MONASH University

MONASH BUSINESS SCHOOL

ETC3580: Advanced Statistical Modelling

Week 9: Nonparametric regression

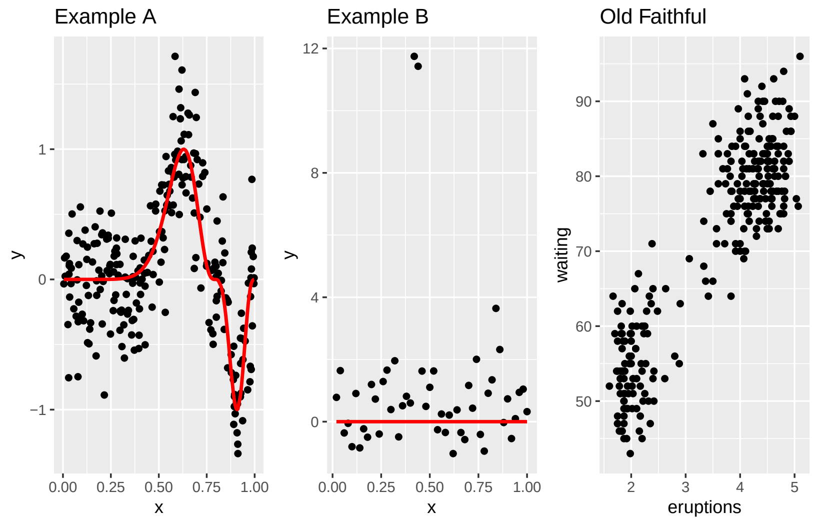
Outline

Nonlinear regression

$$y_i = f(x_i) + \varepsilon_i$$

- How to estimate f?
- Could assume $f(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3$
- Or $f(x) = \beta_0 + \beta_1 x^{\beta_2}$
- OK if you *know* the right form.
- But often better to assume only that f is continuous and smooth.

Examples



Example A
y
1
0
−1
0.00
0.25
0.50
0.75
1.00
x
Example B
y
12
8
4
0
0.00
0.25
0.50
0.75
1.00
x
Old Faithful
waiting
90
80
70
60
50
2
3
4
5
eruptions

Outline

Kernel estimators

Nadaraya–Watson estimator

$$\hat{f}_h(x) = \frac{\displaystyle\sum_{j=1}^{n} K\left(\frac{x - x_j}{h}\right) y_j}{\displaystyle\sum_{j=1}^{n} K\left(\frac{x - x_j}{h}\right)}$$

- K is a kernel function where $\int K = 1$, $K(a) = K(-a)$, and $K(0) \geq K(a)$, for all a.
- $\hat{f}$ is a weighted moving average
- Need to choose K and h.

Common kernels

Uniform

$$K(x) = \begin{cases} \frac{1}{2} & -1 < x < 1 \\ 0 & \text{otherwise.} \end{cases}$$

Epanechnikov

$$K(x) = \begin{cases} \frac{3}{4}(1 - x^2) & -1 < x < 1 \\ 0 & \text{otherwise.} \end{cases}$$

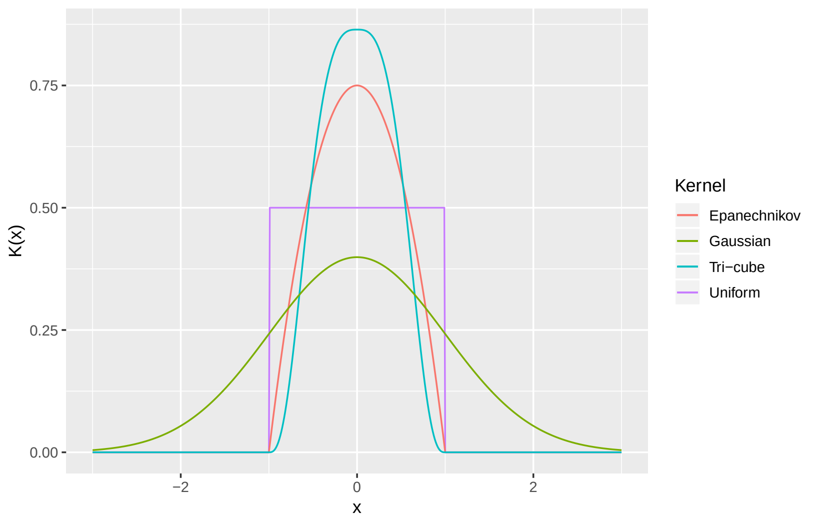
Tri-cube

$$K(x) = \begin{cases} c(1 - |x|^3)^3 & -1 < x < 1 \\ 0 & \text{otherwise.} \end{cases}$$

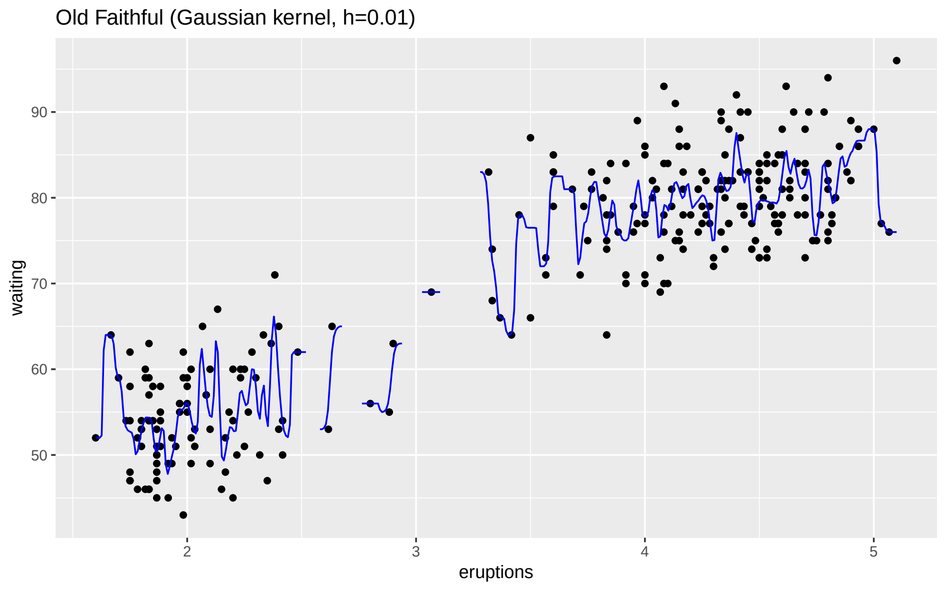
Gaussian

$$K(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2}$$

Common kernels



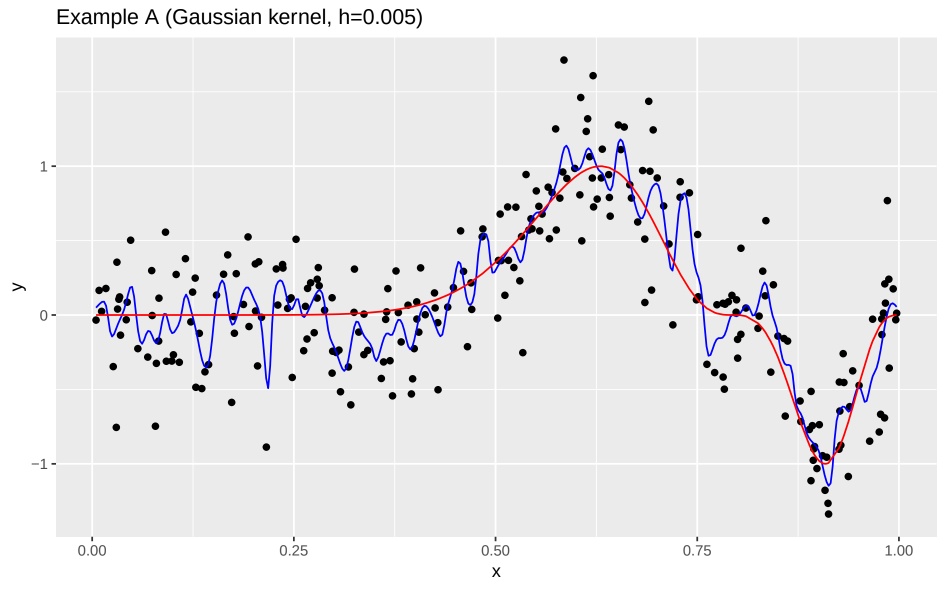
Old Faithful



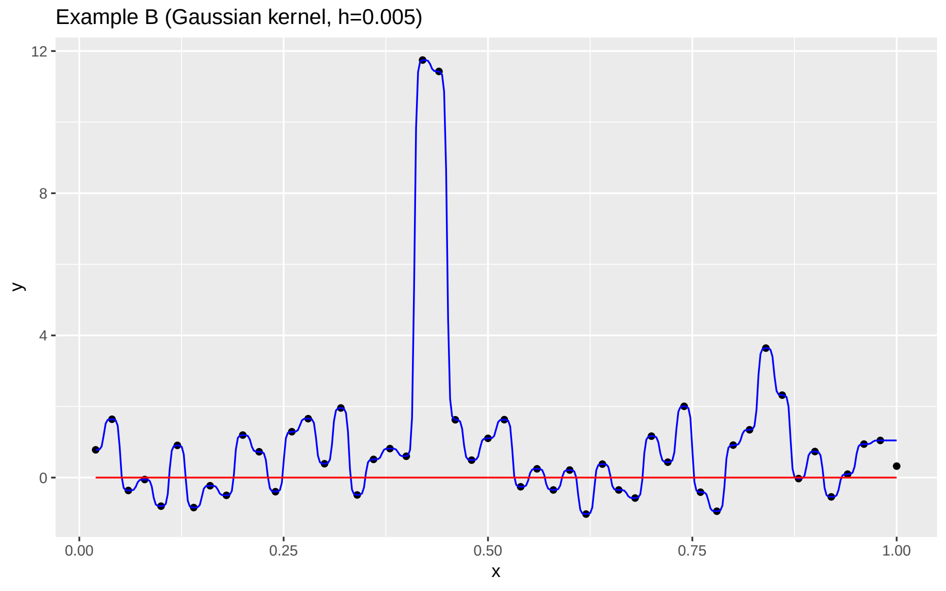
Kernel smoothing

- A smooth kernel is better, but otherwise the choice of kernel makes little difference.
- Optimal kernel (minimizing MSE) is Epanechnikov. It is also fast.
- The choice of h is crucial.

Example A



Example B



Cross-validation

$$CV(h) = \frac{1}{n}\sum_{j=1}^{n}(y_j - \hat{f}_h^{(-j)}(x_j))^2$$

- $(-j)$ indicates jth point omitted from estimate
- Pick h that minimizes CV.
- Works ok provided there are no duplicate (x, y) pairs. But occasionally odd results.

MSE

Let $y = f(x) + \varepsilon$ where $\varepsilon \sim IID(0, \sigma^2)$. Then

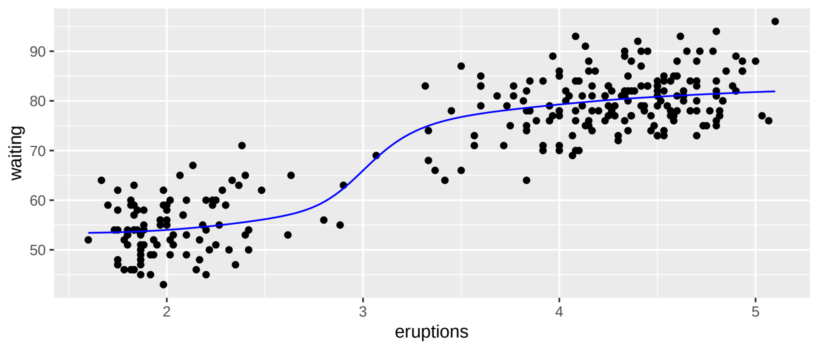
$$\text{MSE}(h) = \text{E}[f(x) - \hat{f}_h(x)]^2 \approx \frac{\sigma^2 r_K}{nh} + \frac{v_K^2 h^4 [f''(x)]^2}{4}$$

- $r_K = \int K^2(x)dx, \qquad v_K = \int x^2 K(x)dx$
- Consistent estimator if $nh \to \infty$ and $h \to 0$ as $n \to \infty$.
- $h_{\text{optimal}} \approx \left(\dfrac{r_K}{n[f''(x)]^2 v_K^2} \right)^{1/5}$

Kernel smoothing in R

Many packages available. One of the better ones is **KernSmooth**:

```
fit <- locpoly(faithful$eruptions, faithful$waiting,
       degree=0, bandwidth=0.3) %>% as.tibble
ggplot(faithful) +
  geom_point(aes(x=eruptions,y=waiting)) +
  geom_line(data=fit, aes(x=x,y=y), col='blue')
```



Outline

Local polynomials

Kernel smoothing is a local constant method:

$$\mathrm{WLS}(x) = \sum_{j=1}^{n} w_j(x)(y_j - a_0)^2$$

where $w_j(x) = \dfrac{K\left(\frac{x-x_j}{h}\right)}{\sum_{i=1}^{n} K\left(\frac{x-x_i}{h}\right)}$

is minimized by

$$\hat{f}(x) = \hat{a}_0 = \sum_{j=1}^{n} w_j(x) y_j$$

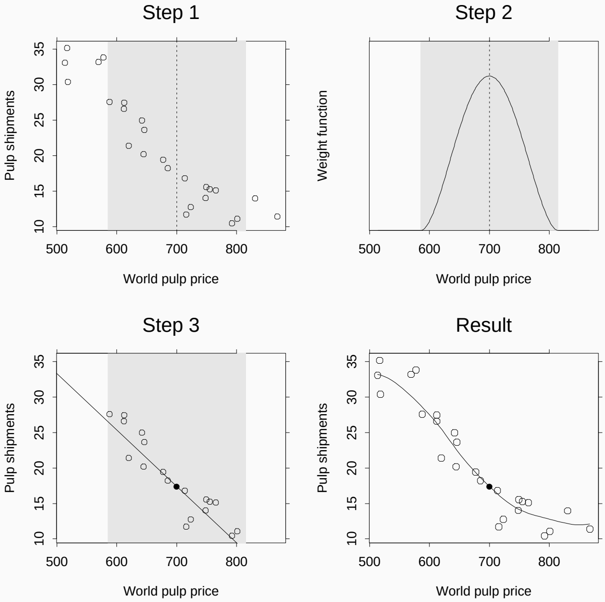
Local polynomials

We can compute local linear instead:

$$\mathrm{WLS}(x) = \sum_{j=1}^{n} w_j(x)(y_j - a_0 - a_1(x_j - x))^2$$

$$\hat{f}(x) = \hat{a}_0$$

Local polynomials



Local polynomials

$$\mathrm{WLS}(x) = \sum_{j=1}^{n} w_j(x)(y_j - \sum_{k=0}^{p} a_k(x_j - x)^p)^2$$

$$\hat{f}(x) = \hat{a}_0$$

- Local linear and local quadratic are commonly used.
- Robust regression can be used instead
- Less biased at boundaries than kernel smoothing
- Local quadratic less biased at peaks and troughs than local linear or kernel

Local polynomials in R

- One useful implementation is `KernSmooth::locpoly(x, y, degree, bandwidth)`
- Uses Gaussian kernel.
- `dpill` can be used to choose the `bandwidth` h if `degree=1`.
- Many people seem to use trial and error — finding the largest h that captures what they think they see by eye.

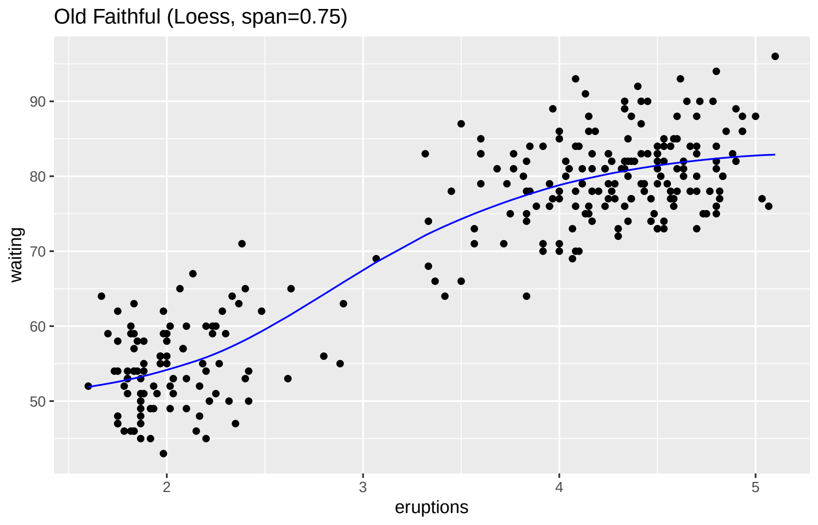
Loess

Best known implementation is **loess** (locally quadratic)

```
fit <- loess(y ~ x, span=0.75, degree=2,
  family="gaussian", data)
```

- Uses tri-cube kernel and variable bandwidth.
- `span` controls bandwidth. Specified in terms of percentage of data covered.
- `degree` is order of polynomial
- Use `family="symmetric"` for a robust fit

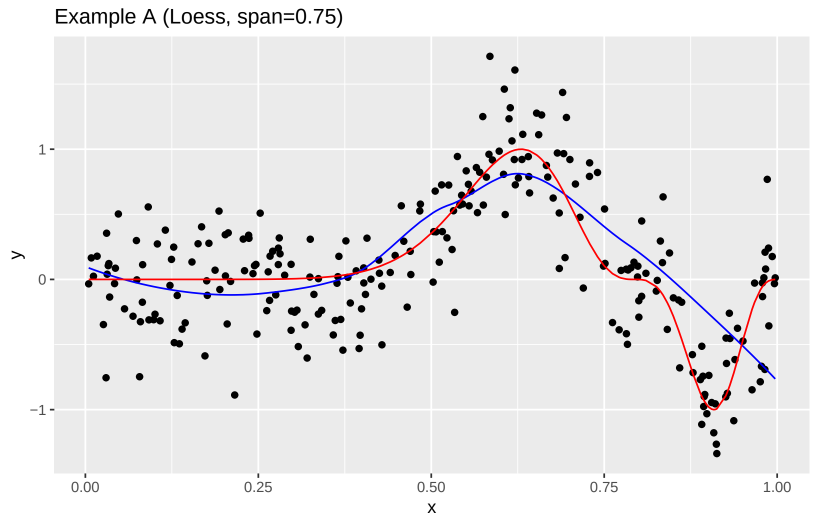
Loess


Old Faithful (Loess, span=0.75)
waiting
90
80
70
60
50
2
3
4
5
eruptions

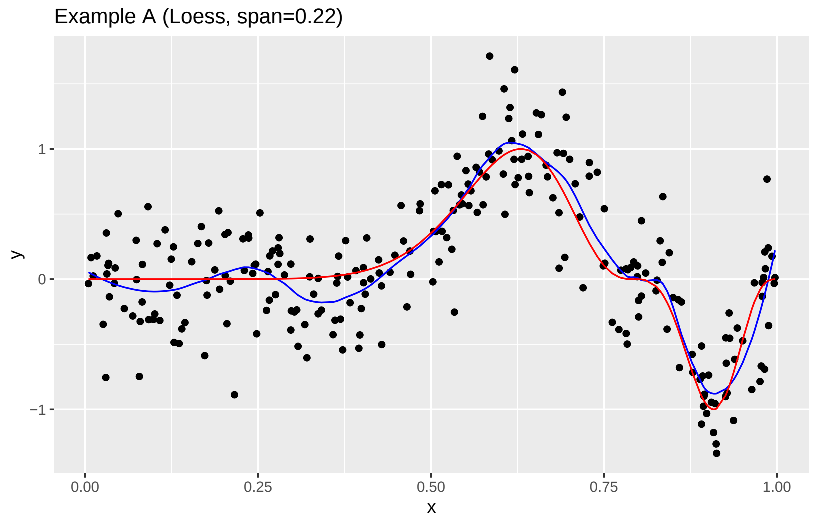
Loess in R

```r
smr <- loess(waiting ~ eruptions, data=faithful)
ggplot(faithful) +
    geom_point(aes(x=eruptions,y=waiting)) +
    ggtitle("Old Faithful (Loess, span=0.75)") +
    geom_line(aes(x=eruptions, y=fitted(smr)),
      col='blue')
```

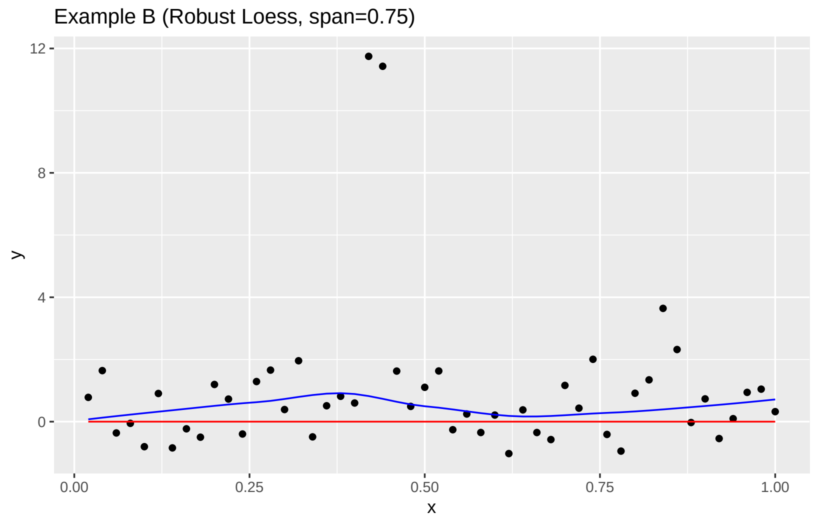
Loess



Loess

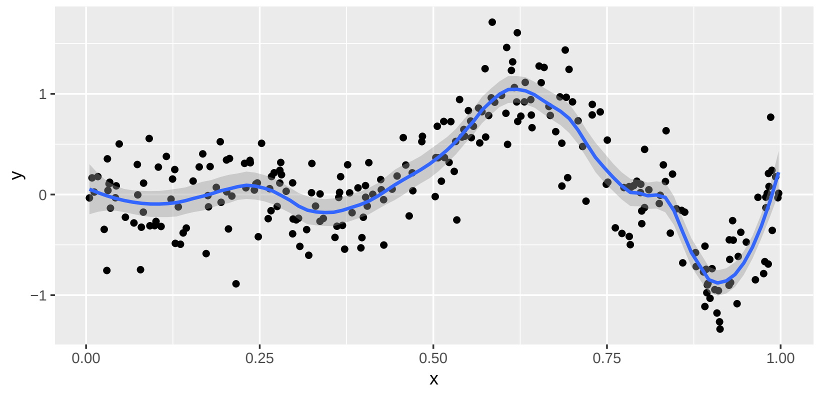


Loess



Loess and geom_smooth()

```
ggplot(exa) +
    geom_point(aes(x=x,y=y)) +
    geom_smooth(aes(x=x,y=y), method='loess',
      span=0.22)
```

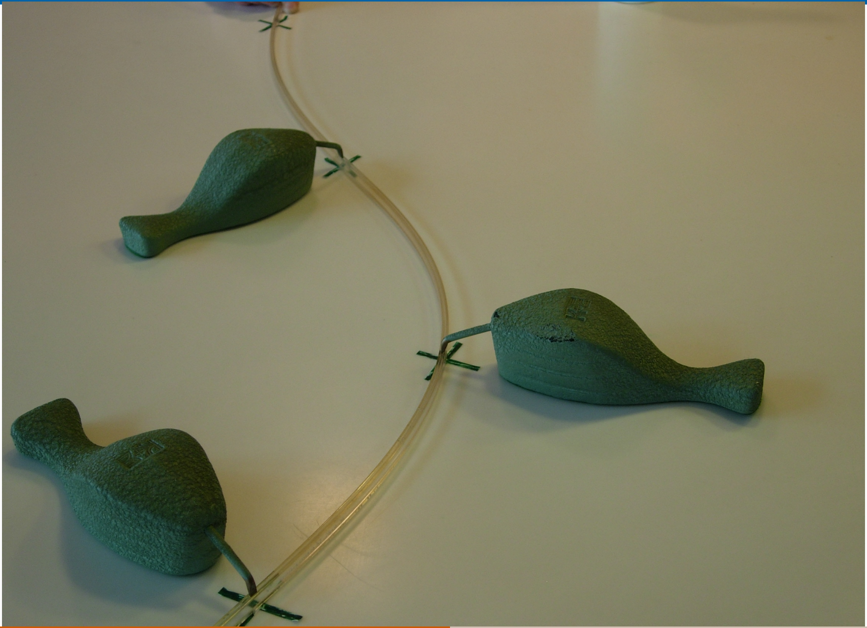


Loess and geom_smooth()

- Because local polynomials use local linear models, we can easily find standard errors for the fitted values.
- Connected together, these form a pointwise confidence band.
- Automatically produced using `geom_smooth`

Outline

Interpolating splines



Interpolating splines

Interpolating splines

Interpolating splines

A spline is a continuous function $f(x)$ interpolating all points (κ_j, y_j) for $j = 1, \dots, K$ and consisting of polynomials between each consecutive pair of 'knots' κ_j and κ_{j+1}.

Interpolating splines

A spline is a continuous function $f(x)$ interpolating all points (κ_j, y_j) for $j = 1, \dots, K$ and consisting of polynomials between each consecutive pair of 'knots' κ_j and κ_{j+1}.

- Parameters constrained so that $f(x)$ is continuous.
- Further constraints imposed to give continuous derivatives.
- Cubic splines most common, with f', f'' continuous.

Outline

Smoothing splines

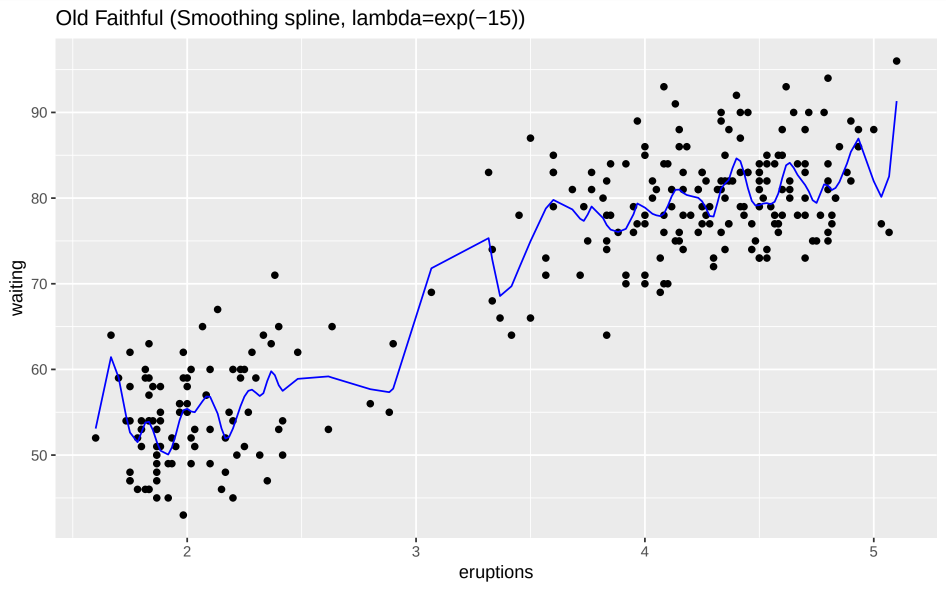
Let $y = f(x) + \varepsilon$ where $\varepsilon \sim IID(0, \sigma^2)$. Then

Choose $\hat{f}$ to minimize

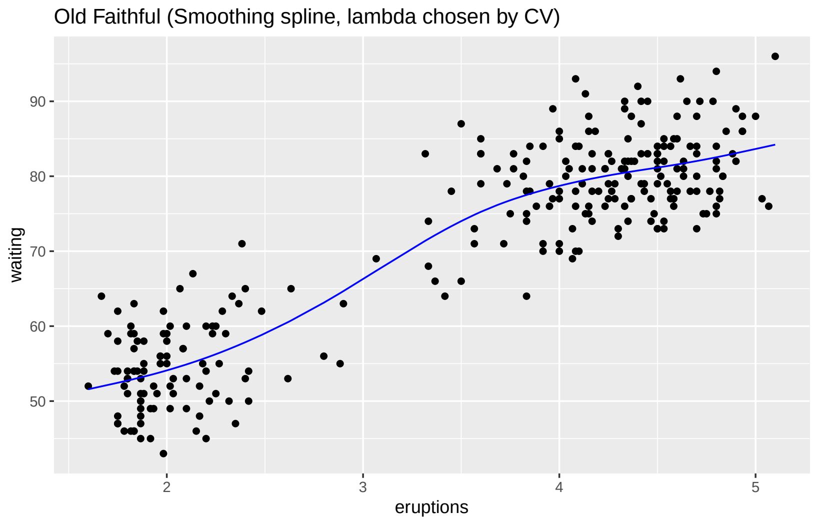
$$\frac{1}{n}\sum_i (y_i - f(x_i))^2 + \lambda \int [f''(x)]^2 dx$$

- λ is smoothing parameter to be chosen
- $\int [f''(x)]^2 dx$ is a measure of roughness.
- Solution: $\hat{f}$ is a cubic spline with knots $\kappa_i = x_i$, $i = 1, \dots, n$ (ignoring duplicates).
- Other penalties lead to higher order splines
- Cross-validation can be used to select λ.

Smoothing splines



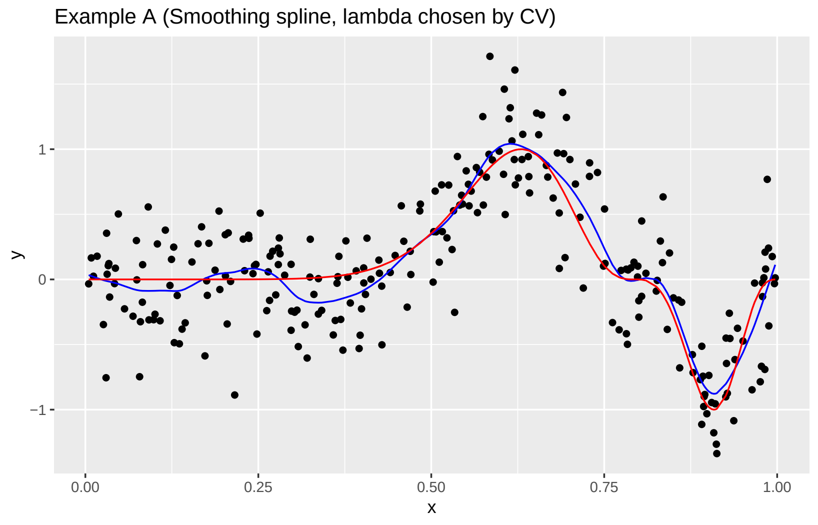
Smoothing splines



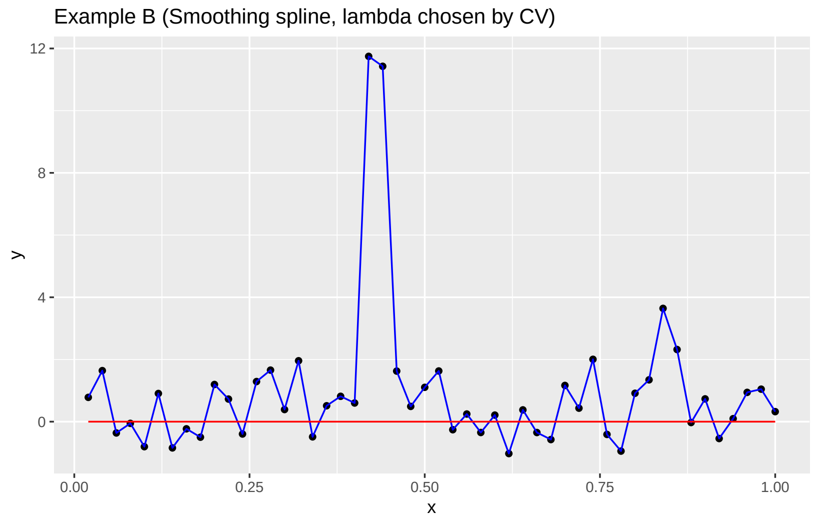
Smoothing splines

```r
smr <- smooth.spline(
  faithful$eruptions,
  faithful$waiting,
  cv=TRUE)
smr <- data.frame(x=smr$x,y=smr$y)
ggplot(faithful) +
  geom_point(aes(x=eruptions,y=waiting)) +
  ggtitle("Old Faithful (Smoothing spline, lambda chosen by
  geom_line(data=smr, aes(x=x, y=y), col='blue')
```

Smoothing splines



Smoothing splines



Outline

Regression splines

- Fewer knots than smoothing splines
- Need to choose the knots rather than a smoothing parameter.
- Can be estimated as a linear model once knots are selected.

General cubic regression splines

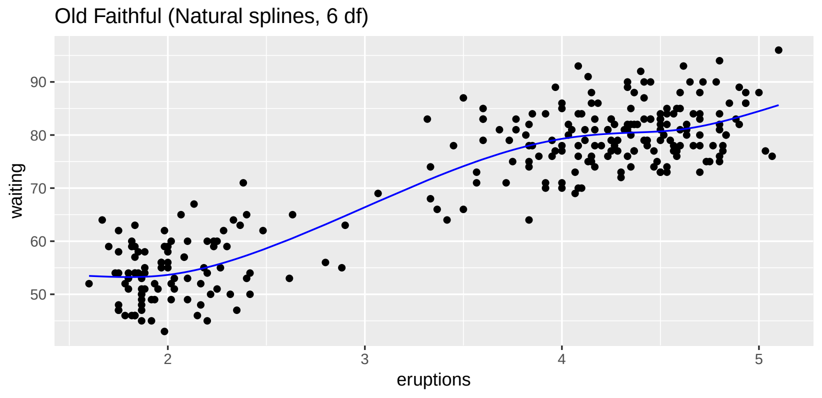
- Let $\kappa_1 < \kappa_2 < \cdots < \kappa_K$ be "knots" in interval (a, b).
- Let $x_1 = x$, $x_2 = x^2$, $x_3 = x^3$, $x_j = (x - \kappa_{j-3})^3_+$ for $j = 4, \ldots, K + 3$.
- Then the regression of y on $x_1, \ldots, x_{K+3}$ is piecewise cubic, but smooth at the knots.
- Choice of knots can be difficult and arbitrary.
- Automatic knot selection algorithms very slow.
- Often use equally spaced knots. Then only need to choose K.

B-splines and natural splines

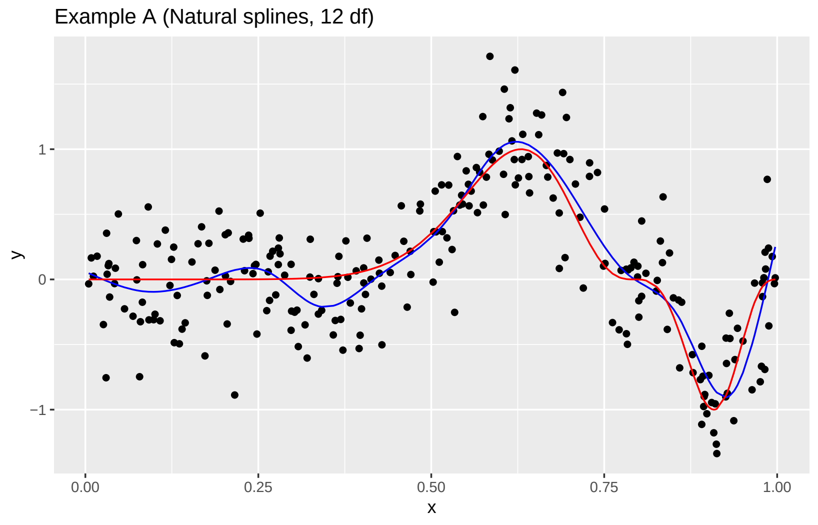
- B-splines provide an equivalent set of basis functions.
- Natural cubic splines are a variation on B-splines with linear boundary conditions.
- These are usually more stable
- Implemented in `splines::ns` function in R
- Can specify knots explicitly, or `df`. Then `df-2` knots are selected at quantiles of x.

Natural splines in R

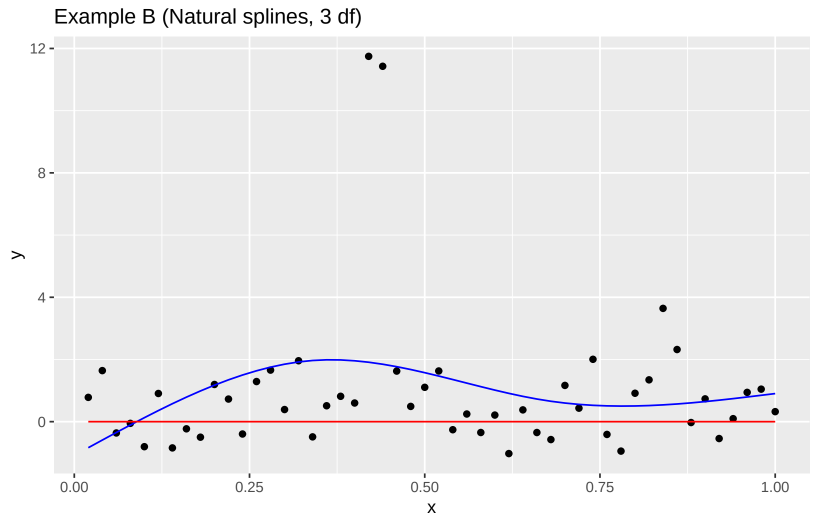
```
fit <- lm(waiting ~ ns(eruptions, df=6), faithful)
ggplot(faithful) +
    geom_point(aes(x=eruptions,y=waiting)) +
    ggtitle("Old Faithful (Natural splines, 6 df)") +
    geom_line(aes(x=eruptions, y=fitted(fit)), col='blue')
```



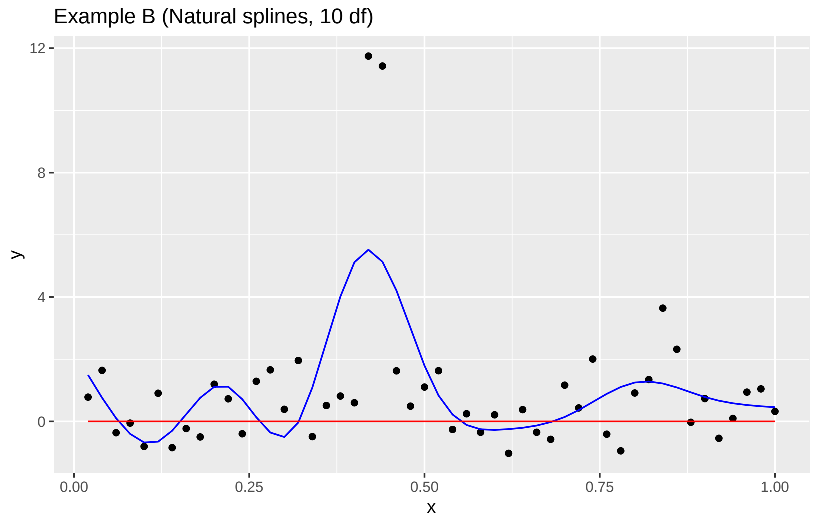
Natural splines in R



Natural splines in R

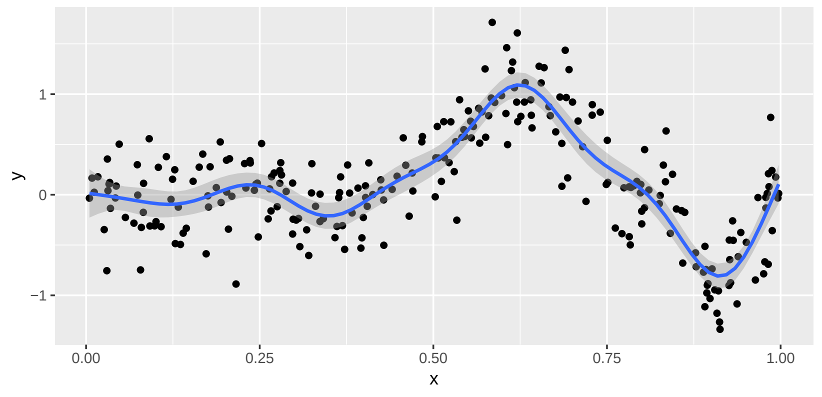


Natural splines in R



Splines and geom_smooth()

```
ggplot(exa) +
    geom_point(aes(x=x,y=y)) +
    geom_smooth(aes(x=x,y=y), method='gam',
      formula = y ~ s(x,k=12))
```



Splines and geom_smooth()

- Because regression splines use local linear models, we can easily find standard errors for the fitted values.
- Connected together, these form a pointwise confidence band.
- Automatically produced using `geom_smooth`

Outline

Multivariate predictors

$$y_i = f(\boldsymbol{x}_i) + \varepsilon_i, \qquad \boldsymbol{x} \in \mathbb{R}^d$$

Most methods extend naturally to higher dimensions.

- Multivariate kernel methods
- Multivariate local quadratic surfaces
- Thin-plate splines (2-d version of smoothing splines)

Multivariate predictors

$$y_i = f(\boldsymbol{x}_i) + \varepsilon_i, \qquad \boldsymbol{x} \in \mathbb{R}^d$$

Most methods extend naturally to higher dimensions.

- Multivariate kernel methods
- Multivariate local quadratic surfaces
- Thin-plate splines (2-d version of smoothing splines)

Problem

The curse of dimensionality!

Curse of dimensionality

Most data lie near the boundary

```r
x <- matrix(runif(1e6,-1,1), ncol=100)
boundary <- function(z) { any(abs(z) > 0.95) }
```

```r
mean(apply(x[,1,drop=FALSE], 1, boundary))
```

```
## [1] 0.0532
```

```r
mean(apply(x[,1:2], 1, boundary))
```

```
## [1] 0.0985
```

```r
mean(apply(x[,1:5], 1, boundary))
```

```
## [1] 0.2285
```

Curse of dimensionality

Most data lie near the boundary

```r
x <- matrix(runif(1e6,-1,1), ncol=100)
boundary <- function(z) { any(abs(z) > 0.95) }
```

```r
mean(apply(x[,1:10], 1, boundary))
```

```
## [1] 0.4031
```

```r
mean(apply(x[,1:50], 1, boundary))
```

```
## [1] 0.9221
```

```r
mean(apply(x[,1:100], 1, boundary))
```

```
## [1] 0.9933
```

Curse of dimensionality

Data are sparse

```
x <- matrix(runif(1e6,-1,1), ncol=100)
nearby <- function(z) { all(abs(z) < 0.5) }
mean(apply(x[,1,drop=FALSE], 1, nearby))
```

```
## [1] 0.4966
```

```
mean(apply(x[,1:2], 1, nearby))
```

```
## [1] 0.2397
```

```
mean(apply(x[,1:5], 1, nearby))
```

```
## [1] 0.0286
```

Curse of dimensionality

Data are sparse

```r
x <- matrix(runif(1e6,-1,1), ncol=100)
nearby <- function(z) { all(abs(z) < 0.5) }
mean(apply(x[,1:10], 1, nearby))
```

```
## [1] 7e-04
```

```r
mean(apply(x[,1:50], 1, nearby))
```

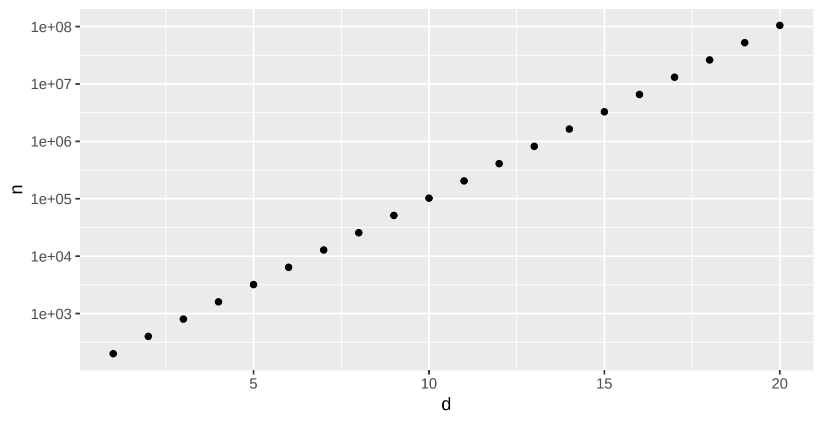
```
## [1] 0
```

```r
mean(apply(x[,1:100], 1, nearby))
```

```
## [1] 0
```

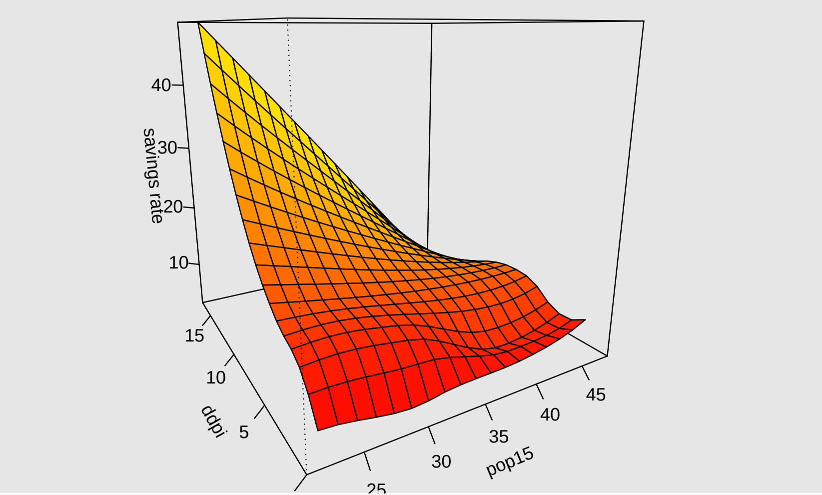
Curse of dimensionality

- Available data in a window is proportional to n^{-d}.
- Let $h = 0.5$, and suppose we need 100 observations to estimate our model locally.



Bivariate smoothing

```r
lomod <- loess(sr ~ pop15 + ddpi, data=savings)
```



Bivariate smoothing

```r
library(mgcv)
smod <- gam(sr ~ s(pop15, ddpi), data=savings)
```