Methods of Applied Statistics I

STA2101H F LEC9101

Week 11

December 1 2021

Today

Start Zoom

1. Upcoming events
2. Recap on GLMs
3. GLM examples
4. case-control studies
5. nonparametric regression

Upcoming

- Monday Dec 6 3.30 Data Science ARES series
  The Rigorous and Human Life of Data Link

Dr. Cecilia Aragon, U Washington

Upcoming

- Monday Dec 6 3.30 Data Science ARES series
  The Rigorous and Human Life of Data Link

Dr. Cecilia Aragon, U Washington

- Friday Dec 3 Toronto Data Workshop Zoom link Leanne Trimble is a data librarian at the Map & Data Library
- Friday Dec 10 Toronto Data Workshop

Nathan Taback U of T

... Upcoming

- Thursday Dec 2 3.30
  A modern take on Huber regression

  Po-Ling Loh, U Cambridge

Zoom Link

Project

- Part I 3–5 pages, non-technical
    1. a description of the scientific problem of interest
    2. how (and why) the data being analyzed was collected
    3. preliminary description of the data (plots and tables)
    4. non-technical summary for a non-statistician of the analysis and conclusions

- Part II 3–5 pages, technical
    1. models and analysis
    2. summary for a statistician of the analysis and conclusions

- Part III Appendix

  R script or .Rmd file; additional plots; additional analysis; References

12 point font

$1\frac{1}{2}$ sp

Figures @ end

Tables @ "

or in between

- 40 points total

- Part I:
  description of data and scientific problem 5
  suitability of plots and tables 5
  quality of the presentation 5

clear, non-technical, concise but thorough

`![path to an figurefilename](text)`

- Part II:
  summary of the modelling and methods 5
  suitability and thoroughness of the analysis 10

justification for choices

model checks, data checks

- Part III:
  relevance of additional material 5
  complete and reproducible submission 5

Recap: GLMs

n $\quad p < n$

- response y_i, covariates x_i^T — $1 \times p$ vector
- $E(y_i) = \mu_i$, $\boxed{g(\mu_i) = x_i^T \beta} = \eta_i$ $\quad \boxed{\text{var}(y_i) = \phi_i V(\mu_i)}$ — $V(\cdot)$ variance function
- ϕ_i is either known, or constant, or $\phi_i = a_i \phi$ — a_i known

$$f(y_i; \phi_i | x_i)$$

$$e^{\frac{\theta_i y_i - b(\theta_i)}{\phi_i} + c(\phi_i, y_i)}$$

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- inference for β based on likelihood theory: Wald $\hat{\beta} - \beta \dot{\sim} N(0, \ldots)$

  $\ell'(\hat{\beta}) = 0, \qquad \widehat{\text{var}}(\hat{\beta}) = \{-\ell''(\hat{\beta})\}^{-1} \qquad (\hat{\beta}-\beta)^T j(\hat{\beta})(\hat{\beta}-\beta) \dot{\sim} \chi^2_p$

  $\hat{\beta}_j \dot{\sim} N(\beta_j, \widehat{\text{var}}(\hat{\beta})_{jj})$

- $w(\beta) = 2\{\ell(\hat{\beta}) - \ell(\beta)\} \dot{\sim} \chi^2_p \qquad 2\{\ell_p(\hat{\beta}_j) - \ell_p(\beta_j)\} \dot{\sim} \chi^2_d$ — profile log-likelihood

  LRT

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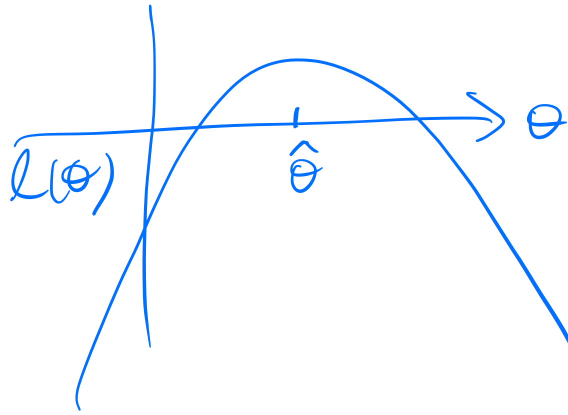
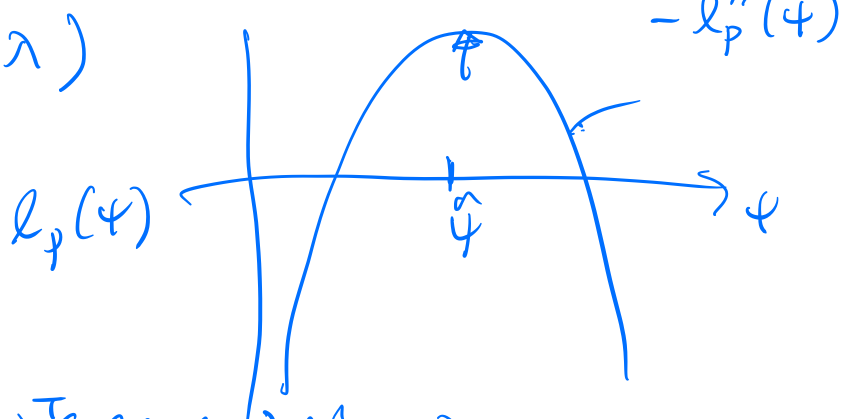
- model-checking as with linear models:
  deviance residuals or Pearson residuals, measures of influence — Cook's distance

$\theta \in \mathbb{R}$



$\theta = (\underline{\underline{\psi}}, \lambda)$



Wald $(\hat\psi - \psi)^T\{-\ell_p''(\hat\psi)\}(\hat\psi - \psi)$

LRT $\quad 2\{\ell_p(\hat\psi) - \ell_p(\psi)\}$

$$j = \begin{bmatrix} j_{\psi\psi} & j_{\psi\lambda} \\ j_{\lambda\psi} & j_{\lambda\lambda} \end{bmatrix}$$

$$\ell_p''(\hat\psi) = \underline{\frac{\partial^2}{\partial\psi}\{\ell(\psi, \hat\lambda_\psi)\}}$$

$$j^{-1}(\theta) = \frac{1}{ad-bc}\begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$$

$N(X\beta, \sigma^2 I)$ $\qquad \ell_p(\sigma^2) = -\frac{n}{2}\log\sigma^2 + \frac{RSS}{2\sigma^2}$

(ntbc)

$\hat\sigma^2 = \frac{1}{n}RSS$ (profile)

$\tilde\sigma^2 = \frac{1}{n-p}RSS$

$g(\mu_i) = x_i^T \beta$

$(y_1, \underline{x}_1) \ldots (y_n, \underline{x}_n)$ β_7 : offset. b7[i].

$$L(\underset{\sim}{\theta}; \psi \mid \underline{x}) = \prod f(y_i; \psi, \lambda \mid x_i)$$

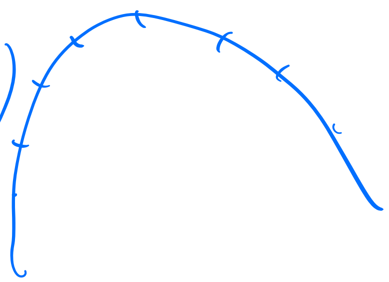
$$L_p(\psi) = L(\psi, \hat{\lambda}_\psi) - \psi_1$$

ψ_2

$\vdots$

ψ_n

$L_p(\psi)$



$\longrightarrow$ confint $\Longleftarrow$ profile conf. intervals

$(\, ,)$

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- model-checking as with linear models:
  deviance residuals or Pearson residuals, measures of influence — Cook's distance

- model-building as with linear models:
  forward/backward/stepwise, analysis of deviance, AIC, subject-matter knowledge

Iterratively re-weighted least squares

$$\hat{\beta} = (X^T W X)^{-1} X^T W z; \quad z = X\beta + \underline{W^{-1}} u; \qquad z(\beta) = X\beta + W^{-1}(\beta)u(\beta); X\beta = \eta$$

$$\text{Var}(\hat{\beta}) \doteq (X^T W X)^{-1}$$

W is diagonal

$p \times p$ $p \times n$ $n \times n$ $n \times p$

derived rvs.

$$W_{ii} = \frac{1}{\phi a_i \{g'(\mu_i)\}^2 V(\mu_i)}$$

$$u_i = \frac{y_i - \mu_i}{\phi a_i g'(\mu_i) V(\mu_i)}$$

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$\mu_i = E(y_i)$

initial values?: $\mu_{init} = y, \quad \eta_{init} = X\beta_{init} = g(y)$

SM §10.3.2; ELM §6.2

Clarification re GLM fitting

$$\hat{\beta} = (X^T W^{-1} X) X^T W z$$

iteration

$$\hat{\beta}^{(t+1)} = (X^T W^{(t)} X)^{-1} X^T W^{(t)} z^{(t)} \qquad z^{(t)} = X\hat{\beta}^{(t)} + W^{-1(t)} u^{(t)};$$

$$W^{(t)} = W(\hat{\beta}^{(t)}), \quad u^{(t)} = u(\hat{\beta}^{(t)})$$

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At convergence,

$$\hat{\beta} = (X^T \hat{W} X)^{-1} X^T \hat{z}$$

$$\widehat{\mathrm{Var}}(\hat{\beta}) \doteq (X^T \hat{W} X)^{-1}$$

W is diagonal

IJALM

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$$W_{ii} = \frac{1}{\phi a_i \{g'(\mu_i)\}^2 V(\mu_i)}, \qquad u_i = \frac{y_i - \mu_i}{\phi a_i g'(\mu_i) V(\mu_i)}$$

... GLMs special sauce

- for Poisson and binomial responses, the saturated model has residual deviance > 0
- this provides a goodness-of-fit test of the regression model

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  it is estimated from the residuals after fitting the regression model   Pearson residuals

$$\tilde{\phi} = \frac{1}{n-p} \sum \frac{(y_i - \hat{\mu}_i)^2}{g'^2(\hat{\mu}_i)V(\hat{\mu}_i)} \quad \text{(ntbc)}$$

(not MLE) X^2 Pearson's

... GLMs special sauce

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- quasi- Poisson or binomial introduces an overdispersion parameter that inflates the estimated variance of $\hat{\beta}_j$

$$\hat{\beta} = (X^T W X)^{-1} X^T W z$$

$$\widehat{\mathrm{var}}\,\hat{\beta} = \tilde{\phi}\, \cancel{V(\hat{\mu})}\, (X^T W X)^{-1}$$

$$\widehat{\mathrm{var}}\,\hat{\beta} = (X^T W X)^{-1} \tilde{\phi}$$

... GLMs special sauce

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- connection to (weighted) least squares enables fast convergence of algorithm, direct generalization of diagnostics

IJALM

Gamma glm; Binary deviance (HW6); HW7,8

- ELM §7.1: "The canonical parameter is $-1/\mu$, so the canonical link is $\eta = -1/\mu$. However, we typically remove the minus (which is fine provided we take account of this in any derivations) and just use the inverse link"

- $E(y_i) = \mu_i, \qquad \theta_i = -1/\mu_i, \qquad \mathrm{var}(y_i) = \mu_i^2/\nu = \phi/\theta_i^2$
- if $g(\mu_i) = \theta_i$, then $g'(\mu_i) = 1/V(\mu_i) \longrightarrow g'(\mu_i) = 1/\mu_i^2$
- $\sum(y_i - \hat{\mu}_i)x_{ij} = 0, \quad j = 1, \ldots, p$

- if μ_i increases, $E(y_i)$ increases, θ_i increases, seems all consistent

Gamma glm; Binary deviance (HW6); HW7,8

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- binary response; deviance = $-2\sum_{i=1}^n\{p_i(\hat{\beta})\log[p_i(\hat{\beta})/\{1-p_i(\hat{\beta})\}] + \log(1-p_i(\hat{\beta})\}$
  $= \dots \qquad = \qquad -2\sum[p_i(\hat{\beta})x_i^T\hat{\beta} + \log\{1-p_i(\hat{\beta})\}]$

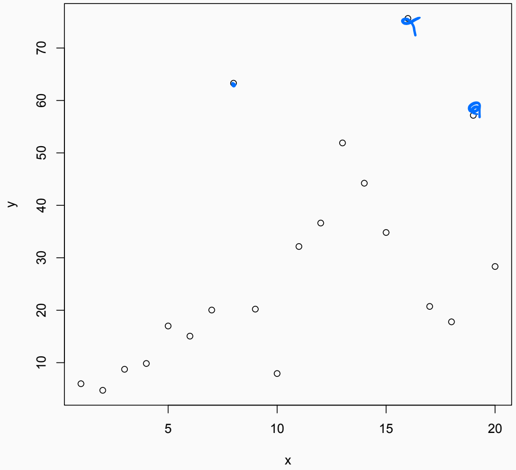
Aside ...

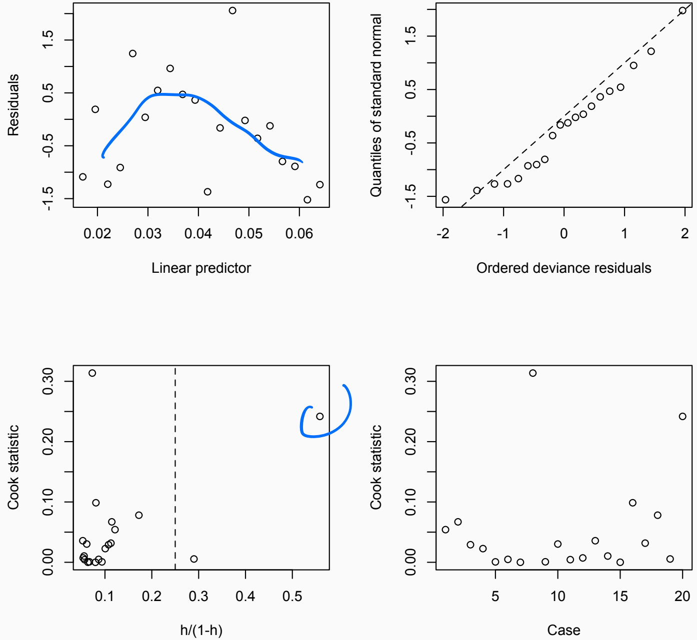
$$
\begin{aligned}
D &= 2\sum\left[y_i \log\left(\frac{y_i}{m_i\hat{p}_i}\right) + (m_i - y_i)\log\left\{\frac{m_i - y_i}{m_i(1-\hat{p}_i)}\right\}\right] \\
&= 2\sum\left\{y_i \log\left(\frac{y_i}{\hat{p}_i}\right) + (1 - y_i)\log\left(\frac{1 - y_i}{1-\hat{p}_i}\right)\right\} \\
&= 2\left\{\sum_{y_i=0}\log\left(\frac{1}{1-\hat{p}_i}\right) + \sum_{y_i=1}\log\left(\frac{1}{\hat{p}_i}\right)\right\} \\
&= -2\left\{\sum_{y_i=0}\log(1-\hat{p}_i) + \sum_{y_i=1}\log(\hat{p}_i)\right\} \\
&= -2\left\{\sum_{i=1}^{n}\log(1-\hat{p}_i) + \sum_{y_i=1}\log\left(\frac{\hat{p}_i}{1-\hat{p}_i}\right)\right\} \\
&= -2\left\{\sum_{i=1}^{n}\log(1-\hat{p}_i) + \sum_{i=1}^{n} y_i x_i^T\hat{\beta}\right\} = -2\left\{\sum_{i=1}^{n}\log(1-\hat{p}_i) + \sum_{i=1}^{n}\hat{p}_i x_i^T\hat{\beta}\right\}
\end{aligned}
$$

Quick example

```
n <- 20
b0 <- 3; b1 <- 2
x <- 1:20; y <- x
eta <- b0 + b1*x
mu = 1/eta
for(i in 1:20){y[i] <- rgamma(1,shape = 3, rate = 3/mu[i])}
plot(x,y)

gamglm <- glm(y ~ x, family = Gamma(link = inverse))

summary(gamglm)

plot.glm.diag(gamglm)
```

… Quick example





More GLM examples

$$g(\mu_i) = \log(\mu_i) = x_i^T\beta$$

$$\mu_i = e^{x_i^T\beta}$$

$\longrightarrow$ glmex.Rmd

see glmex.pdf

$$\frac{1}{\mu_i} = x_i^T\beta$$

$$\mu_i = \underline{\underline{(x_i^T\beta)^{-1}}}$$

multinomial regr Ch 3 ELM (cntbc)

$\longrightarrow$ casecontrol.pdf

two-way tables

factor A

factor B

	1	2	3
1	y_{11}		
2		...	
3			
4			

# of obs's in category

? $A \perp B$?

loglinear models

$\longrightarrow$ A, B as joint responses

logistic or Poisson reg.

or explanatory to y

Nonlinear least squares

- $y_i = \eta(x_i; \beta) + \epsilon_i$

Example 10.9 $\eta(x_i; \beta) = \beta_0\{1 - \exp(-x_i/\beta_1)\}$

- SM shows how this can also be fit using IRWLS

$E(y_i \mid x_i)$

$= \eta(x_i; \beta)$

$Var(y_i) = \sigma^2$

10.1 · Introduction

Table 10.1 Calcium uptake (nmoles/mg) of cells suspended in a solution of radioactive calcium, as a function of time suspended (minutes) (Rawlings, 1988, p. 403).

Time (minutes)	Calcium uptake (nmoles/mg)		
0.45	0.34170	−0.00438	0.82531
1.30	1.77967	0.95384	0.64080
2.40	1.75136	1.27497	1.17332
4.00	3.12273	2.60958	2.57429
6.10	3.17881	3.00782	2.67061
8.05	3.05959	3.94321	3.43726
11.15	4.80735	3.35583	2.78309
13.15	5.13825	4.70274	4.25702
15.00	3.60407	4.15029	3.42484

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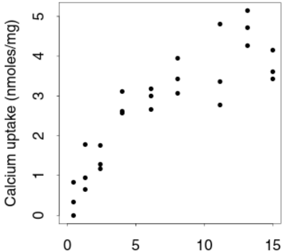

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Example 10.9 $\eta(x_i;\beta) = \beta_0\{1 - \exp(-x_i/\beta_1)\}$

- SM shows how this can also be fit using IRWLS

$\sum_{i=1}^{n}\{y_i - \eta(x_i;\beta)\}^2 = SS(\beta)$

nls (y ~ x , ...)

need to specify $\eta(\cdot)$

need $\beta_0^{(0)}$ $\beta_1^{(0)}$ starting values

$\hat\beta_0$ $\hat\beta_1$

"Allowing for measurement error, which seems to be similar at all levels of *y*"

$(\hat X_\beta^T \hat W \hat X_\beta)^{-1} \hat X_\beta^T \hat W_\beta y$

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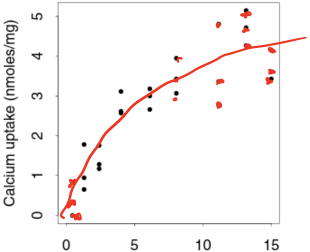

Figure 10.1 Calcium uptake (nmoles/mg) of cells suspended in a solution of radioactive calcium, as a function of time suspended (minutes).

$\frac{dy}{dx} = \beta_0(y -$

$\boxed{\frac{dy}{dx} = (\beta_0 - y)\frac{1}{\beta_1}}$

$f(x_i)$ signal

ϵ noise

- model $y_i = f(x_i) + \epsilon_i, \quad i = 1, \ldots, n \quad x_i$ scalar
- mean function $f(\cdot)$ assumed to be "smooth"

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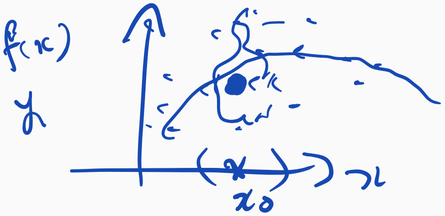
- introduce a kernel function $K(u)$ and define a set of weights

$$w_i = \frac{1}{\lambda} K\left(\frac{x_i - x_0}{\lambda}\right)$$

$i = 1, \dots, n \quad w_i$

- estimate of $f(x)$, at $x = x_0$:

$$\hat{f}_\lambda(x_0) = \frac{\sum_{i=1}^n w_i y_i}{\sum_{i=1}^n w_i}$$



Nonparametric Regression

ELM, Ch. 11; SM, §10.7

- model $y_i = f(x_i) + \epsilon_i, \quad i = 1, \dots, n \quad x_i$ scalar
- mean function $f(\cdot)$ assumed to be "smooth"
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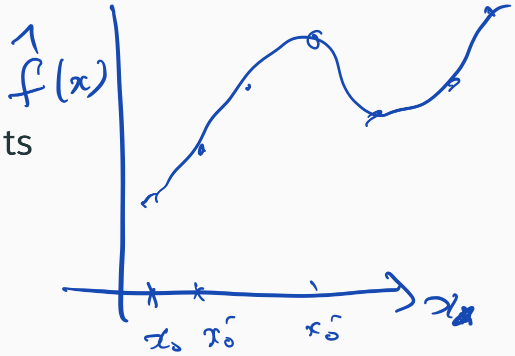
- Nadaraya-Watson estimator – local averaging



local polynomial of degree 0

Kernel smoothers

- choice of bandwidth, λ controls smoothness of est'd function
- larger bandwidth $=$ more smoothing
- kernel estimators are biased
- making the estimate smoother increases bias, decreases variance

Kernel smoothers

ELM §11.1

- choice of bandwidth, λ controls smoothness of function
- larger bandwidth = more smoothing
- kernel estimators are biased
- making the estimate smoother increases bias, decreases variance

$\frac{1}{\lambda} K\left(\frac{x_i - x_0}{\lambda}\right)$

$w_i = e^{-\frac{1}{2}\left(\frac{x_i - x_0}{\lambda}\right)^2} \frac{1}{\sqrt{2\pi}\,\lambda}$

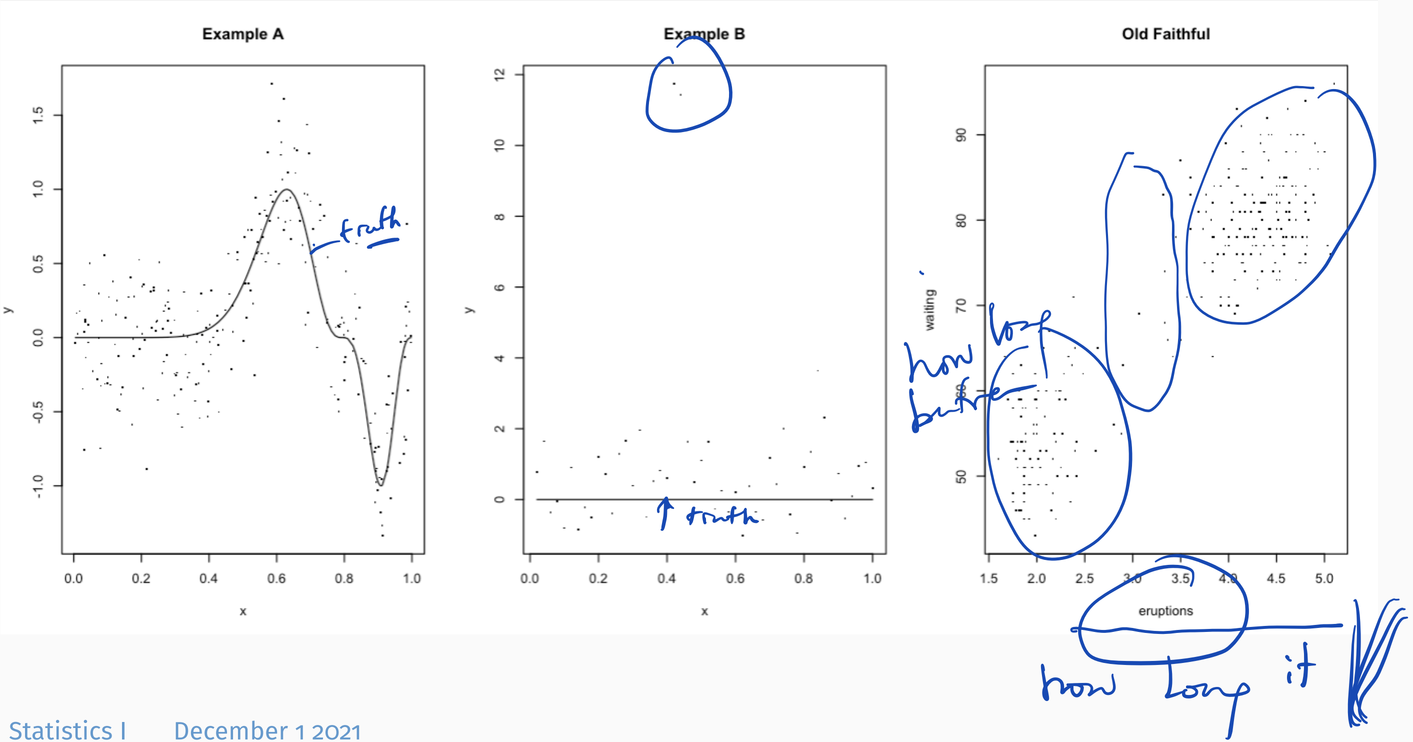
less imp't

- choice of kernel function, $K(\cdot)$, controls smoothness and "local-ness"
- Faraway recommends Epanechnikov kernel $K(x) = \frac{3}{4}(1 - x^2), |x| \leq 1$
- `ksmooth(base)` offers only uniform (box) or normal

- `bkde(KernSmooth)` offers `normal, box, epanech, biweight, triweight`
- `biweight:` $K(x) \propto (1 - |x|^2)^2, |x| \leq 1$ `triweight:` $K(x) \propto (1 - |x|^2)^3, |x| \leq 1$

$\int_{-1}^{1} \frac{3}{4}(1-x^2)\,dx$

Examples


Example A
Example B
Old Faithful
truth
truth
how long before
waiting
eruptions
y
x
how long it

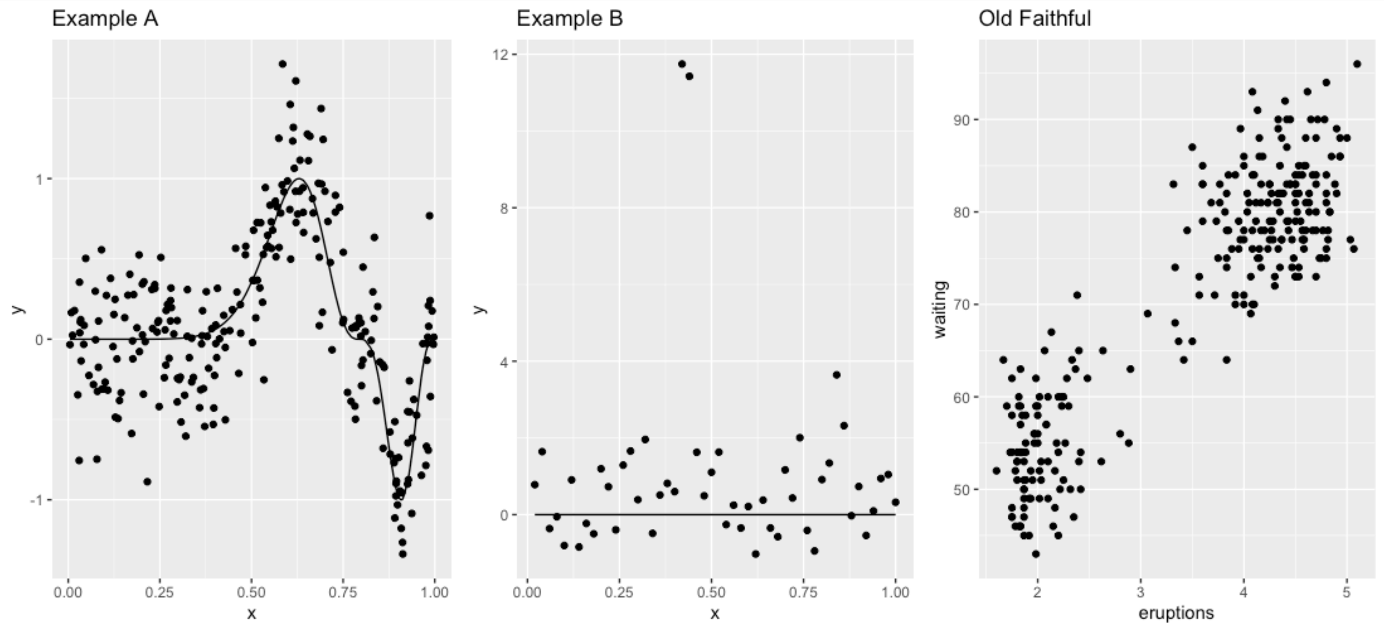
```
exb <- data.frame(exb)

plota <- ggplot(exa) + geom_point(aes(x,y)) +
geom_line(aes(x,m))+ ggtitle("Example A")

plotb <- ggplot(exb) + geom_point(aes(x,y)) +
geom_line(aes(x,m))+ ggtitle("Example B")

plotc <- ggplot(faithful) + geom_point(aes(eruptions,waiting)) +
 ggtitle("Old Faithful")

grid.arrange(plota, plotb, plotc, nrow=1) #in gridExtra library
```


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

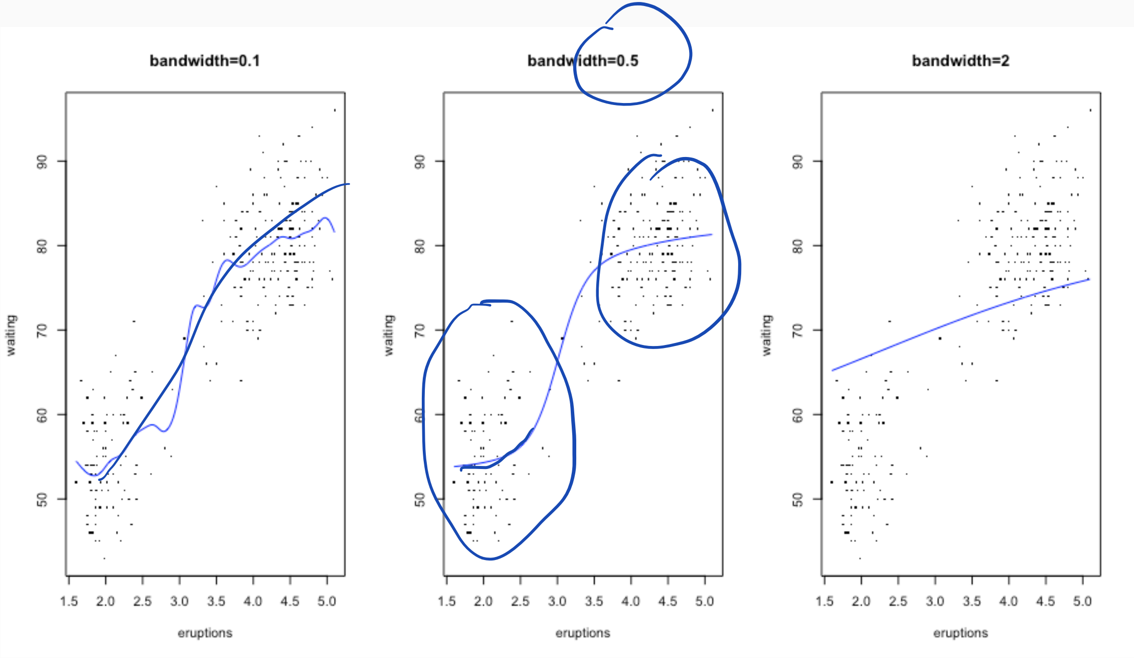
```
with(faithful, plot(eruptions, waiting, cex=2, main = "bandwidth=0.1", pch="."))
lines(locpoly(faithful$eruptions,faithful$waiting,drv=0L,
  degree=0,bandwidth=.1), col = "blue")
```

est $\hat{f}_\lambda$ as above

```
with(faithful, plot(eruptions, waiting, cex=2, main = "bandwidth=0.5", pch="."))
lines(locpoly(faithful$eruptions,faithful$waiting,drv=0L,
  degree=0, bandwidth=.5), col = "blue")

with(faithful, plot(eruptions, waiting, cex=2, main = "bandwidth=2", pch="."))
lines(locpoly(faithful$eruptions,faithful$waiting,drv=0L,
  degree=0, bandwidth=2), col = "blue")
```

... Examples



These are smoother than the plots in ELM using `base::ksmooth`

Bias and MSE

- Nadaraya-Watson: $\hat{f}_\lambda(x) = \Sigma w_i y_i / \Sigma w_i;$ $\qquad w_i = \frac{1}{\lambda} K(\frac{x_i - x_0}{\lambda})$

Bias and MSE

- Nadaraya-Watson: $\hat{f}_\lambda(x) = \Sigma w_i y_i / \Sigma w_i$; $w_i = \frac{1}{\lambda} K(\frac{x_i - x_0}{\lambda})$

- $\hat{f}_\lambda(x)$ is biased

$$E\{\hat{f}_\lambda(x)\} \doteq \frac{1}{2}\lambda^2 f''(x)$$

$$\mathrm{var}\{\hat{f}_\lambda(x)\} \doteq \frac{\sigma^2}{n\lambda \cancel{f(x)}} \int K^2(u)du$$

$g(x)$

$\frac{\sigma^2}{n}$ $\frac{\int_{-1}^{1} K^2(u)du}{\lambda g(x)}$

$$E\hat{f}_\lambda(x) = \sum_{i=1}^{n} \frac{w_i E(y_i)}{\Sigma w_i} = \sum \frac{w_i f(x_i)}{\Sigma w_i}$$

$f(x)$ ✓

$$\doteq \sum \frac{w_i}{\Sigma w_i}\{f(x) + (x_i - x) f'(x) + \frac{1}{2}(x_i - x)^2 f''(x)\}$$

$\to 0$

delta method

- Nadaraya-Watson: $\hat{f}_\lambda(x) = \Sigma w_i y_i / \Sigma w_i$; $\quad w_i = \frac{1}{\lambda} K(\frac{x_i - x_0}{\lambda})$
- $\hat{f}_\lambda(x)$ is biased

$$\int_{-1}^{1} K(u)\,du = 1$$

$$\rightarrow \mathrm{E}\{\hat{f}_\lambda(x)\} \doteq \frac{1}{2}\lambda^2 f''(x)$$

$$\mathrm{var}\{\hat{f}_\lambda(x)\} \doteq \frac{\sigma^2}{n\lambda g(x)} \int K^2(u)\,du$$

$$= \frac{\sigma^2}{n} \cdot \frac{\int_{-1}^{1} K^2(u)\,du}{\lambda\, g(x)}$$

based $n \to \infty$

- could choose λ to minimize MSE $=$ bias^2 $+$ var, at x
- could choose λ to minimize integrated MSE

$g(x)$ is the limiting "density" of the x_i's

- Nadaraya-Watson: $\hat{f}_\lambda(x) = \Sigma w_i y_i / \Sigma w_i$; $w_i = \frac{1}{\lambda} K(\frac{x_i - x_0}{\lambda})$

- $\hat{f}_\lambda(x)$ is biased

$$E\{\hat{f}_\lambda(x)\} \doteq \frac{1}{2}\lambda^2 f''(x)$$

$$\text{var}\{\hat{f}_\lambda(x)\} \doteq \frac{\sigma^2}{n\lambda f_X(x)} \int K^2(u)du$$

g

- could choose λ to minimize MSE $=$ bias^2 $+$ var, at x
- could choose λ to minimize integrated MSE

- more usual to use cross-validation

SM 10.7.1 (no n); ELM 11.1

$$CV(\lambda) = \frac{1}{n}\sum_{i=1}^{n}\{y_i - \hat{f}_{-i}(x_i)\}^2$$

$\hat{f} = \hat{f}_\lambda$

based on $(y_1, \ldots, y_n)$

not y_i

Cross-validation

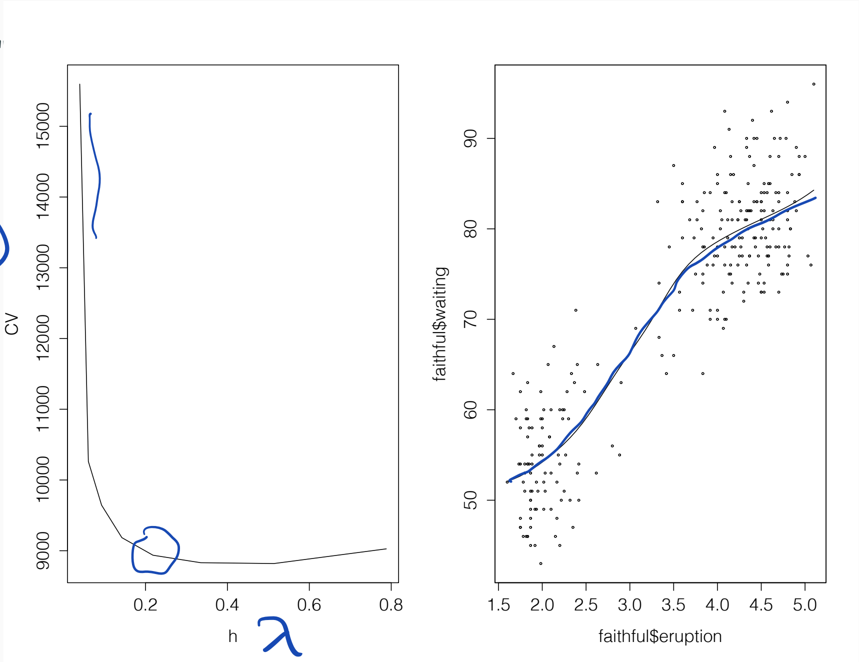
$$\sum (y_i - x_i^T \beta)^2 + \lambda \sum_{i=1}^{n} |\beta_i|$$

```
library(sm)
hm <- hcv(faithful$eruptions,
   faithful$waiting, display = "lines"
sm.regression(faithful$eruptions,
   faithful$waiting, h = hm,
   xlab = "eruptions",
   ylab = "waiting")
```

(CV/λ)

$\lambda_{opt} = 0.22$

$\sum w_i y_i / \sum w_i$



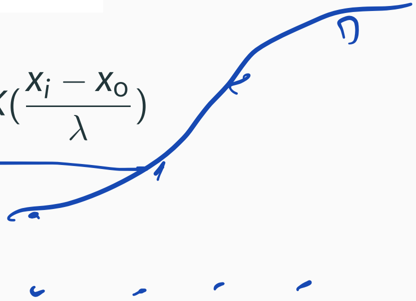
Local Polynomials

- above uses local averaging based on kernel function
- better estimates can be obtained using local regression at point x

Local Polynomials

- above uses local averaging based on kernel function
- better estimates can be obtained using local regression at point x_0
- $$\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} 1 & (x_1 - x_0) & \cdots & (x_1 - x_0)^k \\ \vdots & \vdots & & \vdots \\ 1 & (x_n - x_0) & \cdots & (x_n - x_0)^k \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_k \end{pmatrix} + \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{pmatrix},$$

- above uses local averaging based on kernel function
- better estimates can be obtained using local regression at point x
- $$\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} 1 & (x_1 - x_0) & \cdots & (x_1 - x_0)^k \\ \vdots & \vdots & & \vdots \\ 1 & (x_n - x_0) & \cdots & (x_n - x_0)^k \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_k \end{pmatrix} + \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{pmatrix},$$
- $$\hat{\beta} = (X^T W X)^{-1} X^T W y, \quad W = \mathrm{diag}(w), \quad w_i = \frac{1}{\lambda} K\left(\frac{x_i - x_0}{\lambda}\right)$$
- $$\hat{f}_\lambda(x_0) = \hat{\beta}_0$$



- above uses local averaging based on kernel function
- better estimates can be obtained using local regression at point x
- $$\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} 1 & (x_1 - x_0) & \cdots & (x_1 - x_0)^k \\ \vdots & \vdots & & \vdots \\ 1 & (x_n - x_0) & \cdots & (x_n - x_0)^k \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_k \end{pmatrix} + \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{pmatrix},$$
- $$\hat{\beta} = (X^T W X)^{-1} X^T W y, \quad W = \mathrm{diag}(w), \quad w_i = \frac{1}{\lambda} K\left(\frac{x_i - x_0}{\lambda}\right)$$
- $$\hat{f}_\lambda(x_0) = \hat{\beta}_0$$
- usually evaluate the function at sample points: $\hat{f}_\lambda(x_i), i = 1, \ldots, n$

curve by joining

… local polynomials

- odd-order polynomials work better than even; usually local linear fits are used

- kernel function is often a Gaussian density, or the tricube kernel

$$K(u) = (1 - |u|^3)^3, \quad |u| \leq 1$$

✓

(not to be confused with tri-weight)

(aargh!)

... local polynomials

- odd-order polynomials work better than even; usually local linear fits are used
- kernel function is often a Gaussian density, or the tricube kernel

$$K(u) = (1 - |u|^3)^3, \quad |u| \leq 1$$

- as with N-W (local averaging) estimators, choice of bandwidth controls smoothness
- **loess** is the most widely used, and is the default in `ggplot2`

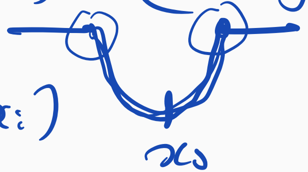
local linear regression

robust regression ($k=1$)

downweight outliers

$$\min \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i)^2 \quad \text{(locally)}$$

$$\min \sum_{i=1}^{n} \rho(y_i - \beta_0 - \beta_1 x_i)$$



... local polynomials

SM 10.7; ELM 11.3

$$\rho(x) = \begin{cases} |x|, & |x|<1 \\ 1, & |x|>1 \end{cases}$$

- odd-order polynomials work better than even; usually local linear fits are used

- kernel function is often a Gaussian density, or the tricube kernel

$$K(u) = (1 - |u|^3)^3, \quad |u| \leq 1$$

- as with N-W (local averaging) estimators, choice of bandwidth controls smoothness
- **loess** is the most widely used, and is the default in `ggplot2`

- fits a local linear regression, but not by least squares

- uses a robust version of least squares that downweights outliers
- the result is that the bandwidth can change with x

… local polynomials

- $\hat{\beta} = (X^T W X)^{-1} X^T W y$ $\qquad W = \text{diag}(w_1, \dots, w_n)$
- $\hat{f}_\lambda(x_0) = \hat{\beta}_0 = \sum_{i=1}^n S(x_0; x_i, \lambda) y_i$
- $S(x_0; x_1, \lambda), \dots, S(x_0; x_n, \lambda)$ first row of “hat” matrix
- this makes it relatively easy to analyse the behaviour of local polynomial smoothers

SM §10.7

- $\hat{\beta} = (X^T WX)^{-1} X^T Wy$ $\qquad W = \text{diag}(w_1, \ldots, w_n)$
- $\hat{f}_\lambda(x_0) = \hat{\beta}_0 = \sum_{i=1}^n S(x_0; x_i, \lambda) y_i$
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  SM §10.7
- and to simplify the expression for the cross-validation criterion $CV(\lambda)$

- $\hat{\beta} = (X^T WX)^{-1} X^T Wy$ $\qquad W = \text{diag}(w_1, \ldots, w_n)$
- $\boxed{\hat{f}_\lambda(x_0) = \hat{\beta}_0 = \sum_{i=1}^n S(x_0; x_i, \lambda) y_i}$
- $S(x_0; x_1, \lambda), \ldots, S(x_0; x_n, \lambda)$ first row of "hat" matrix
- this makes it relatively easy to analyse the behaviour of local polynomial smoothers

SM §10.7

- and to simplify the expression for the cross-validation criterion $CV(\lambda)$
- fitting at each sample value gives

$$\boxed{\hat{f}_\lambda(x_i) = \sum_{j=1}^n S(x_i; x_j, \lambda) y_j}$$

$\frac{w_i y_i}{\sum w_i}$

smoothing matrix

- $$CV(\lambda) = \sum_{i=1}^{n} \{y_i - \hat{f}_{-i}(x_i)\}^2$$

- $$CV(\lambda) = \sum_{i=1}^{n} \{y_i - \hat{f}_{-i}(x_i)\}^2$$
- for local polynomials
$$CV(\lambda) = \sum_{i=1}^{n} \left\{ \frac{y_i - \hat{f}_\lambda(x_i)}{1 - S_{ii}(\lambda)} \right\}^2$$

-
$$CV(\lambda) = \sum_{i=1}^{n}\{y_i - \hat{f}_{-i}^{(\lambda)}(x_i)\}^2$$

$\frac{1}{n}\sum \ldots$

$\min_{\lambda} CV(\lambda)$

- for local polynomials

$$CV(\lambda) = \sum_{i=1}^{n}\left\{\frac{y_i - \hat{f}_\lambda(x_i)}{\boxed{1 - S_{ii}(\lambda)}}\right\}^2$$

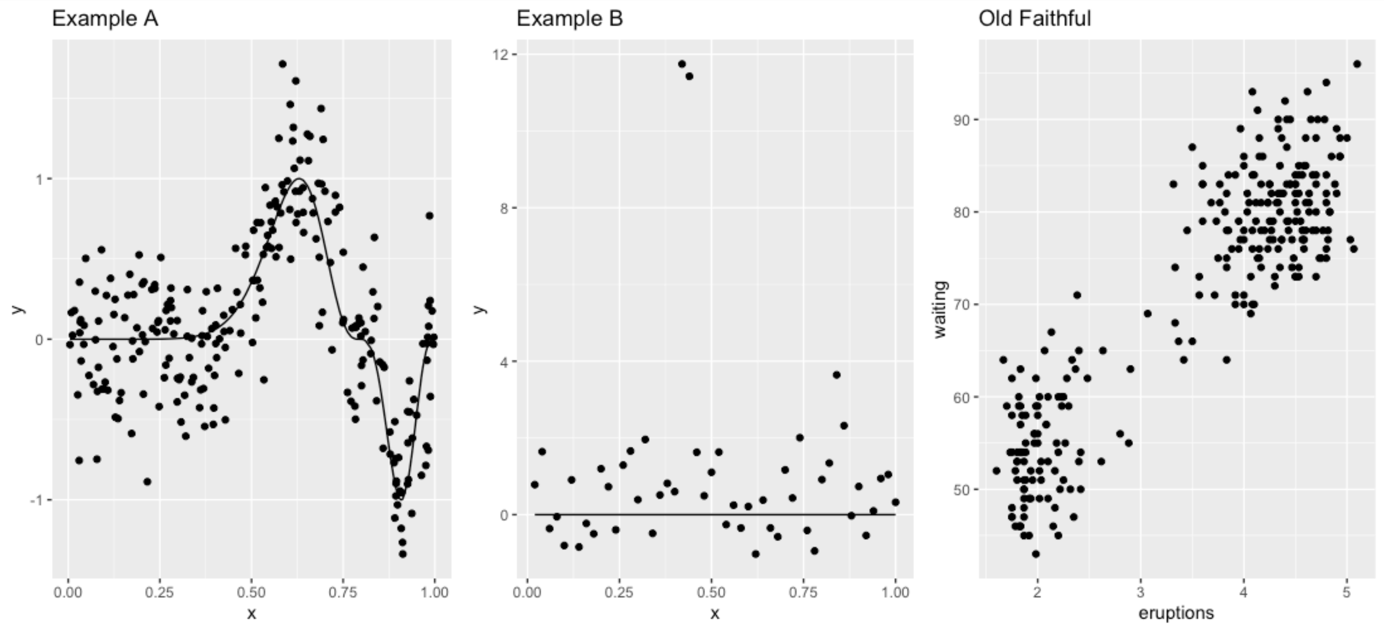
$S_{n \times n}$

- even simpler

$$GCV(\lambda) = \sum_{i=1}^{n}\left\{\frac{y_i - \hat{f}_\lambda(x_i)}{1 - \underline{\mathrm{tr}(S_\lambda)/n}}\right\}^2$$

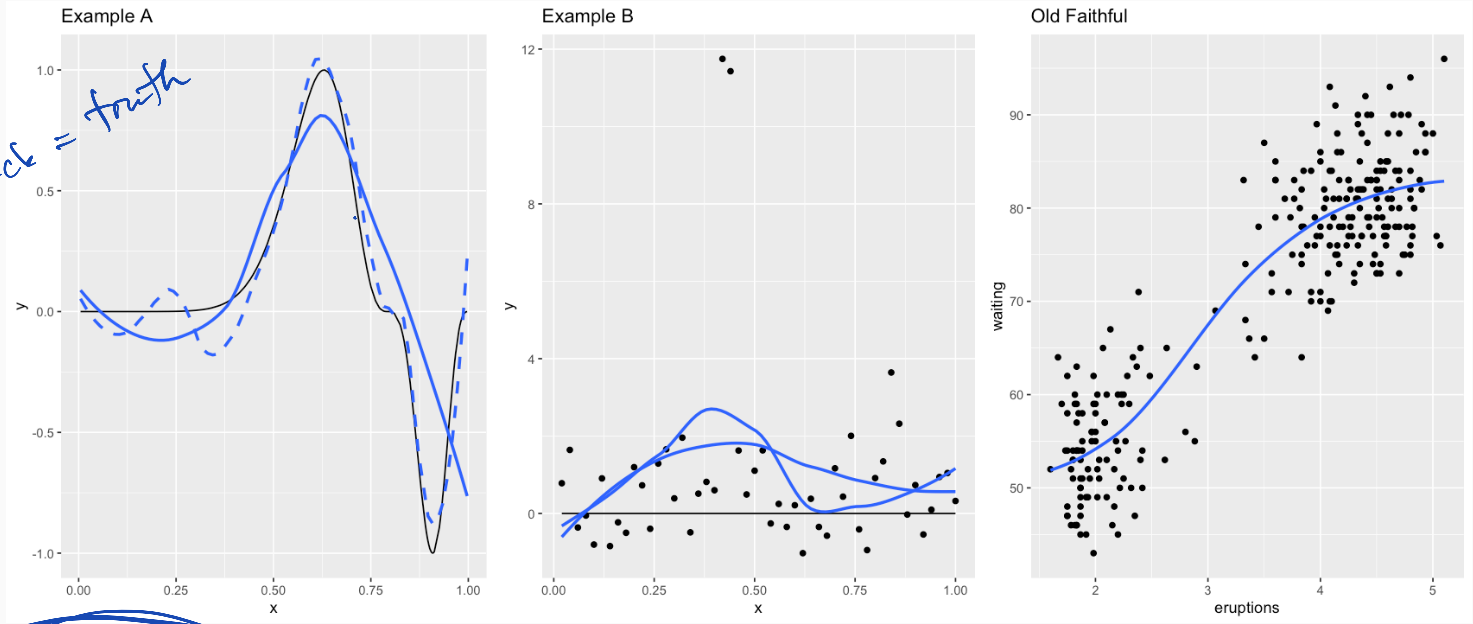
"generalized"

- $$CV(\lambda) = \sum_{i=1}^{n} \{y_i - \hat{f}_{-i}(x_i)\}^2$$
- for local polynomials
$$CV(\lambda) = \sum_{i=1}^{n} \left\{ \frac{y_i - \hat{f}_\lambda(x_i)}{1 - S_{ii}(\lambda)} \right\}^2$$
- even simpler
$$GCV(\lambda) = \sum_{i=1}^{n} \left\{ \frac{y_i - \hat{f}_\lambda(x_i)}{1 - \mathrm{tr}(S_\lambda)/n} \right\}^2$$
- $$\hat{f}_\lambda(x_i) = \sum_{j=1}^{n} S(x_i; x_j, \lambda) y_j$$



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

Examples loess



geom_smooth in ggplot uses local polynomial fitting (loess)

loc. lin. reg. but ~~with~~ robustified

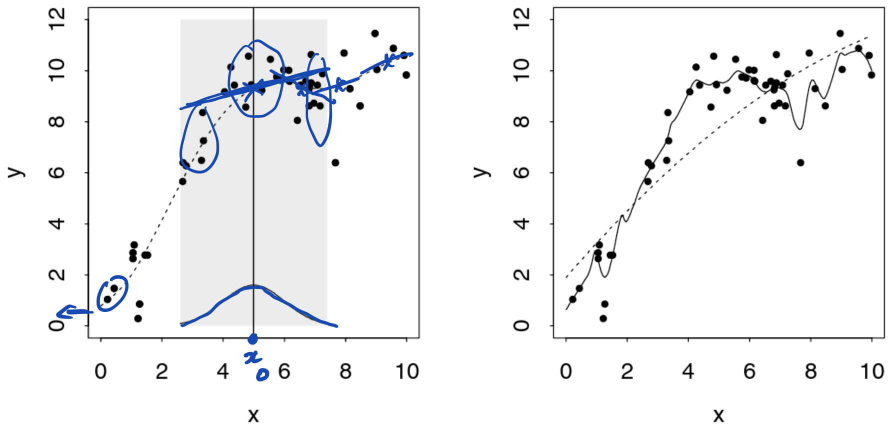


Figure 10.14 Construction of a local linear smoother. Left panel: observations in the shaded part of the panel are weighted using the kernel shown at the foot, with $h = 0.8$, and the solid straight line is fitted by weighted least squares. The local estimate is the fitted value when $x = x_0$, shown by the vertical line. Two hundred local estimates formed using equi-spaced x_0 were interpolated to give the dotted line, which is the estimate of $g(x)$. Right panel: local linear smoothers with $h = 0.2$ (solid) and $h = 5$ (dots).

Recall that a kernel function $w(u)$ is a unimodal density function symmetric about $u = 0$ and with unit variance. One choice of w is the standard normal density. Another is a rescaled form of the *tricube* function

$$w(u) = \begin{cases} (1-|u|^3)^3, & |u| \le 1, \\ 0, & \text{otherwise}, \end{cases} \tag{10.37}$$

Example

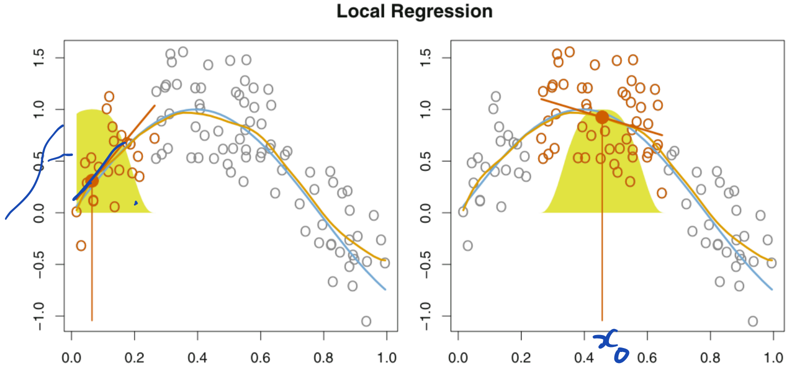


FIGURE 7.9. *Local regression illustrated on some simulated data, where the blue curve represents $f(x)$ from which the data were generated, and the light orange curve corresponds to the local regression estimate $\hat{f}(x)$. The orange colored points are local to the target point x_0, represented by the orange vertical line. The yellow bell-shape superimposed on the plot indicates weights assigned to each point, decreasing to zero with distance from the target point. The fit $\hat{f}(x_0)$ at x_0 is obtained by fitting a weighted linear regression (orange line segment), and using the fitted value at x_0 (orange solid dot) as the estimate $\hat{f}(x_0)$.*

Inference after fitting local polynomials

- model: $y_i = f(x_i) + \epsilon_i, \quad i = 1, \ldots, n$; $\mathrm{E}(\epsilon_i) = 0$; $\mathrm{var}(\epsilon_i) = \sigma^2$

Inference after fitting local polynomials

- model: $y_i = f(x_i) + \epsilon_i, \quad i = 1, \ldots, n$; $\mathrm{E}(\epsilon_i) = 0$; $\mathrm{var}(\epsilon_i) = \sigma^2$
- $\hat{f}_\lambda(x_0) = \hat{\beta}_0 = \sum_{i=1}^n S(x_0; x_i, \lambda) y_i$

Inference after fitting local polynomials

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- $\hat{f}_\lambda(x_0) = \hat{\beta}_0 = \sum_{i=1}^n S(x_0; x_i, \lambda) y_i$
- $E\{\hat{f}_\lambda(x_0)\} =$

Inference after fitting local polynomials

- model: $y_i = f(x_i) + \epsilon_i, \quad i = 1, \dots, n$; $E(\epsilon_i) = 0$; $\text{var}(\epsilon_i) = \sigma^2$
- $\hat{f}_\lambda(x_0) = \hat{\beta}_0 = \sum_{i=1}^n S(x_0; x_i, \lambda) y_i$
- $E\{\hat{f}_\lambda(x_0)\} =$
- $\text{var}\{\hat{f}_\lambda(x_0)\} =$

Inference after fitting local polynomials

- model: $y_i = f(x_i) + \epsilon_i, \quad i = 1, \ldots, n$; $\mathrm{E}(\epsilon_i) = 0$; $\mathrm{var}(\epsilon_i) = \sigma^2$
- $\hat{f}_\lambda(x_0) = \hat{\beta}_0 = \sum_{i=1}^n S(x_0; x_i, \lambda) y_i$
- $\mathrm{E}\{\hat{f}_\lambda(x_0)\} =$
- $\mathrm{var}\{\hat{f}_\lambda(x_0)\} =$
- how many parameters did we fit?

Inference after fitting local polynomials

- model: $y_i = f(x_i) + \epsilon_i, \quad i = 1, \dots, n$; $E(\epsilon_i) = 0$; $\text{var}(\epsilon_i) = \sigma^2$
- $\hat{f}_\lambda(x_0) = \hat{\beta}_0 = \sum_{i=1}^n S(x_0; x_i, \lambda) y_i$
- $E\{\hat{f}_\lambda(x_0)\} =$ ✓
- $\text{var}\{\hat{f}_\lambda(x_0)\} =$ ✓
- how many parameters did we fit?
- by analogy with least squares, estimates of 'degrees of freedom' are $\nu_1 = \text{tr}(S_\lambda)$, or $\nu_2 = \text{tr}(S_\lambda^T S_\lambda)$

$$\tilde{\sigma}^2 = \frac{1}{n - 2\nu_1 + \nu_2} \sum \{y_i - \hat{f}_\lambda(x_i)\}^2$$

lin reg.

$p = tr(H)$

$= tr(H^T H)$

"p"

$= 2\nu_1 - \nu_2$

$n - p$

SM (10.39)

- $E\{\hat{f}_\lambda(x_0)\} = \sum_{i=1}^n S(x_0; x_i, \lambda) f(x_i)$ $\qquad$ $\text{var}\{\hat{f}_\lambda(x_0)\} = \frac{\sigma^2}{n} \sum_{i=1}^n S^2(x_0; x_i, \lambda)$

$= f(x_i)$

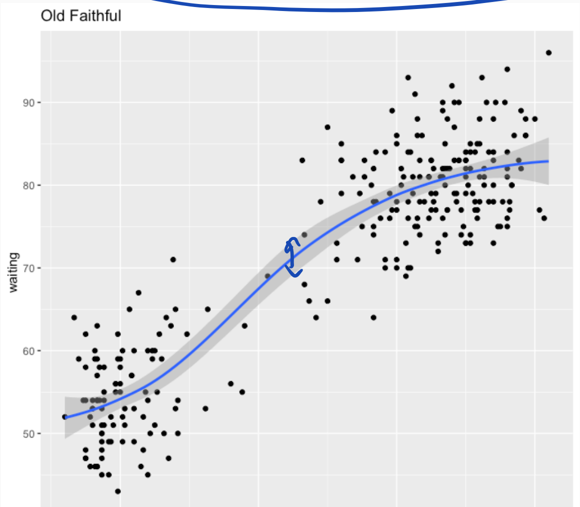
loc. const

$\lambda^2 f''(x_0)$

$$\hat{f}_\lambda^{(x_0)} = \sum_{i=1}^n S(x_i; x_0) y_i$$

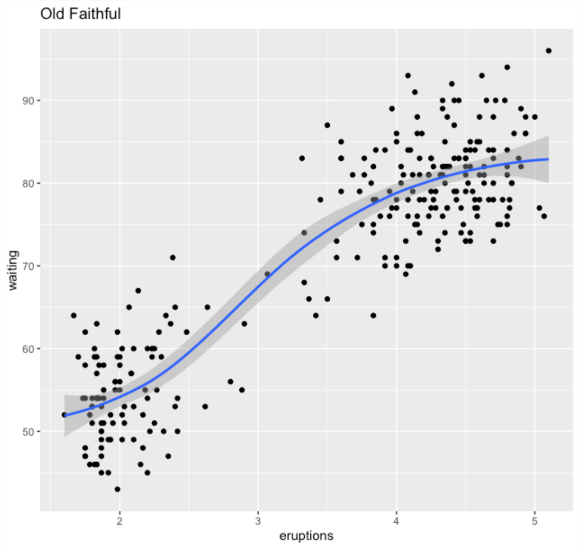
$$\frac{\hat{f}_\lambda(x_0) - E\{\hat{f}_\lambda(x_0)\}}{\widehat{\text{var}}\{\hat{f}_\lambda(x_0)\}^{1/2}} \dot{\sim} N(0, 1)$$

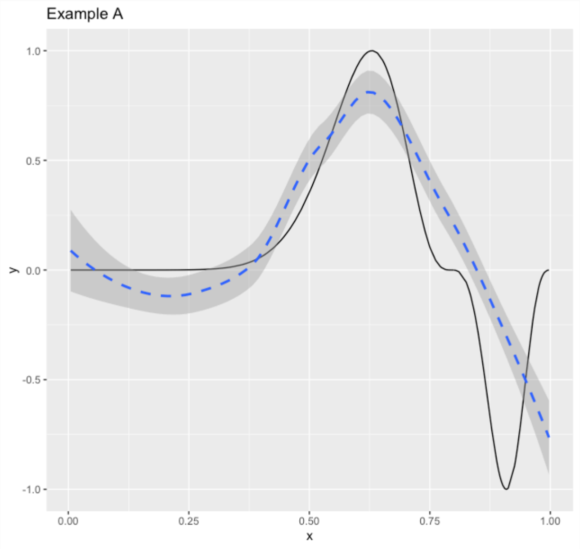
pointwise at each x_0



$$\tilde{\sigma}^2 = \frac{1}{n - 2\nu_1 + \nu_2} RSS$$

… inference after fitting local polynomials





- model $y_i = f(x_i) + \epsilon_i$ $\qquad f(\cdot)$ "flexible"
- above $f(\cdot)$ is estimated at several points using local constants or local linear regression

KernSmooth::locpoly

- another popular approach is to use some very flexible, but parametric form, for f
- for example, $f(x) = \sum_{m=1}^{M} \beta_m \phi_m(x)$

Regression splines

- model $y_i = f(x_i) + \epsilon_i$ $f(\cdot)$ "flexible"
- above $f(\cdot)$ is estimated at several points using local constants or local linear regression KernSmooth::locpoly

- another popular approach is to use some very flexible, but parametric form, for f
- for example, $f(x) = \sum_{m=1}^{M} \beta_m \phi_m(x)$
- examples of ϕ_m: $1, x, x^2, x^3$; $1, \sin(x), \cos(x), \sin(2x), \cos(2x)$;
- piecewise polynomials: e.g. knots at $\xi_1, \xi_2 \in [0, 1]$
- basis functions $\phi(x) : 1, x, x^2, = x^3, (x - \xi_1)^3_+, (x - \xi_2)^3_+$

- model $y_i = f(x_i) + \epsilon_i$ $\quad f(\cdot)$ “flexible”
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- examples of ϕ_m: $1, x, x^2, x^3$; $\quad 1, \sin(x), \cos(x), \sin(2x), \cos(2x)$;
- piecewise polynomials: e.g. knots at $\xi_1, \xi_2 \in [0, 1]$
- basis functions $\phi(x) : 1, x, x^2, = x^3, (x - \xi_1)_+^3, (x - \xi_2)_+^3$

- ELM p.219 builds these “by hand”
- `splines::bs()` builds cubic splines automatically

Smoothing splines

- $y_i = f(x_i) + \epsilon_i, \quad i = 1, \ldots, n$

- $y_i = f(x_i) + \epsilon_i, \quad i = 1, \ldots, n$
- choose $f(\cdot)$ to solve

$$\min_f \sum_{i=1}^{n} \{y - f(x_i)\}^2 + \lambda \int_a^b \{f''(t)\}^2 dt, \quad , \lambda > 0$$

Smoothing splines

- $y_i = f(x_i) + \epsilon_i, \quad i = 1, \ldots, n$
- choose $f(\cdot)$ to solve

$$\min_f \sum_{i=1}^{n} \{y - f(x_i)\}^2 + \lambda \int_a^b \{f''(t)\}^2 dt, \quad , \lambda > 0$$

- solution is a cubic spline, with knots at each observed x_i value

see SM Figure 10.18 for a non-regularized solution

Smoothing splines

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- solution is a cubic spline, with knots at each observed x_i value

see SM Figure 10.18 for a non-regularized solution

- has an explicit, finite dimensional solution

Smoothing splines

- $y_i = f(x_i) + \epsilon_i, \quad i = 1, \ldots, n$
- choose $f(\cdot)$ to solve

$$\min_f \sum_{i=1}^{n} \{y - f(x_i)\}^2 + \lambda \int_a^b \{f''(t)\}^2 dt, \quad , \lambda > 0$$

- solution is a cubic spline, with knots at each observed x_i value

see SM Figure 10.18 for a non-regularized solution

- has an explicit, finite dimensional solution
- $\hat{f} = \{\hat{f}(x_1), \ldots, \hat{f}(x_n)\} = (I + \lambda K)^{-1} y$

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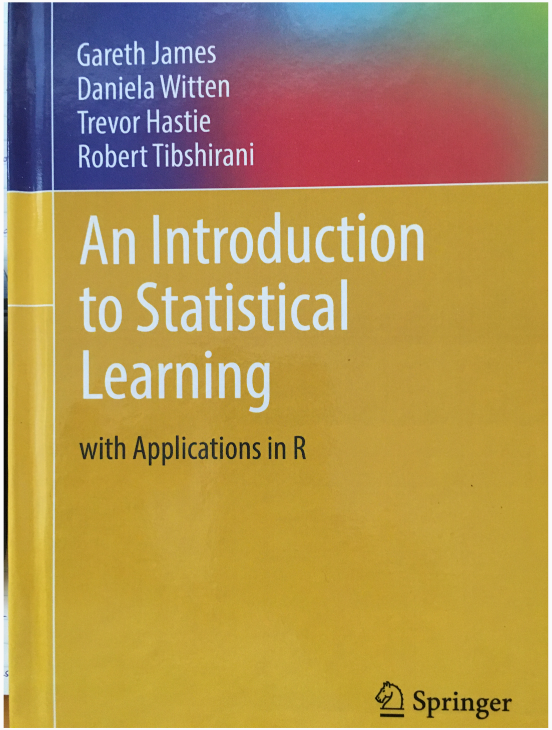
Gareth James
Daniela Witten
Trevor Hastie
Robert Tibshirani
An Introduction to Statistical Learning
with Applications in R
Springer

- $y_i = f(x_i) + \epsilon_i$

- local polynomial regression – `stats::loess`, `KernSmooth::locpoly` ELM 11.3; SM 10.7.1
- regression splines – `splines::bs` , `splines::ns` ELM 11.2b p 218ff
- smoothing splines – `stats:smooth.spline` ELM 11.2a; SM 10.7.2

- penalized splines – `pspline::smooth.Pspline` Peng et al. 2006
- wavelets – `wavethresh::wd` ELM 11.4
- and more... ELM 11.5; ISLR Ch.7

- same ideas can be applied to generalized linear models
- replace linear predictor $\eta_i = x_i^T\beta$ with $f(x_i)$
- use local poly, reg splines, etc. SM Ex. 10.32 logistic regression

Explanation vs Prediction

- regression (and other) models may be fit in order to uncover some structural relationship between the response and one or more predictors
  - How do wages depend on education?
  - How does socio-economic status affect probability of severe covid?
- statistical analysis will focus on estimation and/or testing
- the data provides both an estimate of a model parameter and an estimate of uncertainty

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- or classifying new observations on the basis of their x values
- the statistical analysis will focus on the accuracy and precision of the prediction/classification
- the data used to fit the model does not provide a good assessment of the prediction or classification error — motivates the division of data into training and test sets