~ bs(x,knots=knots))
> X <- model.matrix(bsfit0)
> df <- round(sum(diag(X%*%solve(t(X)%*%X)%*%t(X))),2)
> setup(paste("R's regression spline with",m,"knots &",df,"df"))
> lines(x,predict(bsfit0))
```

> round(vif(bjfit0),2)

x	x^2	x^3	$(x-k_1)_+$^3
34715.01	5734082.57	67249875.68	38208202.68
$(x-k_2)_+$^3	$(x-k_3)_+$^3	$(x-k_4)_+$^3	$(x-k_5)_+$^3
66989.68	3094.03	136.76	3.97

```
> round(vif(bsfit0),2)
bs(x, knots = knots)1 bs(x, knots = knots)2 bs(x, knots = knots)3
                 2.72                  3.81                  4.51
bs(x, knots = knots)4 bs(x, knots = knots)5 bs(x, knots = knots)6
                 3.64                  3.59                  4.10
bs(x, knots = knots)7 bs(x, knots = knots)8
                 2.90                  1.53
```

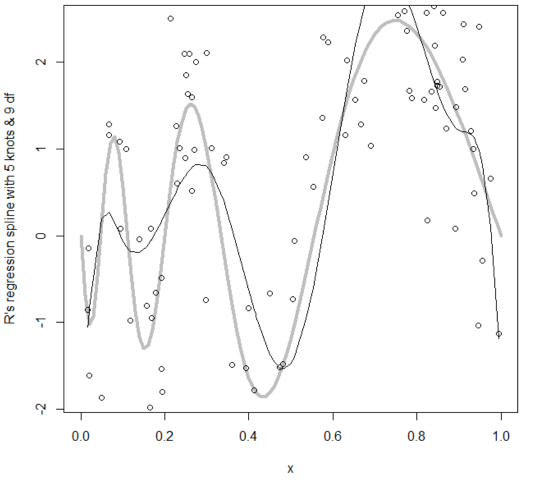


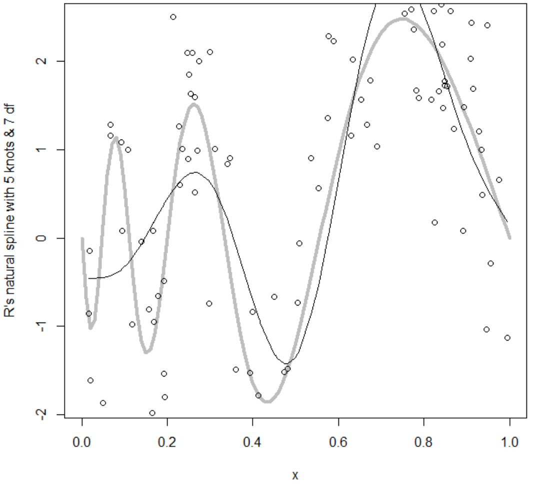


Variations on regression splines…

- ***Natural splines*** spend 2 more df to force $p_1(x)$ and $p_{m+1}(x)$ to be linear

```
> knots <- seq(.1,.9,by=.2)
> m <- length(knots)
> nsfit0 <- lm(y ~ ns(x,knots=knots))
> X <- model.matrix(nsfit0)
> df <- round(sum(diag(X%*%solve(t(X)%*%X)%*%t(X))),2)
> setup(paste("R's natural spline with",m,"knots &",df,"df"))
> lines(x,predict(bsfit0))
```





- If you specify df instead of knots, you get ≈ df equally spaced knots.

```
> df.req <- 9 ## select knots at (df.req – 3) quantiles of x
> bsfit1 <- lm(y ~ bs(x,df=df.req))
> X <- model.matrix(bsfit1)
> df <- round(sum(diag(X%*%solve(t(X)%*%X)%*%t(X))),2)
> setup(paste("R's regression spline with",df.req,"knots requested &",df,"df"))
> lines(x,predict(bsfit1))
> ## plot not shown; similar to others…
```

We increase df by increasing the number of knots

Aside: Residual diagnostics, F-test, LRT, AIC, BIC still work…

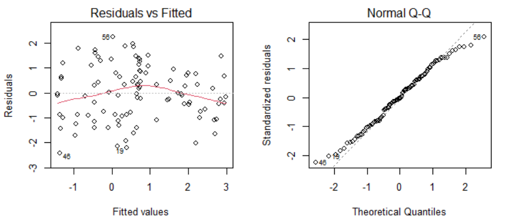
```
> par(mfrow=c(2,2))

> plot(nsfit0)

> plot(bsfit0)

> anova(nsfit0, bsfit0)
```

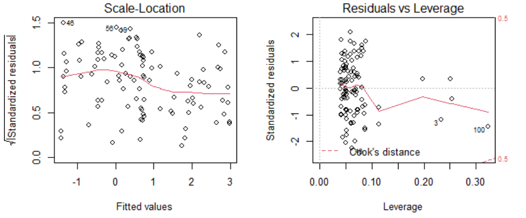
Analysis of Variance Table

Model 1: y ~ ns(x, knots = knots)

Model 2: y ~ bs(x, knots = knots)

	Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)	
1	93	115.16					
2	91	108.05	2	7.1084	2.9933	0.05508	.





Be careful with F-test and LRT that the models are really nested!

Smoothing Splines

- A slightly different approach to splines is to try to find a smooth function $g(x)$ that minimizes the "Ridge-like" penalized RSS

$$\sum_{i=1}^{n} \left(y_i - g(x_i)\right)^2 + \lambda \int g''(t)^2 \, dt \qquad (*)$$

  - Here, λ penalizes wiggliness or roughness: the larger λ is, the more linear $g(x)$ must be.
  - It turns out that

    the function $g(x)$ that minimizes (*) is a natural cubic spline, with knots $t_i = x_i$ at every data point x_i, and coefficients shrunken toward a linear form for $g(x)$.

    (how much shrinkage depends on λ).

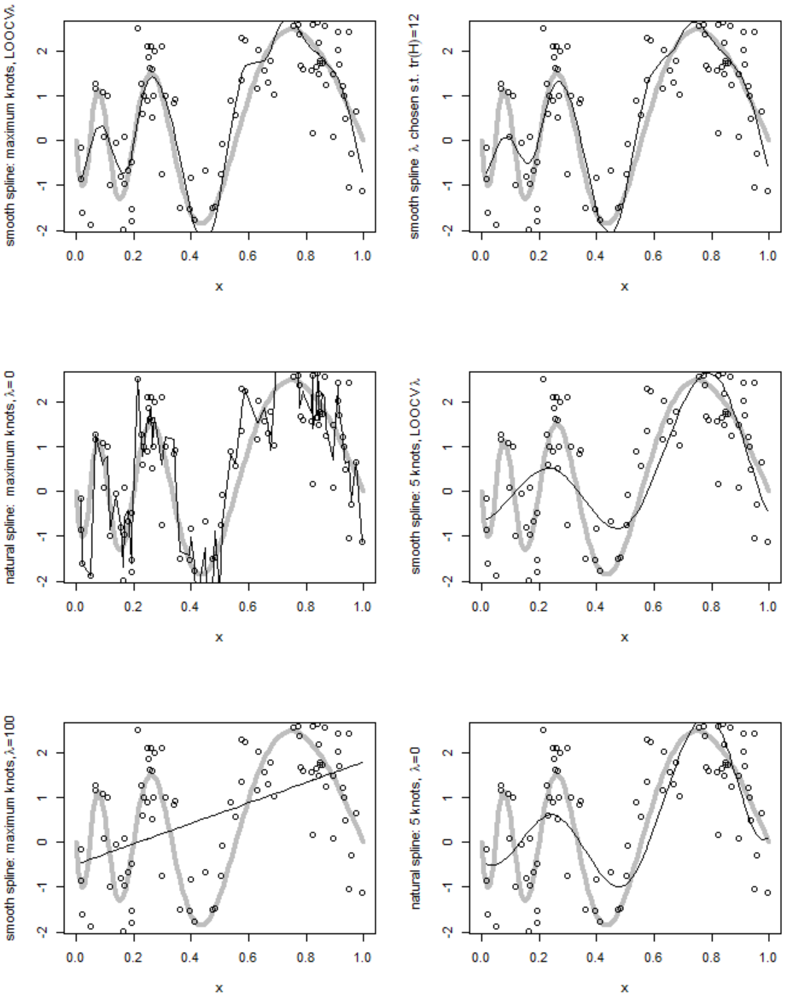
Smoothing Splines and df…

- When $g(x)$ is a natural cubic spline with knots at $t_1, \dots, t_m$, the penalized RSS (*) turns out to be
$$(Y - G\beta)^T(Y - G\beta) + \lambda\beta^T \mathrm{M}\beta$$
- G is the X-matrix from a natural spline basis $g_1(x), \dots, g_{m+2}(x)$, and M is a matrix with entries
$$M_{ij} = \int g''_i(t) g''_j(t) dt$$
- Following the same calculus as for Ridge Regression,
$$\hat{Y} = H_\lambda Y, where$$
$$H_\lambda = G\left(G^T G + \lambda M\right)^{-1} \mathrm{G}^\mathrm{T}$$
$$\textit{(Effective)}\ df = tr(H_\lambda)$$

We *increase* df by increasing the sample size $x_1, \dots, x_n$; we *decrease* df by increasing λ, or by using fewer knots $t_1, \dots, t_m$ (at possibly different locations than the x_i's).

Our running example: smoothing splines

```
> par(mfcol=c(3,2))
> setup(expression(paste("smooth spline: maximum knots, LOOCV  ",
+ lambda)))
> lines(ss <- smooth.spline(x,y,all.knots=T))
> ss$df      ## [1] 14.76477
> setup(expression(paste("natural spline:  maximum knots,  ",
+ lambda==0)))
> lines(ss <- smooth.spline(x,y,lambda=0))
> ss$df     ## [1] 64
> setup(expression(paste("smooth spline: maximum knots,  ",
+ lambda==100)))
> lines(ss <- smooth.spline(x,y,lambda=100))
> ss$df     ## [1] 2.002092
> setup(expression(paste("smooth spline:  ",lambda,
+ "  chosen s.t.  ",tr(H)==12)))
> lines(ss <- smooth.spline(x,y,df=12))
> ss$df    ## [1] 11.99843
> setup(expression(paste("smooth spline: 5 knots, LOOCV  ",
+ lambda)))
> lines(ss <- smooth.spline(x,y,nknots=5))
> ss$df    ## [1] 5.784098
> setup(expression(paste("natural spline: 5 knots,  ",
+ lambda==0)))
> lines(ss <- smooth.spline(x,y,nknots=5,lambda=0))
> ss$df    ## [1] 7
```



smooth.spline() is part of the base R distribution.

By default, smooth.spline() chooses as many equally-spaced knots as it can, up to the sample size n. If you set all.knots=TRUE, smooth.spline() uses all the data points as knots.

Summary

- Two meanings of "Linear" model / linear smoother
  - $y = \beta_0 + \beta_1 x + \varepsilon$, vs. $\hat{Y} = HY$
  - $df = tr(H)$
- Polynomial Regression
- Fixing Collinearity: Orthogonal basis for X
- Ridge Regression as a wiggliness/roughness penalty
  - Effective $df = tr(H_\lambda)$
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