Using splines in regression

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This material is part of the **statsTeachR** *project*

Today's Lecture

- Spline models
- Penalized spline regression

More info:

- Harrel, *Regression Modeling Strategies*, Chapter 2, PDF handout
- *ISL* Chapter 7

Piecewise linear models

A piecewise linear model (also called a change point model or broken stick model) contains a few linear components

- Outcome is linear over full domain, but with a different slope at different points
- Points where relationship changes are referred to as "change points" or "knots"
- Often there's one (or a few) potential change points

Piecewise linear models

Suppose we want to estimate $\mathsf{E}(y|x) = f(x)$ using a piecewise linear model.

- For one knot we can write this as

$$\mathsf{E}(y|x) = \beta_0 + \beta_1 x + \beta_2 (x - \kappa)_+$$

where κ is the location of the change point and

$$(x - \kappa)_+ =$$

Interpretation of regression coefficients

$$\mathsf{E}(y|x) = \beta_0 + \beta_1 x + \beta_2 (x - \kappa)_+$$

- $\beta_0 = \mathbb{E}[y|x = 0]$ (assuming $\kappa > 0$)
- $\beta_1 =$
- $\beta_2 =$
- $\beta_1 + \beta_2 =$

Interpretation of regression coefficients

$$\mathsf{E}(y|x) = \beta_0 + \beta_1 x + \beta_2 (x - \kappa)_+$$

- $\beta_0 = \mathbb{E}[y|x = 0]$ (assuming $\kappa > 0$)
- $\beta_1 =$ Expected change in y for a 1-unit increase in x, when $x < \kappa$
- $\beta_2 =$
- $\beta_1 + \beta_2 =$

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- $\beta_2 =$ Change in slope between $x < \kappa$ and $x > \kappa$
- $\beta_1 + \beta_2 =$

Interpretation of regression coefficients

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- $\beta_0 = \mathbb{E}[y|x = 0]$ (assuming $\kappa > 0$)
- $\beta_1 =$ Expected change in y for a 1-unit increase in x, when $x < \kappa$
- $\beta_2 =$ Change in slope between $x < \kappa$ and $x > \kappa$
- $\beta_1 + \beta_2 =$ Expected change in y for a 1-unit increase in x, when $x \geq \kappa$

Estimation

- Piecewise linear models are low-dimensional (no need for penalization)
- Parameters are estimated via OLS
- The design matrix is ...

Multiple knots

Suppose we want to estimate $\mathsf{E}(y|x) = f(x)$ using a piecewise linear model.

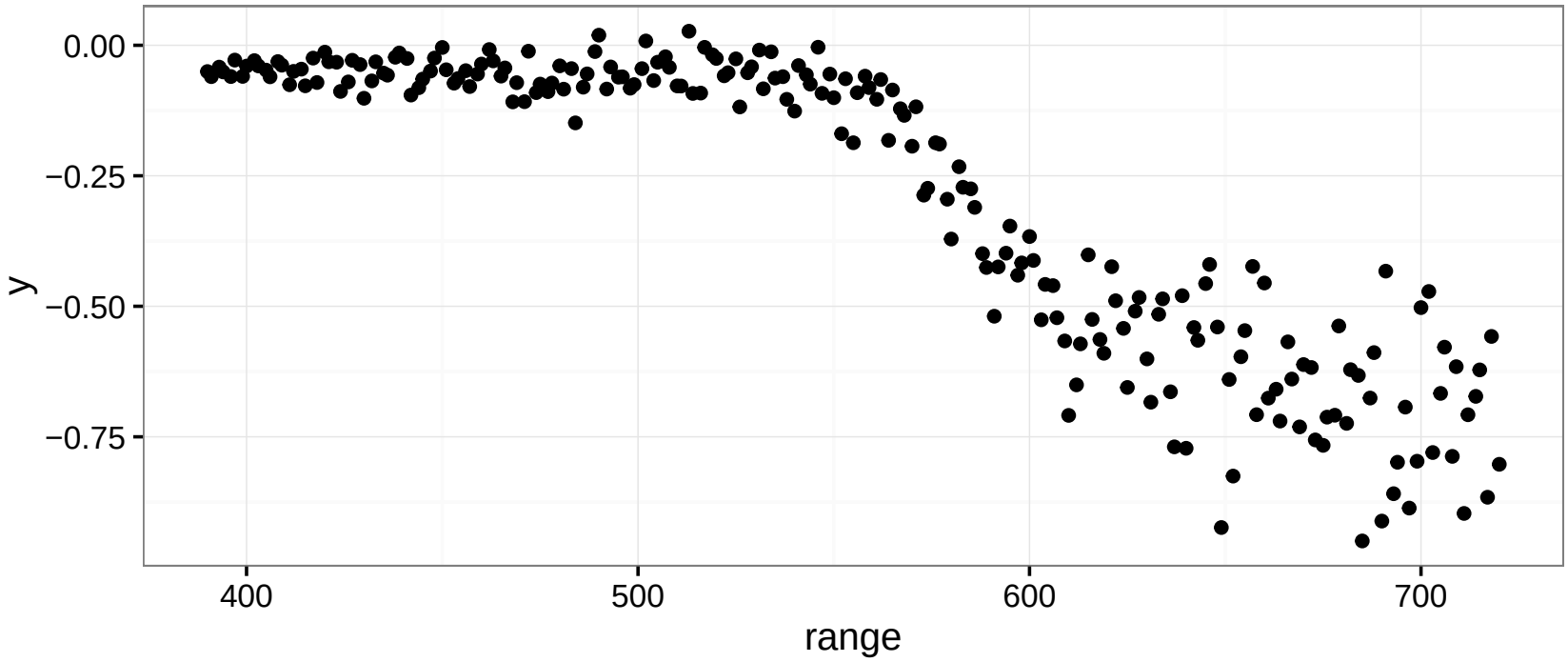
- For multiple knots we can write this as

$$\mathsf{E}(y|x) = \beta_0 + \beta_1 x + \sum_{k=1}^{K} \beta_{k+1}(x - \kappa_k)_+$$

  where $\{\kappa_k\}_{k=1}^{K}$ are the locations of the change points
- Note that knot locations are defined before estimating regression coefficients
- Also, regression coefficients are interpreted conditional on the knots.

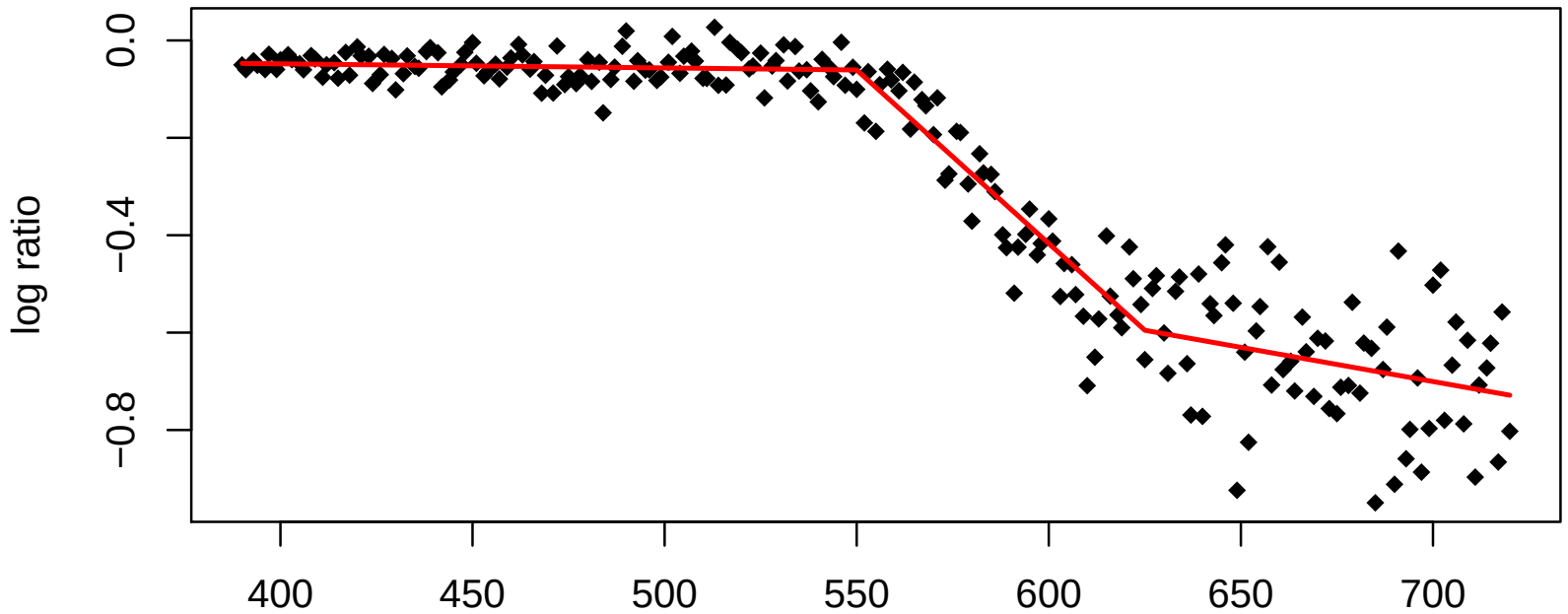
Example: lidar data

```
library(MASS)
library(SemiPar)
data(lidar)
y = lidar$logratio
range = lidar$range
qplot(range, y)
```



Example: lidar data

```
knots <- c(550, 625)
mkSpline <- function(k, x) (x - k > 0) * (x - k)
X.des = cbind(1, range, sapply(knots, FUN=mkSpline, x=range))
colnames(X.des) <- c("intercept", "range", "range1", "range2")
lm.lin = lm(y ~ X.des - 1)
plot(range, y, xlab = "Range", ylab = "log ratio", pch = 18)
points(range, lm.lin$fitted.values, type = 'l', col = "red", lwd = 2)
```



Example: lidar data

```
summary(lm.lin)$coef
```

```
##                     Estimate   Std. Error     t value     Pr(>|t|)
## X.desintercept -1.444288e-02 0.0687353855  -0.2101230 8.337689e-01
## X.desrange     -8.407376e-05 0.0001426647  -0.5893102 5.562663e-01
## X.desrange1    -7.042794e-03 0.0003834218 -18.3682689 4.379404e-46
## X.desrange2     5.723186e-03 0.0005153479  11.1054811 5.554824e-23
```

Piecewise quadratic and cubic models

Suppose we want to estimate $\mathrm{E}(y|x) = f(x)$ using a piecewise quadratic model.

- For multiple knots we can write this as

$$\mathrm{E}(y|x) = \beta_0 + \beta_1 x + \beta_1 x^2 + \sum_{k=1}^{K} \beta_{k+2}(x - \kappa_k)_+^2$$

  where $\{\kappa_k\}_{k=1}^K$ are the locations of the change points
- Similar extension for cubics
- Piecewise quadratic models are smooth and have continuous first derivatives

Pros and cons of piecewise models

Piecewise (linear, quadratic, etc) models have several advantages

- Easy construction of basis functions
- Flexible, and don't rely on determining an appropriate form for $f(x)$ using standard functions
- Allow for significance testing on change point slopes
- Fairly direct interpretations

Disadvantages

- knot specification is often arbitrary

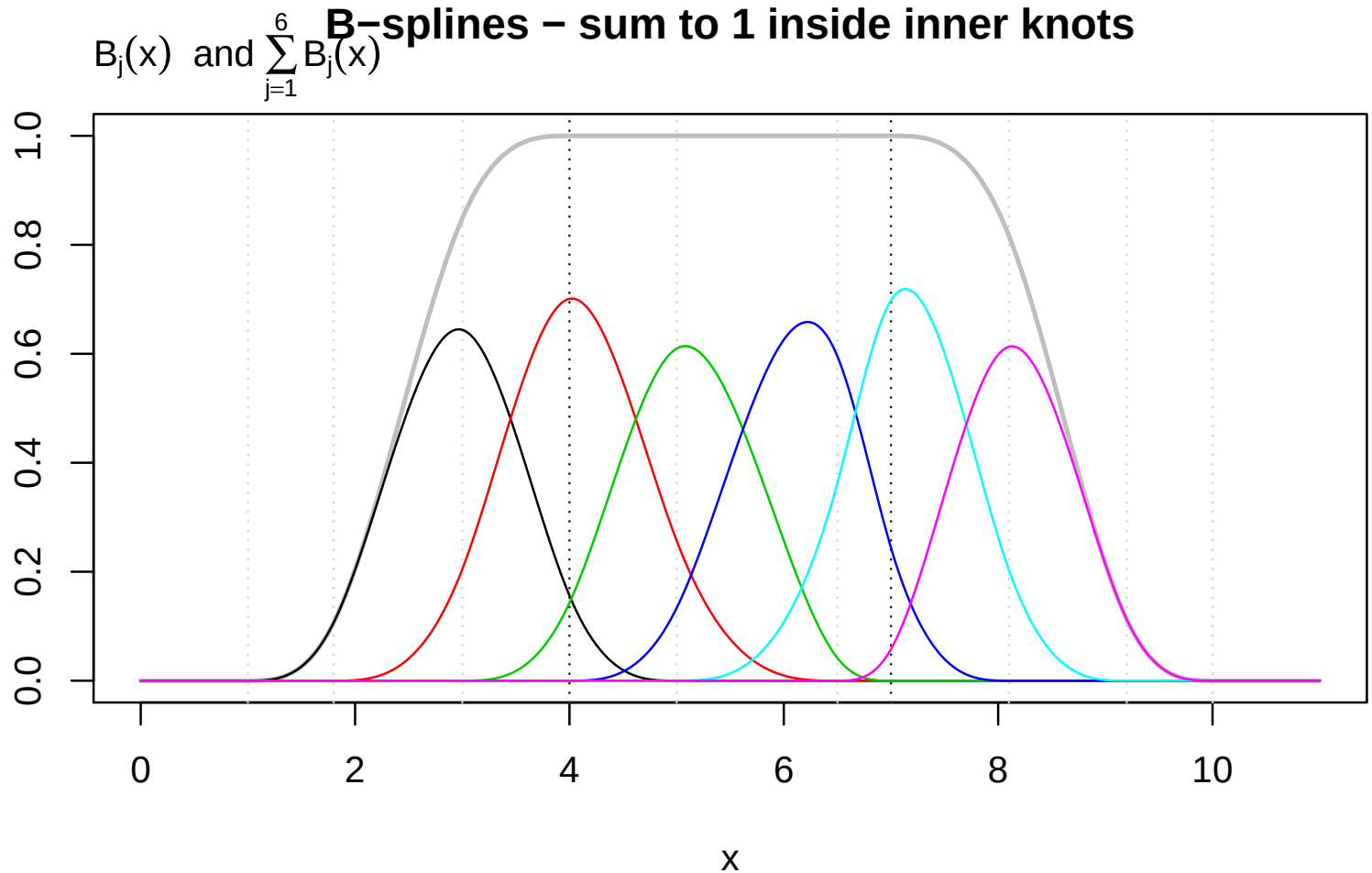
B-splines and natural splines

Characteristics

- Both B-splines and natural splines similarly define a basis over the domain of x
- Can be constrained to have seasonal patterns
- They are made up of piecewise polynomials of a given degree, and have defined derivatives similarly to the piecewise defined functions
- Big advantage over linear splines: parameter estimation is often fairly robust to your choice of knots
- Big disadvantage over linear splines: harder to interpret specific coefficients

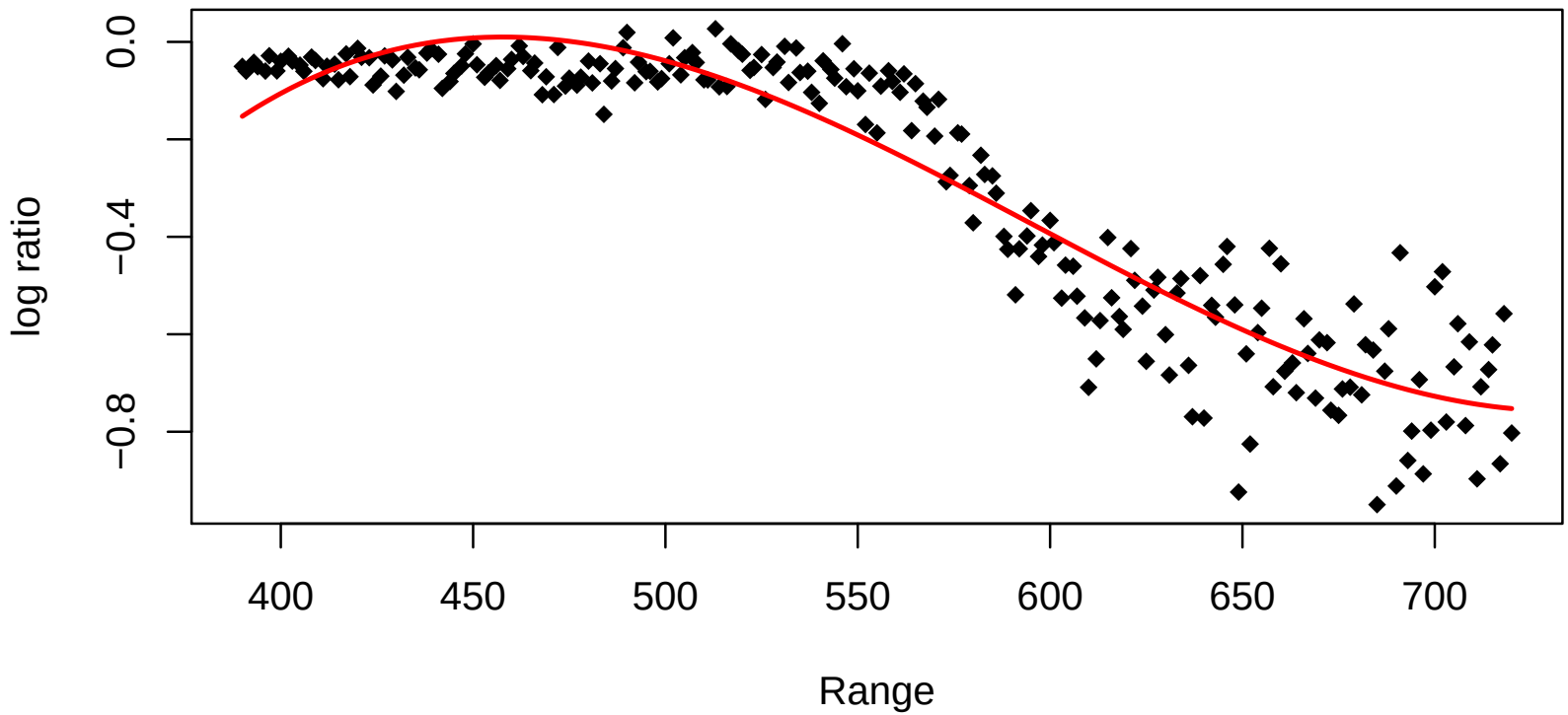
B-splines basis functions

$$\mathrm{E}(y|x) = \beta_0 + \sum_{j=1}^{6} \beta_j B_j(x)$$



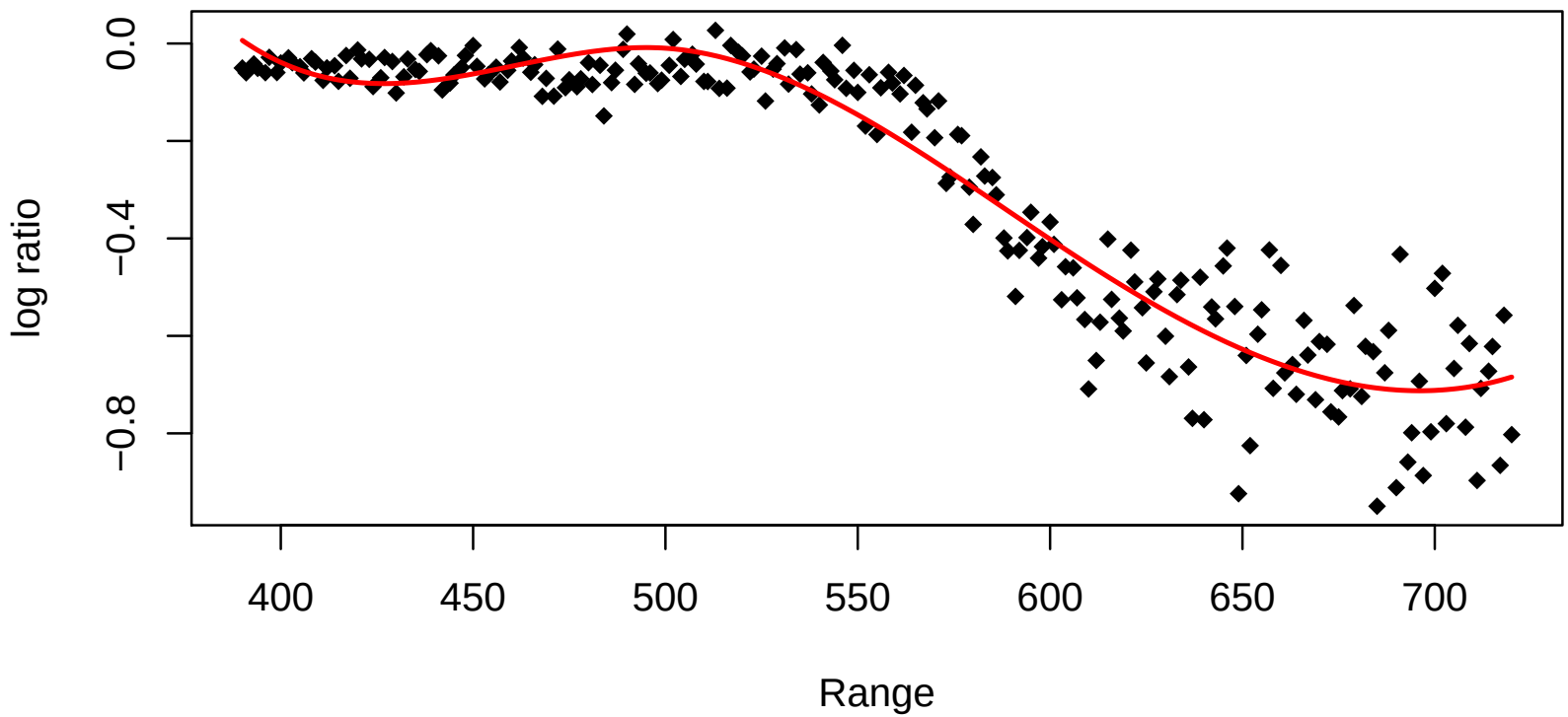
Example: lidar data B-splines

```
require(splines)
lm.bs3 = lm(y ~ bs(range, df=3))
plot(range, y, xlab = "Range", ylab = "log ratio", pch = 18)
points(range, lm.bs3$fitted.values, type = 'l', col = "red", lwd = 2)
```



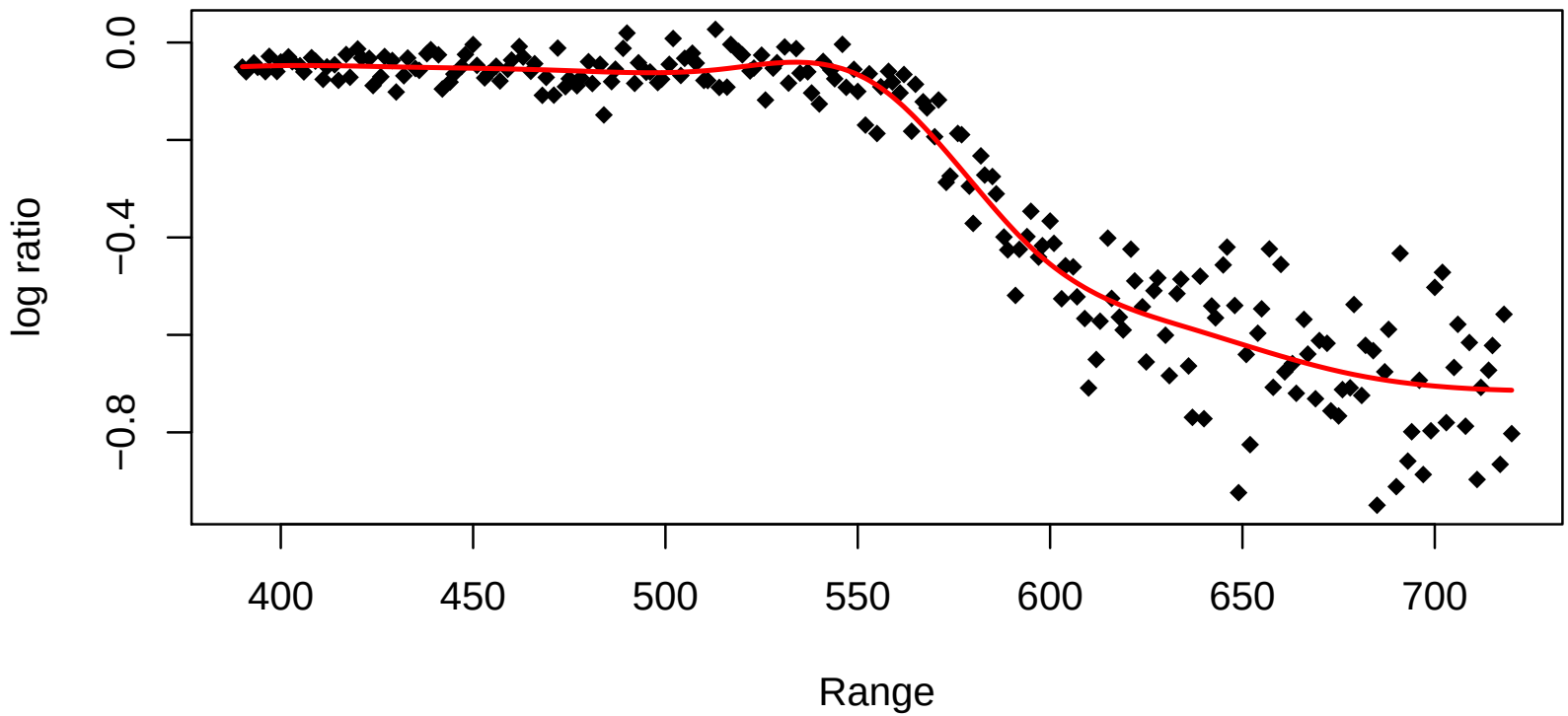
Example: lidar data B-splines

```
lm.bs5 = lm(y ~ bs(range, df=5))
plot(range, y, xlab = "Range", ylab = "log ratio", pch = 18)
points(range, lm.bs5$fitted.values, type = 'l', col = "red", lwd = 2)
```



Example: lidar data B-splines

```
lm.bs10 = lm(y ~ bs(range, df=10))
plot(range, y, xlab = "Range", ylab = "log ratio", pch = 18)
points(range, lm.bs10$fitted.values, type = 'l', col = "red", lwd = 2)
```



Quick intro to penalized splines

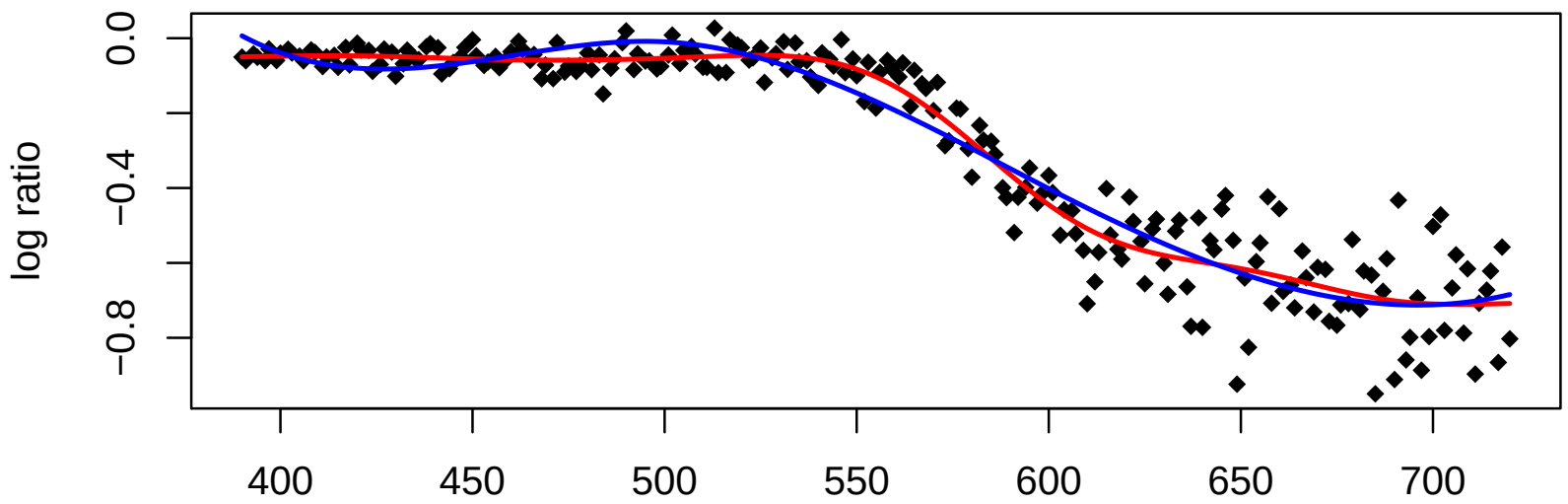
Generalized Additive Models (GAMs)

- A model dependent on unknown smooth functions of predictors.
- Typically estimated using penalized likelihood maximization.
- The basic idea of penalization is to discount models that overfit the data.
- Key feature of GAMs: smoothness can be selected automatically.

Example: lidar data penalized splines

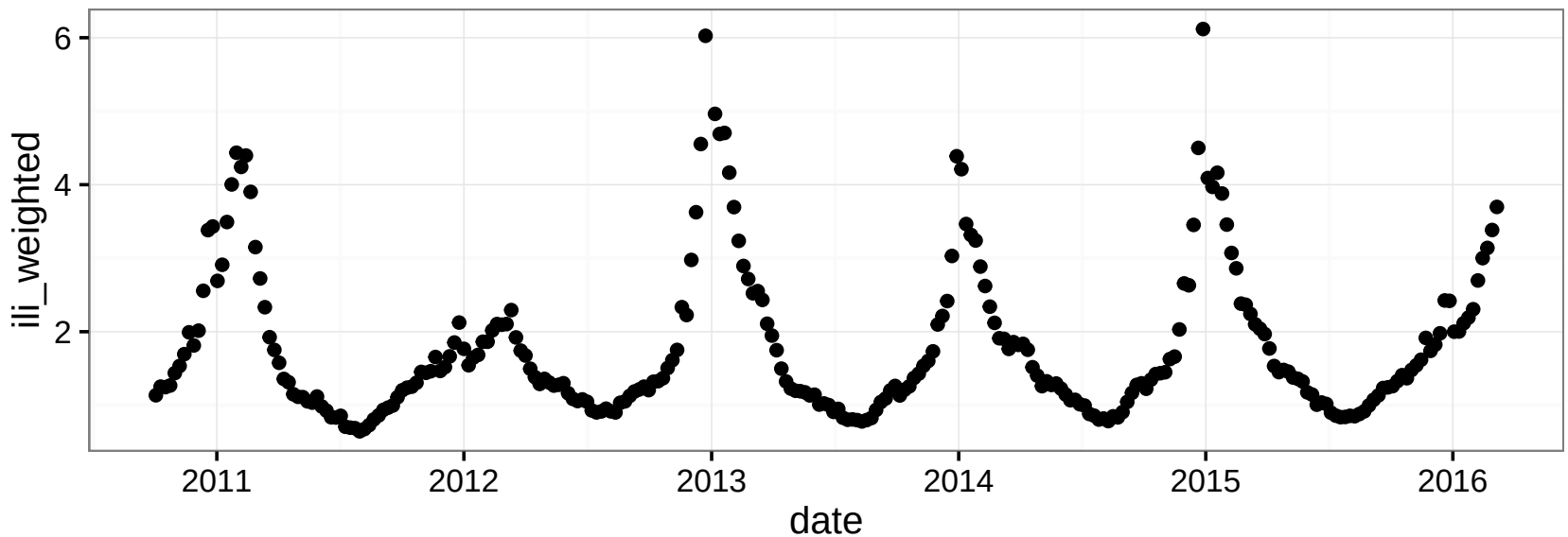
$$\mathbb{E}[y|range] = \beta_0 + s(range)$$

```
library(mgcv) ## try ?mgcv for more info
gam.penspl <-  gam(y ~ s(range)) ## no knots/df specified!
plot(range, y, xlab = "Range", ylab = "log ratio", pch = 18)
points(range, fitted(gam.penspl), type = 'l', col = "red", lwd = 2)
points(range, lm.bs5$fitted.values, type = 'l', col = "blue", lwd = 2)
```



Another setting where splines could be useful

```
library(cdcfluview)
library(dplyr)
library(lubridate)
usflu <- get_flu_data("national", "ilinet", years=2010:2015)
usflu <- mutate(usflu,
                date = as.Date(paste0(YEAR, sprintf("%02d", WEEK), "00"
                               format="%Y%W%w"),
                ili_weighted = X.UNWEIGHTED.ILI,
                dec_date = decimal_date(date),
                time_in_year = dec_date%%1)
ggplot(usflu, aes(x=date, y=ili_weighted)) + geom_point()
```



This is not a "real" time series analysis

These observations are time-series data

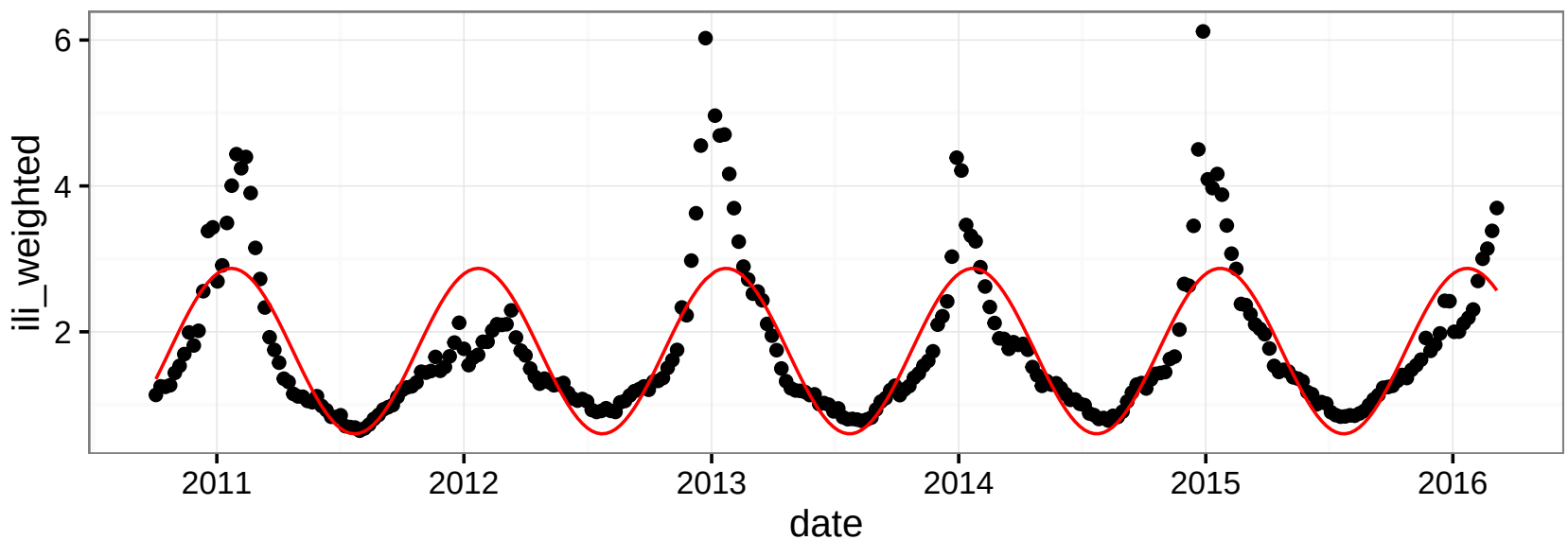
- Time is a "special" covariate: order matters, independence assumption often violated.
- There are more formal and systematic methods of analyzing time-series data that we are not going to discuss today, e.g. ARIMA models. (If interested, consider STAT 597TS.)
- A few nice resources: Hydman and Athanasopoulos's *Forecasting: Principles and Practice*, at https://www.otexts.org/fpp, or Shumway and Stoffer, *Time Series Analysis and Its Applications: with R examples*.

Fit a trigonometric model

We could fit a seasonal model like this:

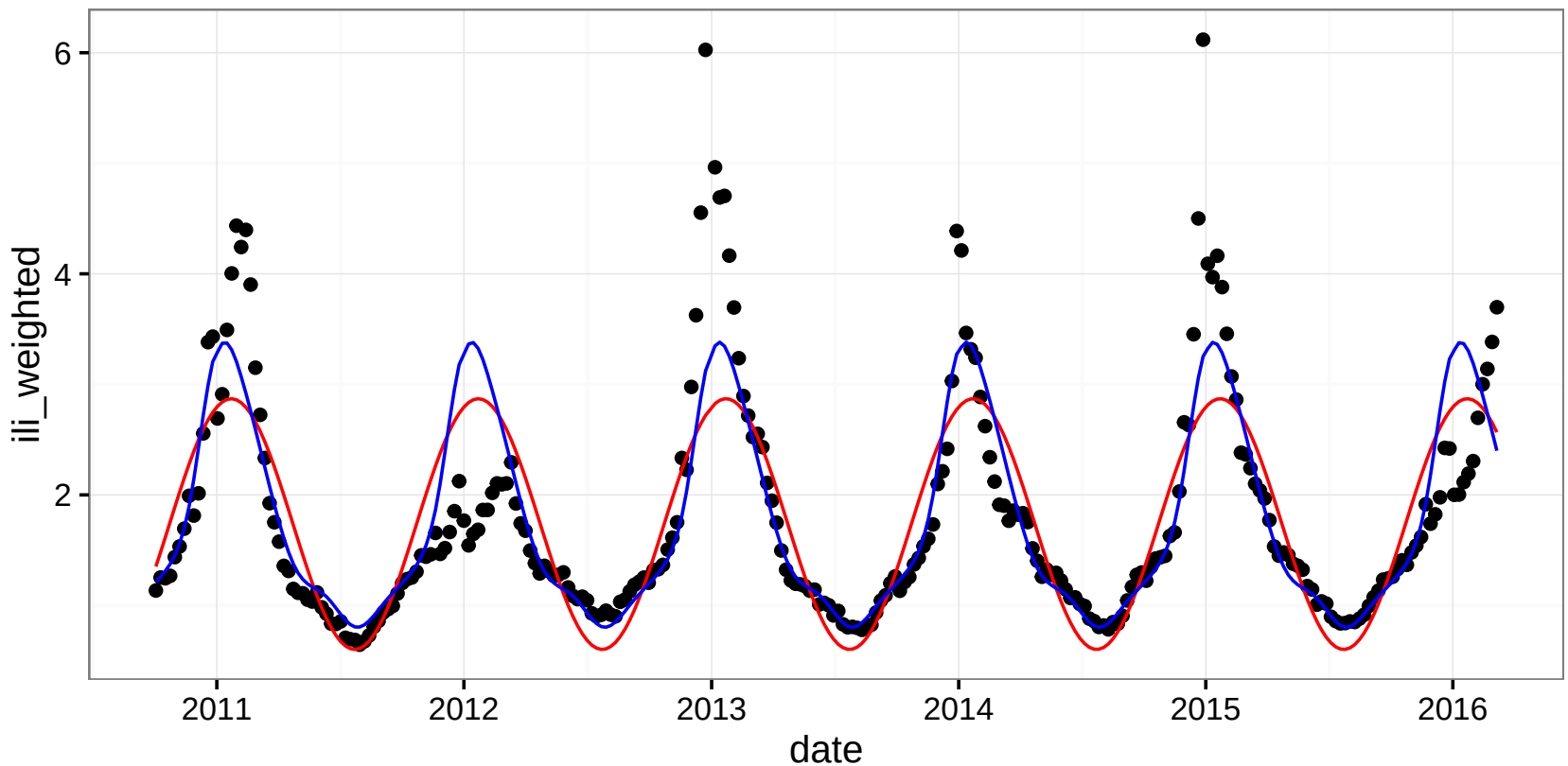
$$\mathbb{E}[y_t] = \beta_0 + \beta_1 \cdot \sin(2\pi t) + \beta_2 \cdot \cos(2\pi t)$$

```
usflu <- usflu[!is.na(usflu$dec_date),] ## remove "week 53"
trig_mdl <- lm(ili_weighted~sin(dec_date*2*pi)+cos(dec_date*2*pi),
               data=usflu)
usflu$trig_preds <- predict(trig_mdl)
ggplot(usflu, aes(x=date, y=ili_weighted)) + geom_point() +
    geom_line(aes(y=trig_preds), color="red")
```



Fit a penalized splines model

```
library(mgcv)
spline_mdl <- gam(ili_weighted ~ s(time_in_year, bs="cc"), data=usflu)
usflu$spl_preds <- predict(spline_mdl)
ggplot(usflu, aes(x=date, y=ili_weighted)) + geom_point() +
    geom_line(aes(y=trig_preds), color="red") +
    geom_line(aes(y=spl_preds), color="blue")
```

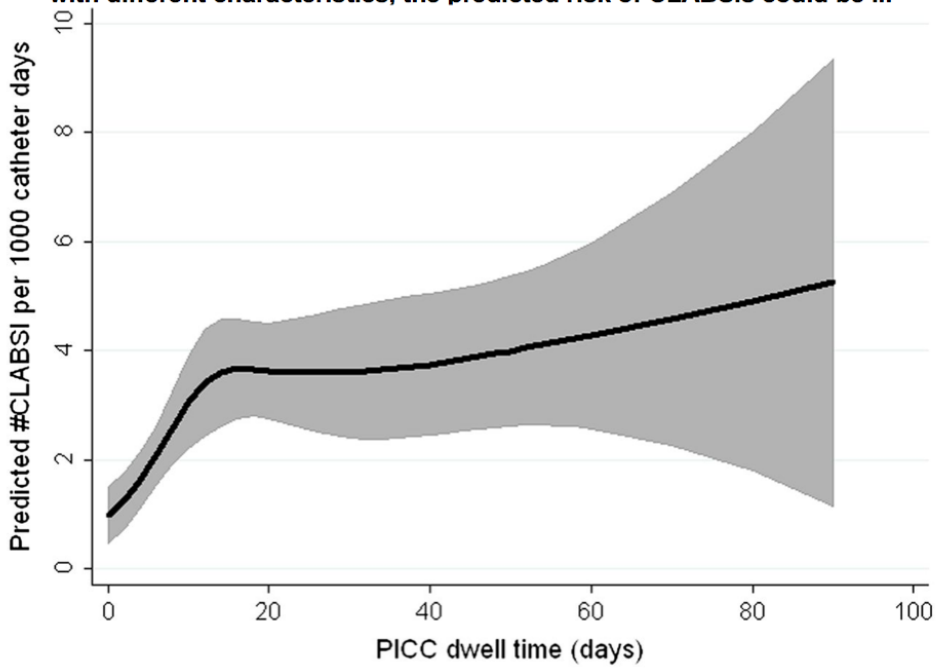


Take-home points for spline approaches (1)

Splines can flexibly model non-linear relationships

- Can improve model fit because of relaxed linearity assumptions.
- Caveat: spline models require careful graphical interpretation, slopes may not be easily available/interpretable

Predicted CLABSI rate (solid line) with 95% CIs (shading) over catheter dwell time for a given hospital, age, birth weight, CLABSI from previous PICC, and concurrent PICC. For a neonate with different characteristics, the predicted risk of CLABSIs could be ...



Aaron M. Milstone et al. Pediatrics 2013;132:e1609-e1615

PEDIATRICS

Take-home points for spline approaches (2)

Do you want control over your knots?

- Your application may have explicit "change-points" (i.e. interrupted time-series)
- In most cases, you do not want your spline model to be sensitive to user input (i.e. knot placement)
- "Penalized splines" can reduce this sensitivity at the cost of more complex model and estimation (More in *ISL* Chapter 7, Biostat Methods 3, anything about Generalized Additive Models (e.g. `mgcv` package and `gam() function`), one of your projects?).

Small group lab exercise

- Without adding any additional predictors into your model, experiment with different types of spline model fits. What is the best model that you can find? What criteria did you use to pick it?
- For that model, plot the residuals. What does the residual plot tell you about the appropriateness of the model from both a scientific and statistical perspective?