Module 5, Part 1: Basis Expansion and Parametric Splines, Bias-Variance Trade-off, and Model Selection

BIOS 526

Reading

- Chapter 5 (Sections 5.1 and 5.2 on parametric splines) of Hastie et al. Elements of Statistical Learning.
- Chapter 5 of James et al. (Cross-validation) Introduction to Statistical Learning

Concepts

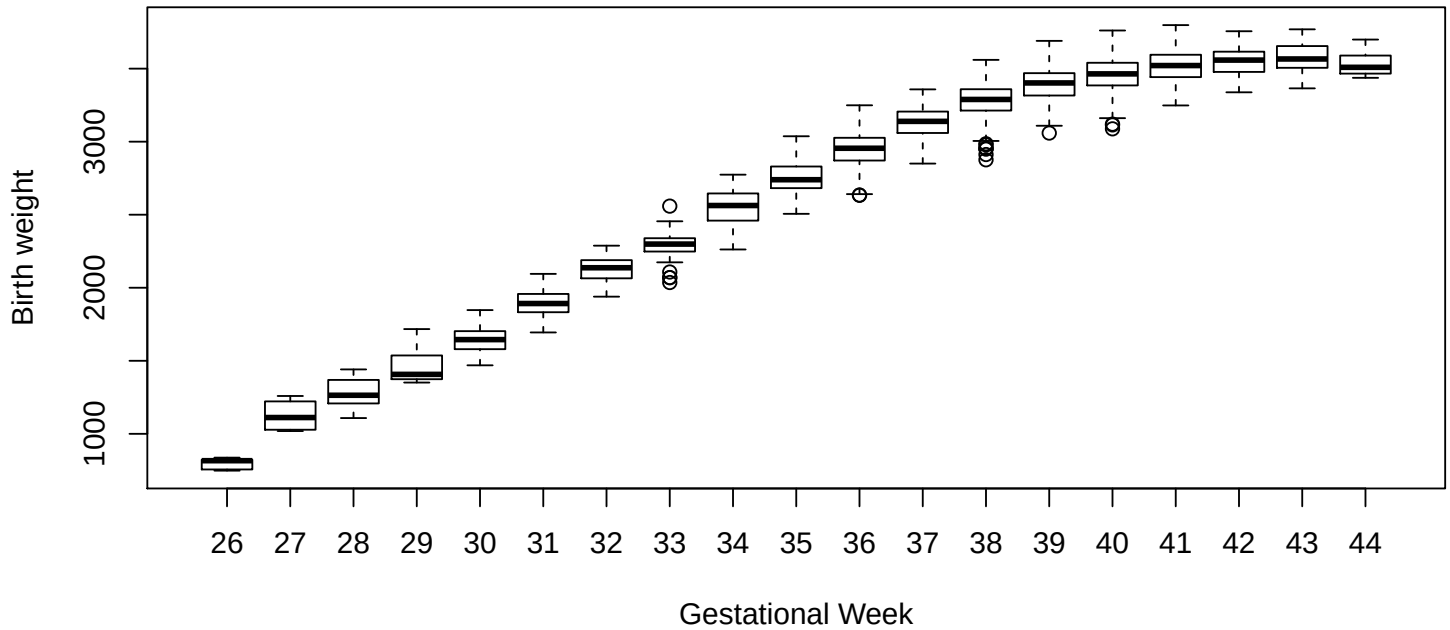
- Basis functions and knots.
- Piecewise linear splines.
- Piecewise cubic splines.
- Bias-Variance Tradeoff.
- Criteria for model prediction performance (CV, GCV, AIC).

Parametric Splines

Motivating Example: Birth Weight and Mother's Age

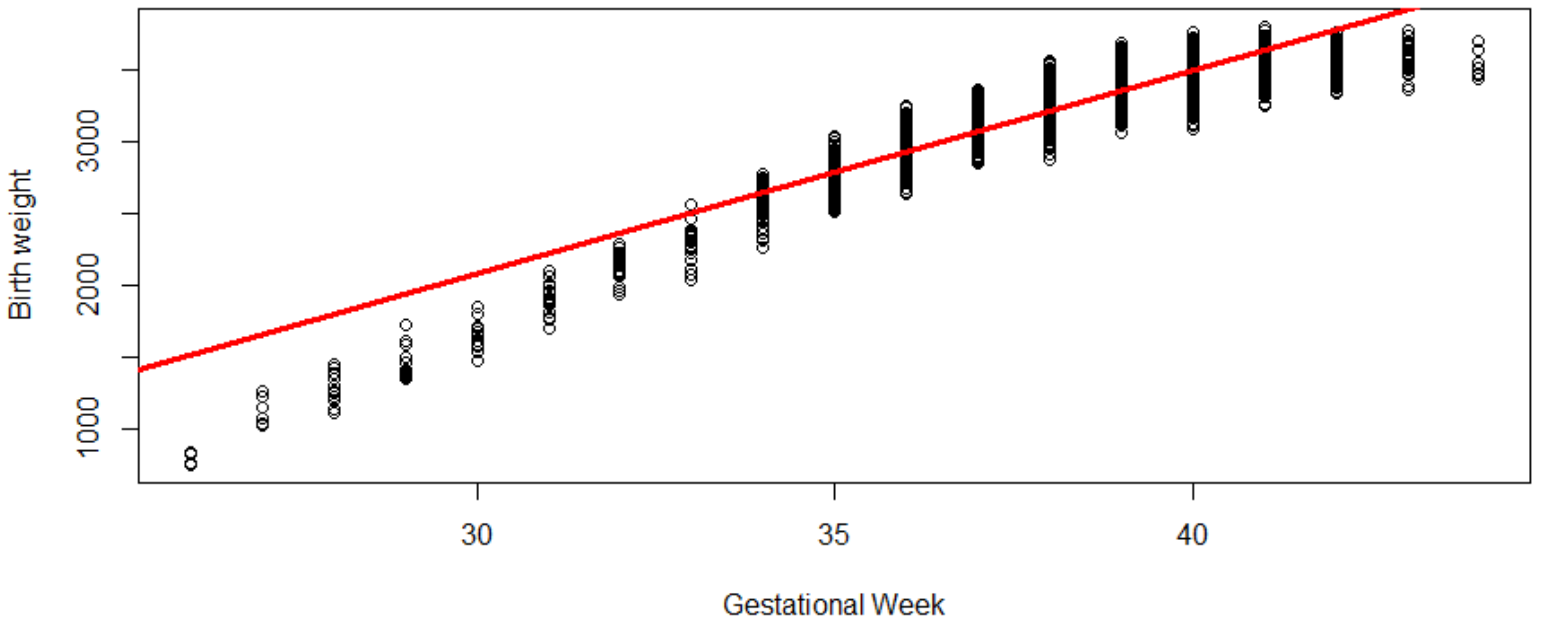
- gw: gestational age in weeks
- age: maternal age at delivery.
- bw: birth weight at delivery in grams.

```
> load ("GAbirth.RData")
> str (dat)
'data.frame':   5000 obs. of  3 variables:
 $ gw : num  41 38 39 40 40 38 40 40 38 37 ...
 $ age: int  33 23 36 30 26 18 19 37 23 25 ...
 $ bw : num  3540 3287 3438 3419 3278 ...
```



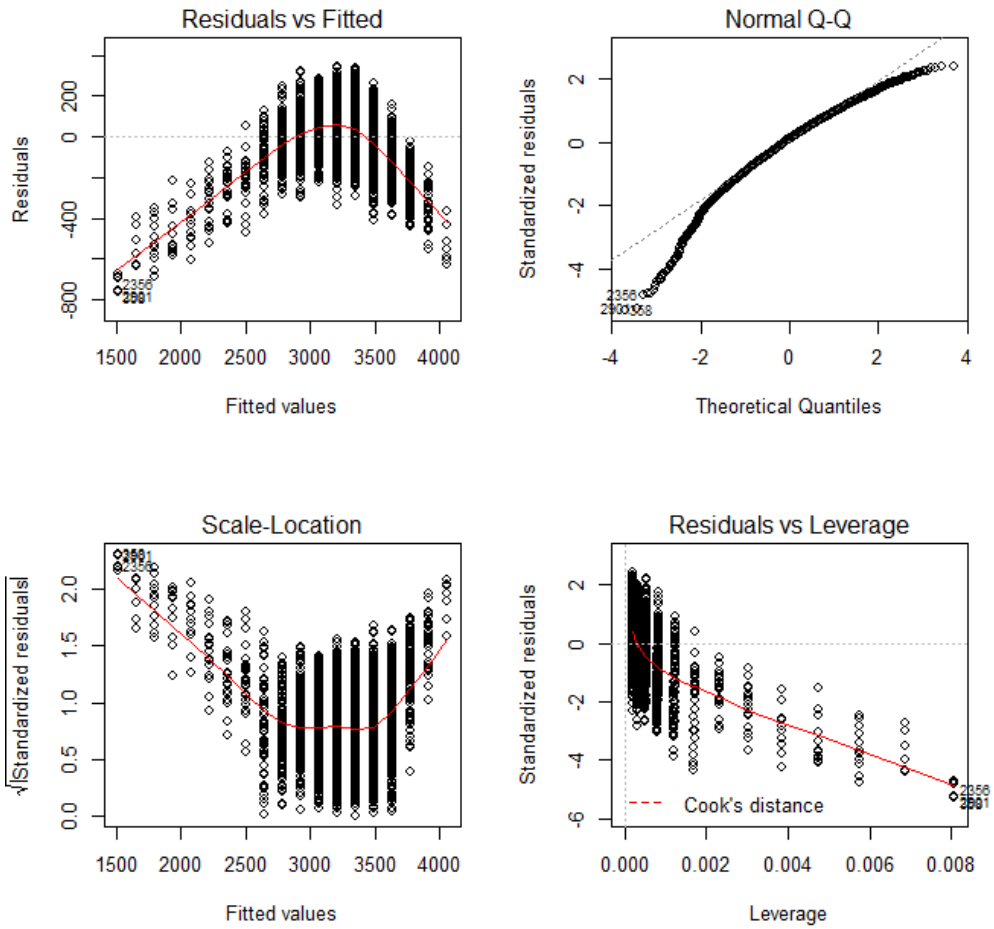
Linear Regression

```
> fit = lm (bw~gw, data = dat)
> summary(fit)
Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) -2177.513     39.351  -55.34   <2e-16 ***
gw            141.808      1.019  139.10   <2e-16 ***

> plot (dat$bw~dat$gw, xlab = "Gestational Week", ylab = "Birth weight")
> abline(fit, col=2, lwd = 3)
```



Linear Regression Diagnostics

```
> par(mfrow = c(2,2)); plot (fit)
```



Basis Expansion

Consider the regression model:

$$y_i = g(x_i) + \epsilon_i \ .$$

One approach: assume $g(x_i)$ is a linear combination of M functions of x_i

We will choose some simple $b_m(x_i)$.

Instead of estimating $g(x_i)$, we estimate the scalars β_m. For sufficiently large M, can do a good job of approximating any $g(x_i)$.

Replace x_i with $b_m(x_i)$, $m = 1, \ldots, M$, in a new regression.

Note $b_m(x_i)$ is simply a transformation of the original variable x_i.

$b_m(x_i)$ is called a basis function.

Basis Expansion, continued

- Basis functions are a core tool in the field of functional data analysis: observations are curves or functions.
- Basis functions extend basis vectors from linear algebra.
- Recall: in OLS, $\hat{\mathbf{Y}} = \mathbf{X}\hat{\boldsymbol{\beta}}$, represent $\mathbf{Y} \in \mathbb{R}^n$ with the rank-p $\text{colspace}(\mathbf{X})$.
- $\mathbf{X}$: each covariate forms a separate vector of the basis.
- Now, we consider a single covariate, but multiple functions of the single covariate.

Basis Expansion Examples

Polynomial

$$y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \beta_3 x_i^3$$

Indicator

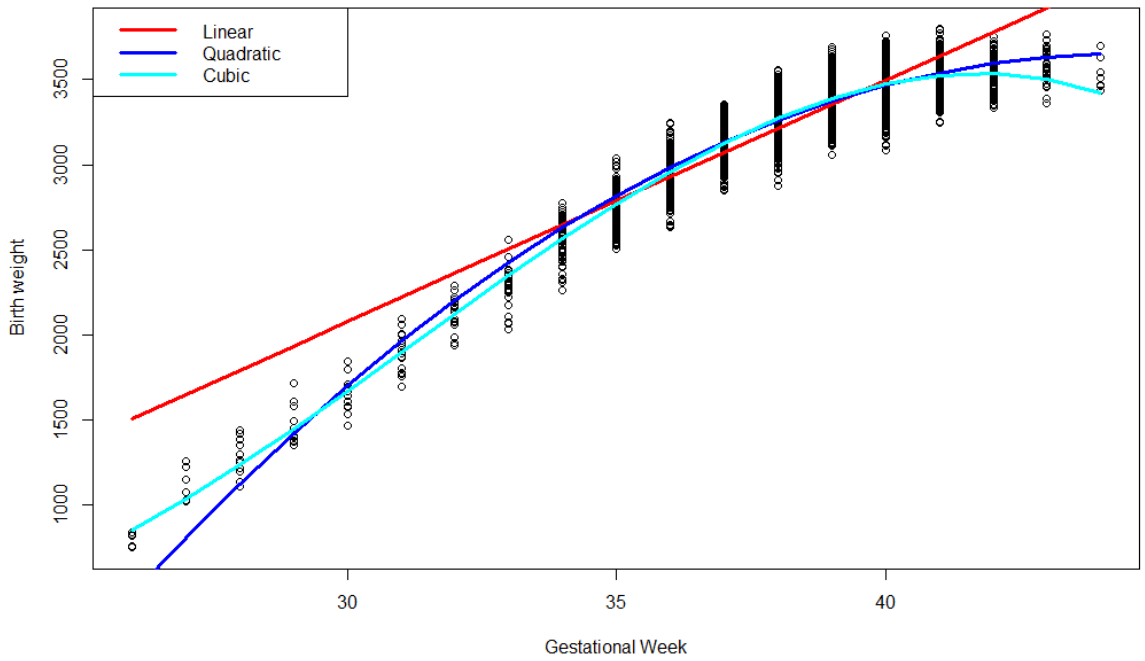
$$y_i = \beta_0 + \beta_1 x_i + \beta_2 I_{x_i > 0}$$

Periodic

$$y_i = \beta_0 + \beta_1 \sin(x_i/K) + \beta_2 \cos(x_i/K)$$

Polynomial Regression

```
> fit2 = lm (bw~gw+I(gw^2), data = dat)
> fit3 = lm (bw~gw+I(gw^2) + I(gw^3), data = dat)
```

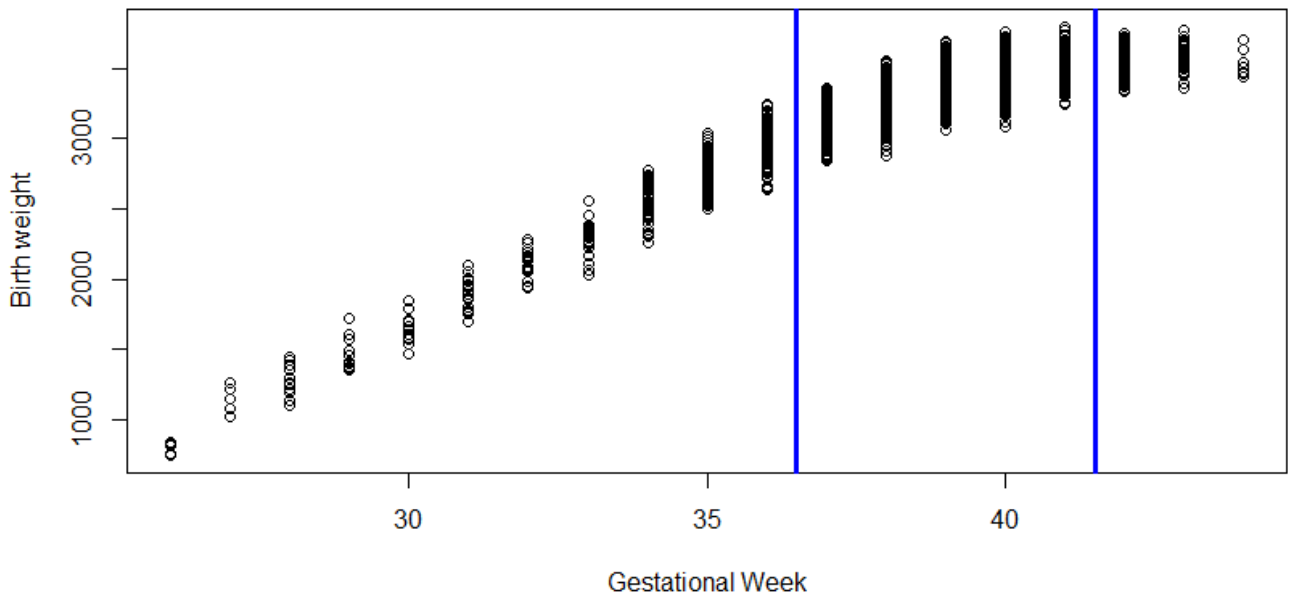


Note that polynomial functions often cannot model the ends very well.

Piecewise Regression

To model non-linear relationship: divide range of the covariate into some suitable regions.

E.g., pregnancy length: preterm (< 37 weeks), full-term (37-41 weeks), and post-term (> 42 weeks).



Model with polynomial functions separately within each region. The interior values that define the regions are called knots.

Piecewise Regression Specification

Piecewise regression is equivalent to a model where the basis functions of x_i interact with dummy variables for regions.

E.g., Piecewise quadratic regression:

$$\begin{aligned} y_i = &\beta_0 + \beta_1 x_i + \beta_2 x_i^2 \\ &+ \beta_3 D_{1i} + \beta_4 x_i \times D_{1i} + \beta_5 x_i^2 \times D_{1i} \\ &+ \beta_6 D_{2i} + \beta_7 x_i \times D_{2i} + \beta_8 x_i^2 \times D_{2i} \end{aligned}$$

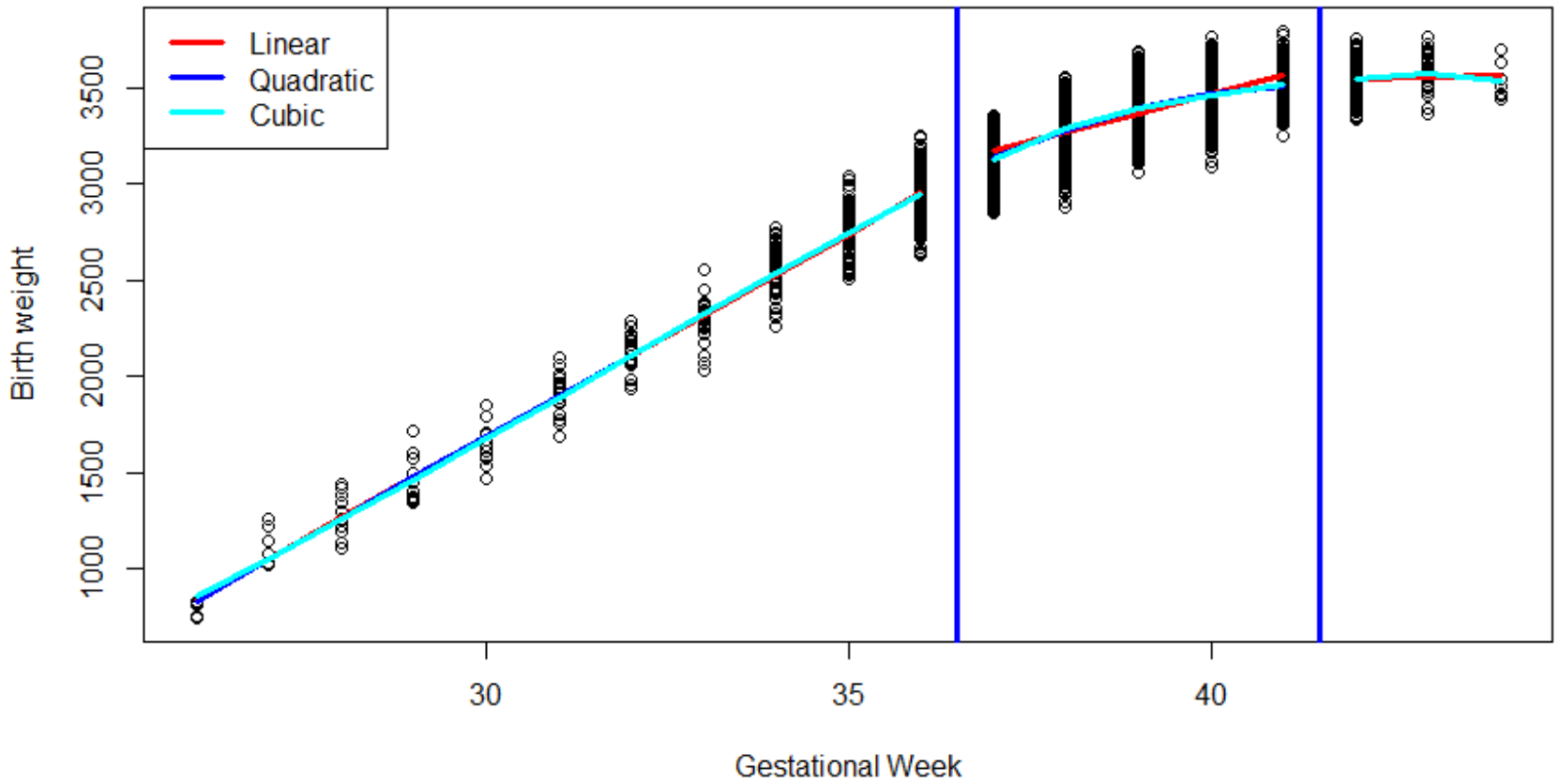
where

$$D_{1i} = \begin{cases} 1 & 37 \leq x_i < 42 \\ 0 & \text{otherwise} \end{cases} \qquad D_{2i} = \begin{cases} 1 & x_i \geq 42 \\ 0 & \text{otherwise} \end{cases}$$

We only need **two** dummy variables for three regions.

Piecewise Regression

- The positive association between pregnancy length and birth weight decreases for higher gestational weeks.
- Here, linear, quadratic, and cubic result in similar trend in each region.



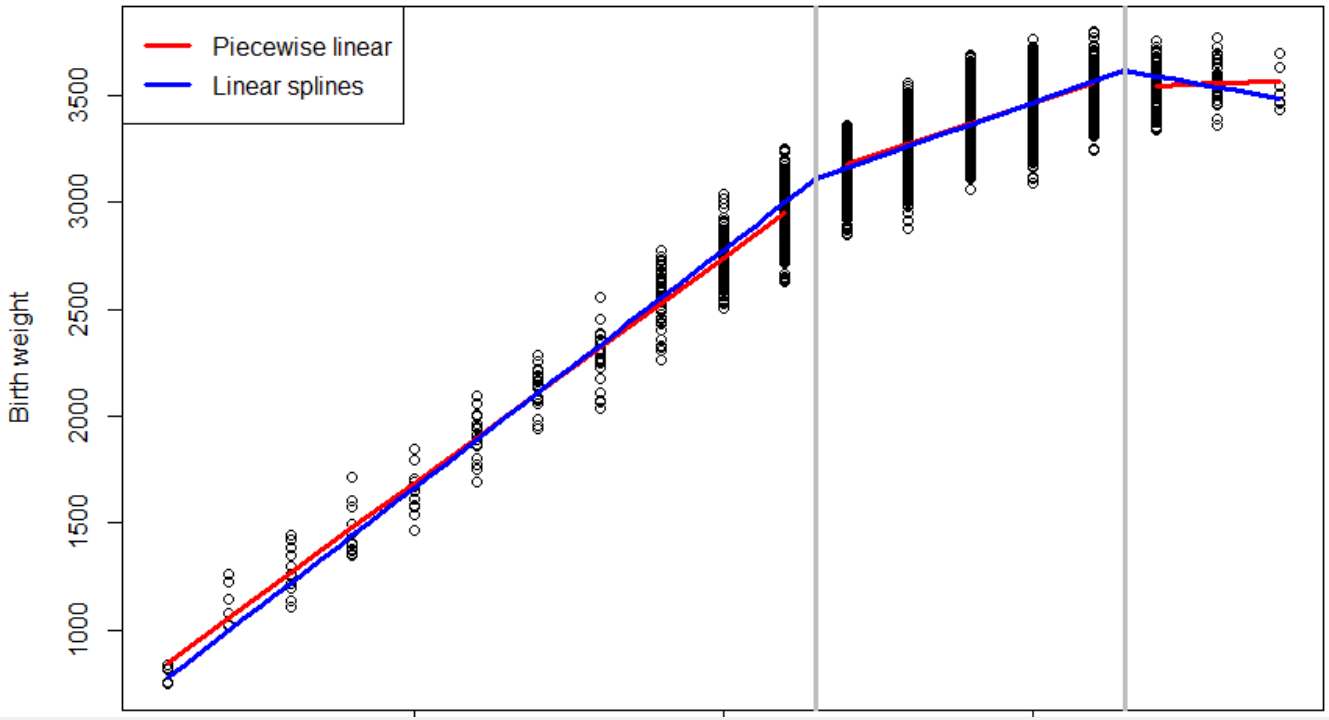
Piecewise Splines

Piecewise polynomials have limitations:

- The regression functions do not match at knot locations.
- Requires many regression coefficients (degrees of freedom).

Splines are basis functions for piecewise regressions that are connected at the interior knots.

Splines are continuous, which makes them aesthetically appealing.



Linear Splines

A linear piecewise spline at knot locations 36.5 and 41.5 is specified as

$$y_i = \beta_0 + \beta_1 x_i + \beta_2 (x_i - 36.5)_+ + \beta_3 (x_i - 41.5)_+$$

Here we only need 4 regression coefficients, instead of 6 in a model that does not force the regression lines to connect at knots.

Count the parameters: 2 parameters per line * 3 lines - 2 constraints = 4 where $(\ldots)_+$ denotes the positive part.

$$(x_i - 36.5)_+ = \begin{cases} x_i - 36.5 & \text{if } x_i \geq 36.5 \\ 0 & \text{otherwise} \end{cases}$$

$$(x_i - 41.5)_+ = \begin{cases} x_i - 41.5 & \text{if } x_i \geq 41.5 \\ 0 & \text{otherwise} \end{cases}$$

Linear Splines: Coefficient Interpretation

$$y_i = \beta_0 + \beta_1 x_i + \beta_2 (x_i - 36.5)_+ + \beta_3 (x_i - 41.5)_+$$

For $x_i < 36.5$:

$$y_i = \beta_0 + \beta_1 x_i \ .$$

For $36.5 < x_i < 42.5$:

$$\begin{aligned} y_i &= \beta_0 + \beta_1 x_i + \beta_2 (x_i - 36.5) \\ &= (\beta_0 - \beta_2 * 36.5) + (\beta_1 + \beta_2) x_i \ . \end{aligned}$$

For $42.5 < x_i$:

$$\begin{aligned} y_i &= \beta_0 + \beta_1 x_i + \beta_2 (x_i - 36.5) + \beta_3 (x_i - 41.5) \\ &= (\beta_0 - \beta_2 * 36.5 - \beta_3 * 41.5) + (\beta_1 + \beta_2 + \beta_3) x_i \ . \end{aligned}$$

β_2 and β_3 represent changes in slope compared to the previous region

Linear Splines: Coefficient Interpretation

```
> Sp1 = (dat$gw - 36.5)*as.numeric(dat$gw >= 36.5 )
> Sp2 = (dat$gw - 41.5)*as.numeric(dat$gw >= 41.5)

> fit7 = lm (bw~ gw+Sp1 + Sp2, data = dat)
> summary (fit7)

Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) -5013.768     62.747  -79.90   <2e-16 ***
gw            222.620      1.757  126.71   <2e-16 ***
Sp1          -121.427      2.549  -47.64   <2e-16 ***
Sp2          -152.948     10.492  -14.58   <2e-16 ***
```

-
-
- After pregnancy week 41.5, birth weight was negatively associated with gestational week by -52 g/week ($CI_{95\%}$ -72, -32).

Cubic Splines

Linear splines are easy to interpret.

The resulting function $g(x_i)$ is not smooth. The first-derivative of

$$g(x_i) = \beta_0 + \beta_1 x_i + \beta_2 (x_i - 36.5)_+ + \beta_3 (x_i - 41.5)_+$$

is discontinuous at the knots.

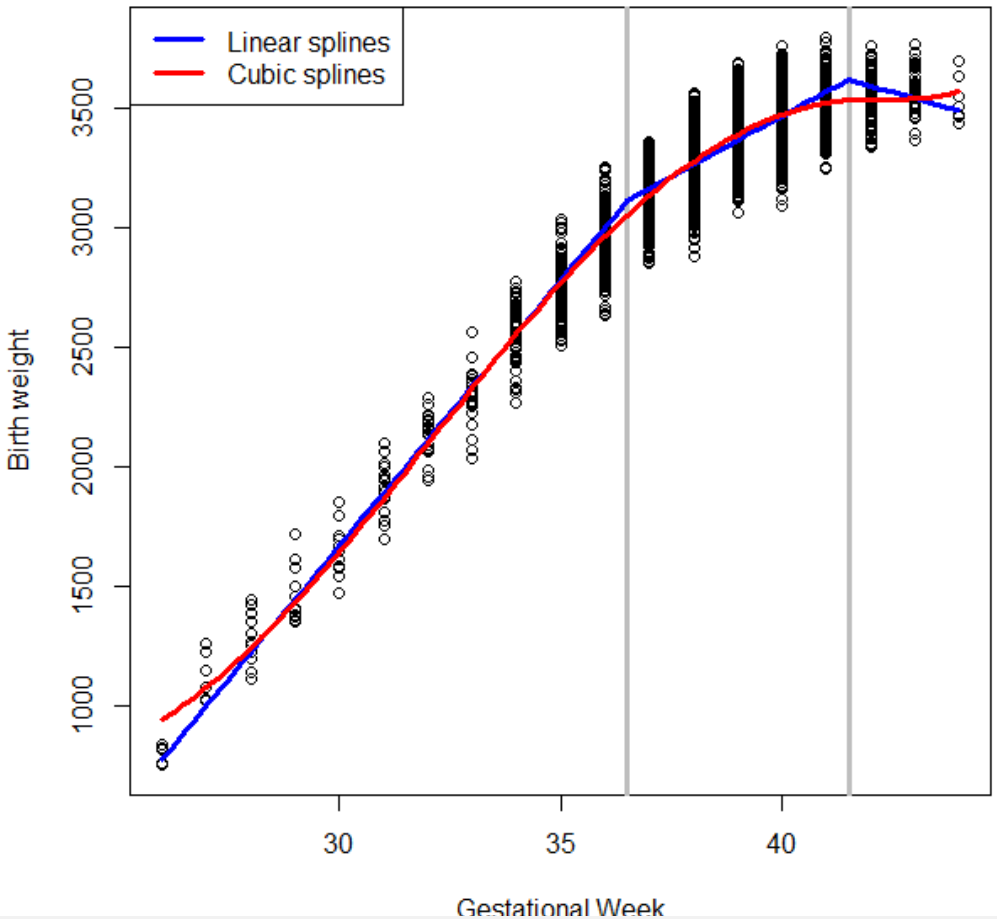
We can also work with piecewise cubic functions that are connected at the knots:

Cubic splines are popular because:

- continuous 2nd-derivatives, typically what we view as *smooth* visually.

Cubic versus Linear Splines

```
> Sp1 = (dat$gw - 36.5)^3*as.numeric(dat$gw >= 36.5 )
> Sp2 = (dat$gw - 41.5)^3*as.numeric(dat$gw >= 41.5)
> fit8 = lm (bw~ gw+I(gw^2) + I(gw^3) + Sp1 + Sp2, data = dat)
```



Polynomial Splines

The general formulation of a d-degree polynomial regression model with M knots, $\kappa_1, \kappa_2, \ldots, \kappa_M$ is

The above is known as the truncated power formulation.

Linear (d = 1):

$$y_i = \beta_0 + \beta_1 x_i + \sum_{m=1}^{M} \beta_{1+m} (x_i - \kappa_m)_+ \ .$$

Quadratic (d = 2):

$$y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \sum_{m=1}^{M} \beta_{2+m} (x_i - \kappa_m)_+^2 \ .$$

Interpreting Polynomial Splines

- Linear splines: a good choice for interpretability – the coefficients at the knots represent the change in slope from the previous region.
- Cubic splines: appears smooth, which is often biologically reasonable. Generally we do not interpret the individual coefficients of the truncated polynomials.

```
lm(formula = bw ~ gw + I(gw^2) + I(gw^3) + Sp1 + Sp2, data = dat)
              Estimate Std. Error t value Pr(>|t|)
(Intercept)  2.890e+04  3.717e+03   7.776 9.02e-15 ***
gw          -2.968e+03  3.335e+02  -8.901  < 2e-16 ***
I(gw^2)      9.972e+01  9.900e+00  10.073  < 2e-16 ***
I(gw^3)     -1.036e+00  9.734e-02 -10.641  < 2e-16 ***
Sp1          7.732e-01  2.482e-01   3.115  0.00185 **
Sp2          7.455e+00  3.471e+00   2.148  0.03177 *
---
Signif. codes:  0 ?***? 0.001 ?**? 0.01 ?*? 0.05 ?.? 0.1 ? ? 1

Residual standard error: 109.8 on 4994 degrees of freedom
Multiple R-squared:  0.881,Adjusted R-squared:  0.8809
F-statistic:  7397 on 5 and 4994 DF,  p-value: < 2.2e-16
```

B-Splines

The truncated power formulation can sometimes experience numerical problems when fitting because:

- the covariates are highly correlated;
- d^{th} power can be small or large with large d.

B-splines can be used to represent the same space as truncated polynomial splines.

Mathematically, these will produce the same predictions as truncated polynomial splines.

Computationally, may be more accurate – avoid overflow errors.

Scaled between 0 and 1. Provide better numerical stability.

Commonly implemented in statistical software but in my experience you can just use cubic splines with modern computers.

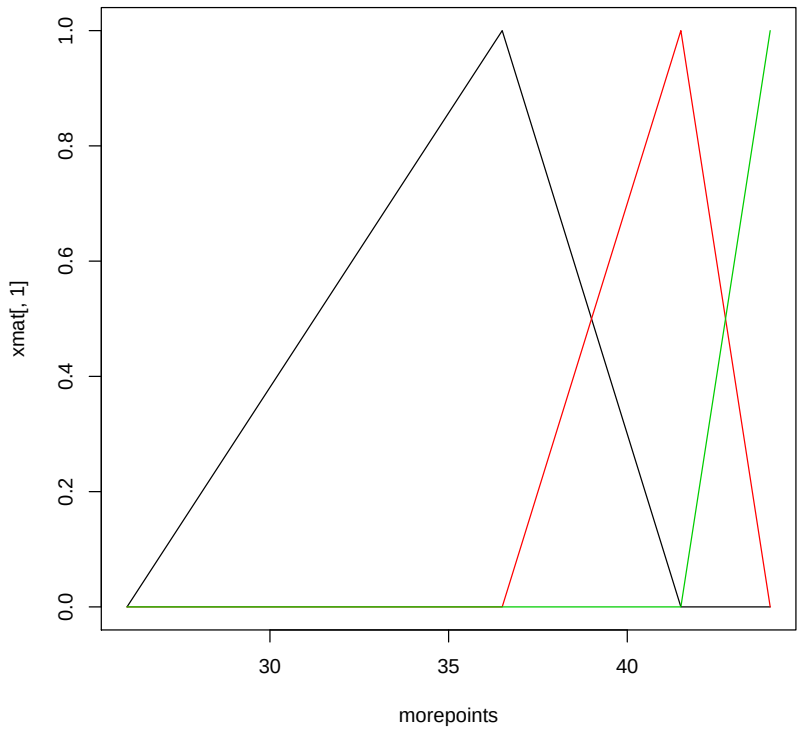
B-Splines and computation

The `bs()` function in R will create the appropriate design matrix.

```
### Load the splines package
library (splines)

### Linear splines
fit1 = lm ( bw ~ bs(gw, knots = c(36.5, 41.5), degree = 1),  data = dat)

### Quadratic splines
fit2 = lm ( bw ~ bs(gw, knots = c(36.5, 41.5), degree = 2),  data = dat)

### Cubic splines
fit3 = lm ( bw ~ bs(gw, knots = c(36.5, 41.5), degree = 3),  data = dat)
```

B-Splines

E.g. of degree 1 (linear) B-spline and degree 3 (cubic) B-spline.
In general, we do not use degree 1 B-splines – piecewise linear splines are fine.
It's the cubic polynomials that blow up. Cubic b-splines are popular.

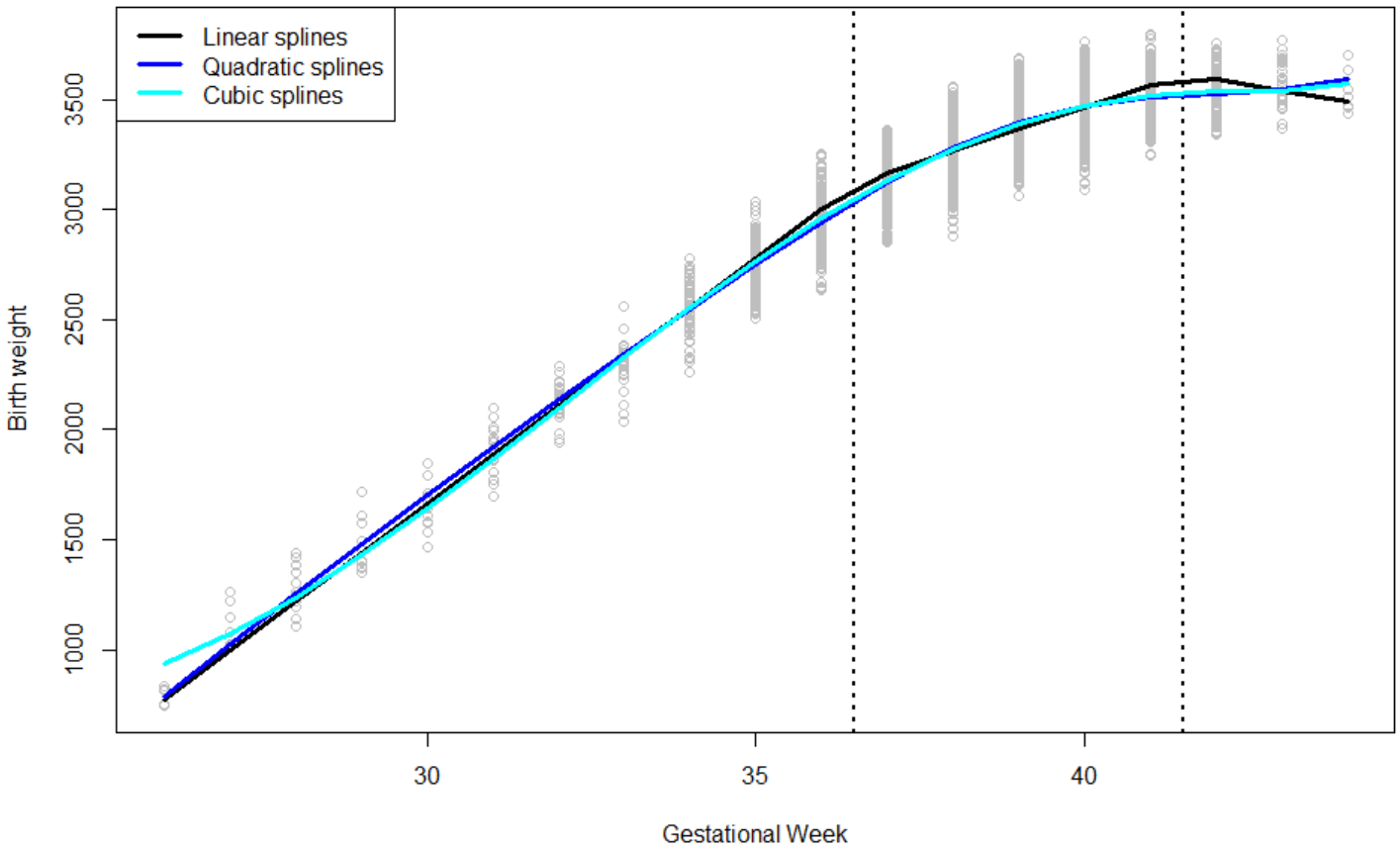


B-Splines

Coefficients are not interpretable.

```
lm(formula = bw ~ bs(gw, knots = c(36.5, 41.5), degree = 3),
    data = dat)

Residuals:
    Min      1Q  Median      3Q     Max
-399.13  -74.61    4.47   77.06  301.40

Coefficients:
                                                Estimate Std. Error t value Pr(>|t|)
(Intercept)                                       937.45      34.65  27.056  < 2e-16
bs(gw, knots = c(36.5, 41.5), degree = 3)1        408.19      57.92   7.048 2.07e-12
bs(gw, knots = c(36.5, 41.5), degree = 3)2       2037.52      32.46  62.779  < 2e-16
bs(gw, knots = c(36.5, 41.5), degree = 3)3       2655.45      38.15  69.608  < 2e-16
bs(gw, knots = c(36.5, 41.5), degree = 3)4       2582.17      35.94  71.851  < 2e-16
bs(gw, knots = c(36.5, 41.5), degree = 3)5       2633.37      52.76  49.912  < 2e-16
---
Signif. codes:  0 ?***? 0.001 ?**? 0.01 ?*? 0.05 ?.? 0.1 ? ? 1

Residual standard error: 109.8 on 4994 degrees of freedom
Multiple R-squared:  0.881,Adjusted R-squared:  0.8809
F-statistic:  7397 on 5 and 4994 DF,  p-value: < 2.2e-16
```

B-Splines



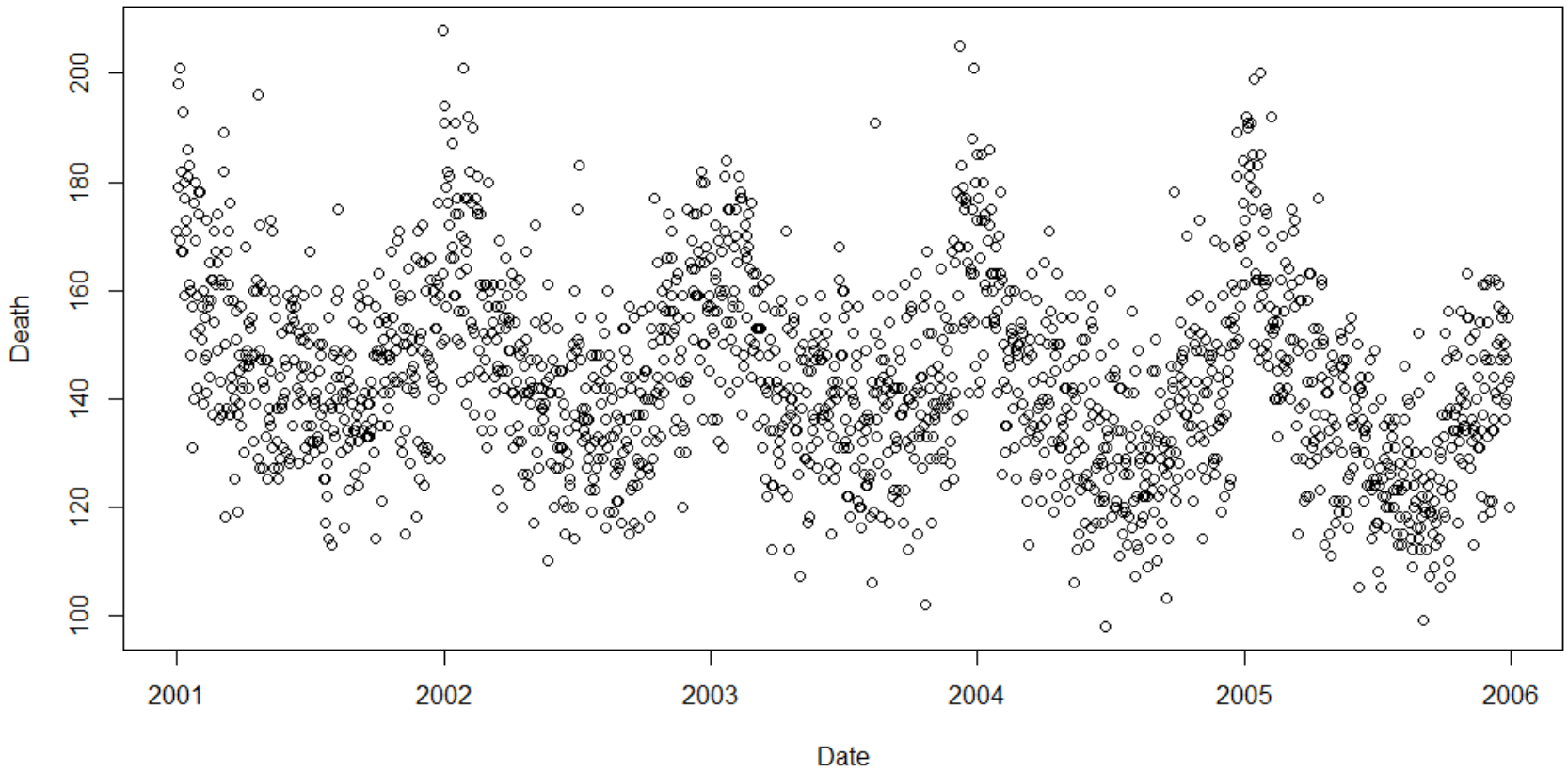
Note:

```
> sum((fit7$fitted-fit9$fitted)^2)
[1] 4.9437e-18
> sum((fit8$fitted-fit11$fitted)^2)
[1] 2.056156e-13
```

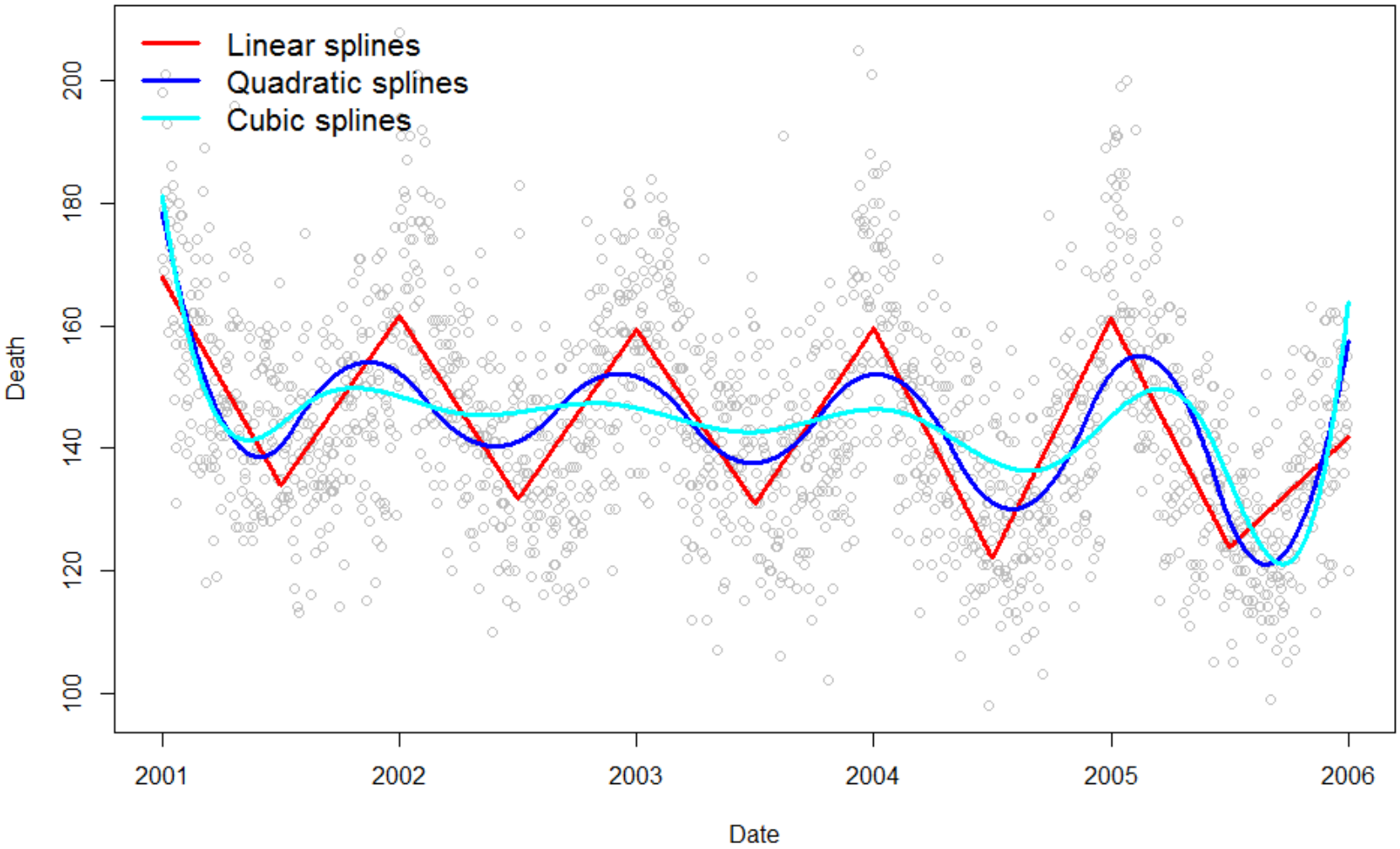
Example: Daily Death Counts in NYC

```
> load ("NYC.RData")
> plot (health$alldeaths~health$date, xlab = "Date", ylab = "Death")
```

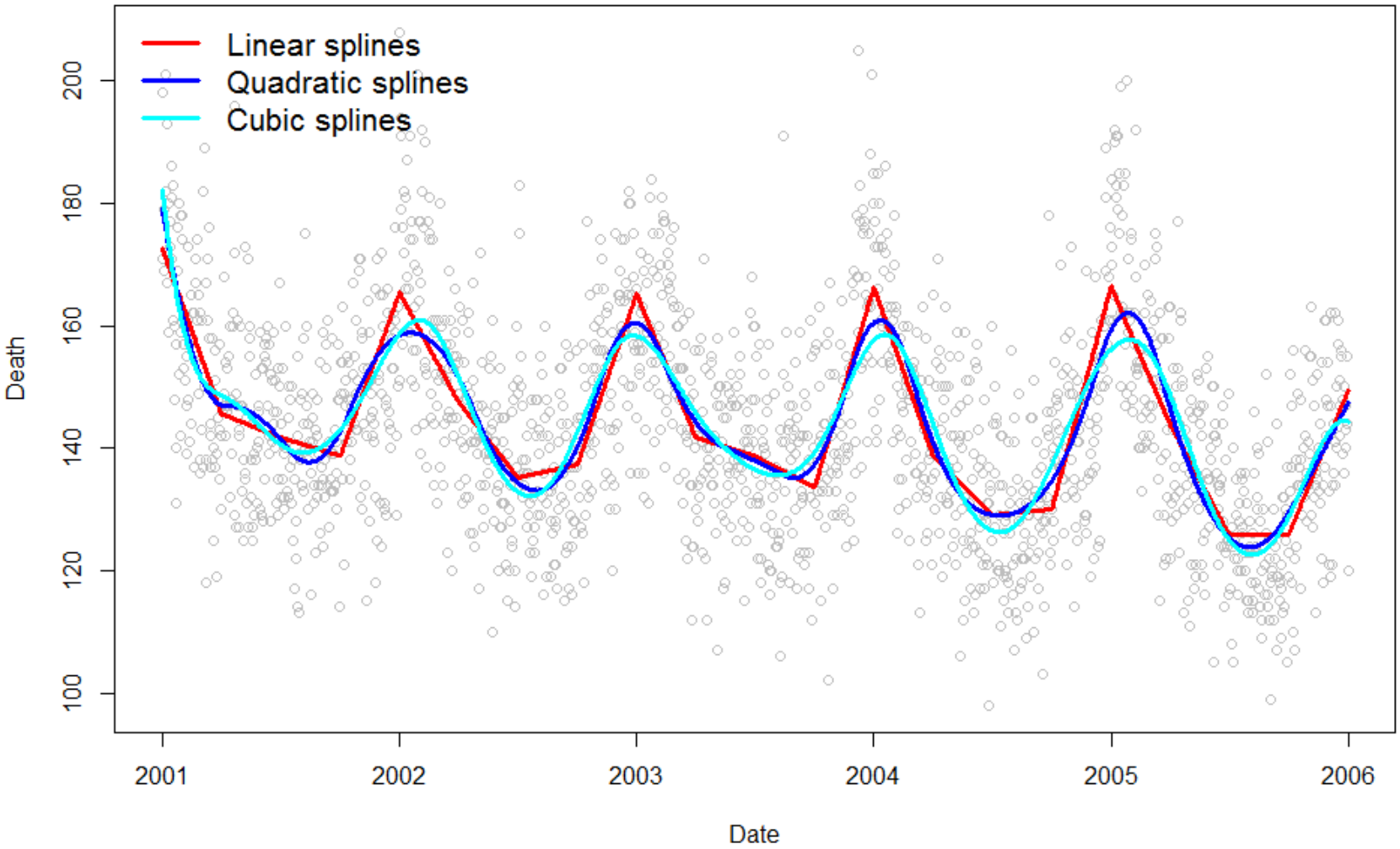
Daily non-accidental mortality counts in 5-county New York City, 2001-2006.



Knots at quantiles, df=10



Knots at quantiles, df = 20



Model Selection

Model Selection

We need to pick:

1. Which basis function? Linear versus cubic.
2. How many knots?
3. Where to put the knots?

Challenge: these models are usually not nested!

Main Ideas:

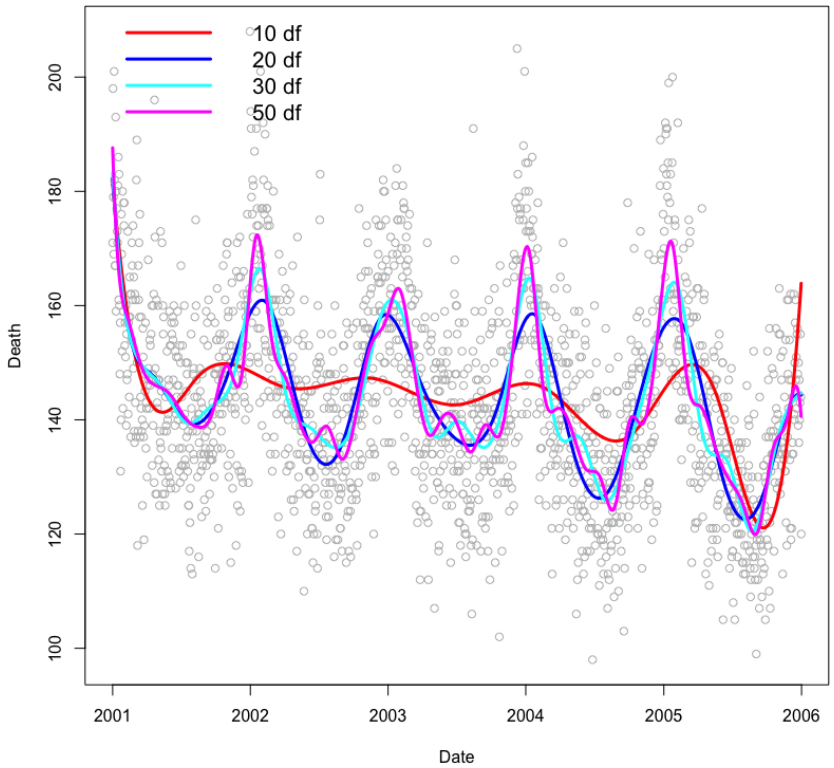
- Choice of basis function usually does not have a large impact on model fit, especially when there are enough knots and $g(x)$ is smooth.
- When there are enough knots, their locations are less important too.

For now, we'll focus on the **how many** question.

Bias-Variance Trade-Off

More knots $\rightarrow$ $\begin{cases} \text{Can better capture fine-scale trends} \\ \text{Need to estimate more coefficients} \end{cases}$

Cubic Splines with Different Number of Knots



Towards the Bias-Variance Decomposition

Assume Y comes from some true model

$$Y = g(X) + \epsilon, \qquad \epsilon \sim (0, \sigma^2) \; .$$

where $g(\cdot)$ is some unknown function.

For given x_i, we estimate Y with $\hat{g}(x_i)$, where here we assume $\hat{g}(x_i) \perp\!\!\!\perp \epsilon$. In other words, x_i is an "unseen" data point.

The expected squared difference between Y and the estimator $\hat{g}(X)$ is the population mean squared error (MSE). For given x_i,

$$\begin{aligned} E[\, \{Y - \hat{g}(X)\}^2 \, | X = x_i \,] &= \texttt{derive...} \\ &= \sigma^2 + E\, \{g(x_i) - \hat{g}(x_i)\}^2 \end{aligned}$$

Derivations

Bias-Variance Decomposition, cont.

$$E\{\, g(x_i) - \hat{g}(x_i)\,\}^2 = ...$$

Derivations

Cross-validation Error

Let $\hat{g}_i^{(-i)}$ be the fitted value of y_i at x_i using all the data except y_i. The ordinary leave-one-out cross-validation (LOOCV) is given by

$$\text{CV} =$$

Intuitively, CV estimates the population MSE, $E[\,(Y - \hat{g}(X))^2\,]$, with a sample MSE.

Note here we are averaging across the values of x_i.

Caveat from Hastie et al: "Discussions of error rate estimation can be confusing, because we have to make clear which quantities are fixed and which are random..."

Overfitting

- If you overfit, then you start to fit the noise in the data, i.e., you estimate $g(x_i) + \epsilon_i$, instead of $g(x_i)$.
- With overfitting, new data are poorly predicted.
- From Bias-Variance perspective:

- In splines, lines that are very wiggly = high variance.
- If you underfit, then you tend to estimate a smoothed version of $g(x_i)$, at extreme, fit a mean s.t. $\hat{g}(x_i) = \frac{1}{n}\sum y_i$.
- From Bias-Variance perspective:

- In splines, lines that vary little = low variance.

Cross-validation Error, OLS

For linear regression, LOOCV can be obtained easily from $\hat{y}_i$, as predicted using estimators from the *full* data:

$$\boxed{\text{CV} = \frac{1}{n}\sum_{i=1}^{n}\frac{(y_i - \hat{y}_i)^2}{(1 - H_{ii})^2}},$$

where H_{ii} is the (i, i)th element of the hat matrix.

(This results from a clever application of a linear algebra trick, not discussed here.)

This is the formula for any design matrix in OLS.

Generalized Cross-validation Error

One variation of LOOCV is the generalized cross-validation (GCV)

$$\text{GCV} =$$

Compared to CV,

- GCV replaces each H_{ii} by the average of all H_{ii}.
- GCV is a weighted version of CV.
- For complicated models (not OLS), CV is computationally costly, as it requires fitting the model many times.
- GCV often easier to calculate.

We want to pick a model which minimizes CV or GCV.

K-Fold CV

- In K-Fold CV, the data are divided into K subsets

$$MSE_k = \frac{1}{n/K} \sum_{i \in \mathcal{S}_k} (y_i - \hat{y}_i^{-\mathcal{S}_k})^2$$

$$CV = \widehat{MSE} = \frac{1}{K} \sum_{k=1}^{K} MSE_k$$

- Each partition has a training dataset with $(K-1) * n/K$ observations and test dataset with n/K observations.
- Then the model is fit K times.
- LOOCV is a special case where the number of folds is n.

Training, validation, and test dataset

Another approach is to divide the dataset into two datasets and use one dataset for estimation (training) and another for testing (test).

Popular splits: 70% (training) and 30% (test), or 80% and 20%.

This is often combined with cross-validation, where CV is applied to the training dataset to obtain the model, and then the model is applied to the unseen data to evaluate accuracy.

The "validation dataset" is the data left out when using cross-validation. In practice, we move across the different folds to tune hyperparameters. E.g., number of knots.

Popular in computer science with huge datasets.

Is there anything wrong with this approach?

K-Fold CV, cont.

- There is another bias-variance tradeoff ("meta" bias-variance tradeoff) regarding the optimal K
- K impacts the MSE of the sample estimate of the MSE,

$$E(MSE - \widehat{MSE})^2$$

  where $\widehat{MSE}$ is from K-fold CV.
- If we let $K = 2$, we will do a poorer job of fitting the model (using less data) $\rightarrow$ upwardly biased $\widehat{MSE}$.
- At the other extreme, LOO has least bias because we are using $n - 1$ observations to estimate the models, but each term in the summand is highly correlated, leading to higher variance.
- General recommendations: 5 or 10-fold CV to balance this tradeoff.
- A discussion is James et al 2013 Chapter 5.

Likelihood-Based Approach

With basis expansion, we assume g_i can be expressed as a linear combination of some linear regressors,

$$\mathbf{Y} \sim N(\mathbf{X}\boldsymbol{\beta}, \sigma^2\mathbf{I}) .$$

The Gaussian (Normal) likelihood is given by

$$f(\boldsymbol{\beta}, \sigma^2) = (2\pi\sigma^2)^{-n/2} \exp\{-\frac{1}{2\sigma^2}(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})'(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})\}$$

with log-likelihood function

$$\log f(\boldsymbol{\beta}, \sigma^2) = -\frac{n}{2}\log(2\pi\sigma^2) - \frac{1}{2\sigma^2}(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})'(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}) .$$

Given our estimated coefficients $\hat{\boldsymbol{\beta}}$, we hope to maximize

$$E\left[\log f(\hat{\boldsymbol{\beta}}, \sigma^2)\right] = -\frac{n}{2}\log(2\pi\sigma^2) - \frac{1}{2\sigma^2}E\left[(\mathbf{X}\boldsymbol{\beta} - \mathbf{X}\hat{\boldsymbol{\beta}})'(\mathbf{X}\boldsymbol{\beta} - \mathbf{X}\hat{\boldsymbol{\beta}})\right] .$$

Mallow's C_p and Akaike Information Criterion

It can be shown that

$$E\left[\log f(\hat{\boldsymbol{\beta}}, \sigma^2)\right] \approx \log f(\hat{\boldsymbol{\beta}}, \sigma^2) + \frac{n}{2} - p.$$

So one approach is to select a model that maximizes the above. If σ^2 is assumed known, this gives rise to the Mallow's C_p criterion:

$$\boxed{C_p = \frac{1}{\sigma^2}(\mathbf{Y} - \hat{\boldsymbol{\beta}}\mathbf{X})'(\mathbf{Y} - \hat{\boldsymbol{\beta}}\mathbf{X}) - n + 2p}\,.$$

In practice, σ^2 is often replaced by its estimate from the largest model considered.

Akaike information criterion (AIC) generalizes this to any likelihood:

$$\boxed{AIC = -2 \times \log f(\hat{\boldsymbol{\beta}}, \hat{\sigma}^2) + 2p}\,,$$

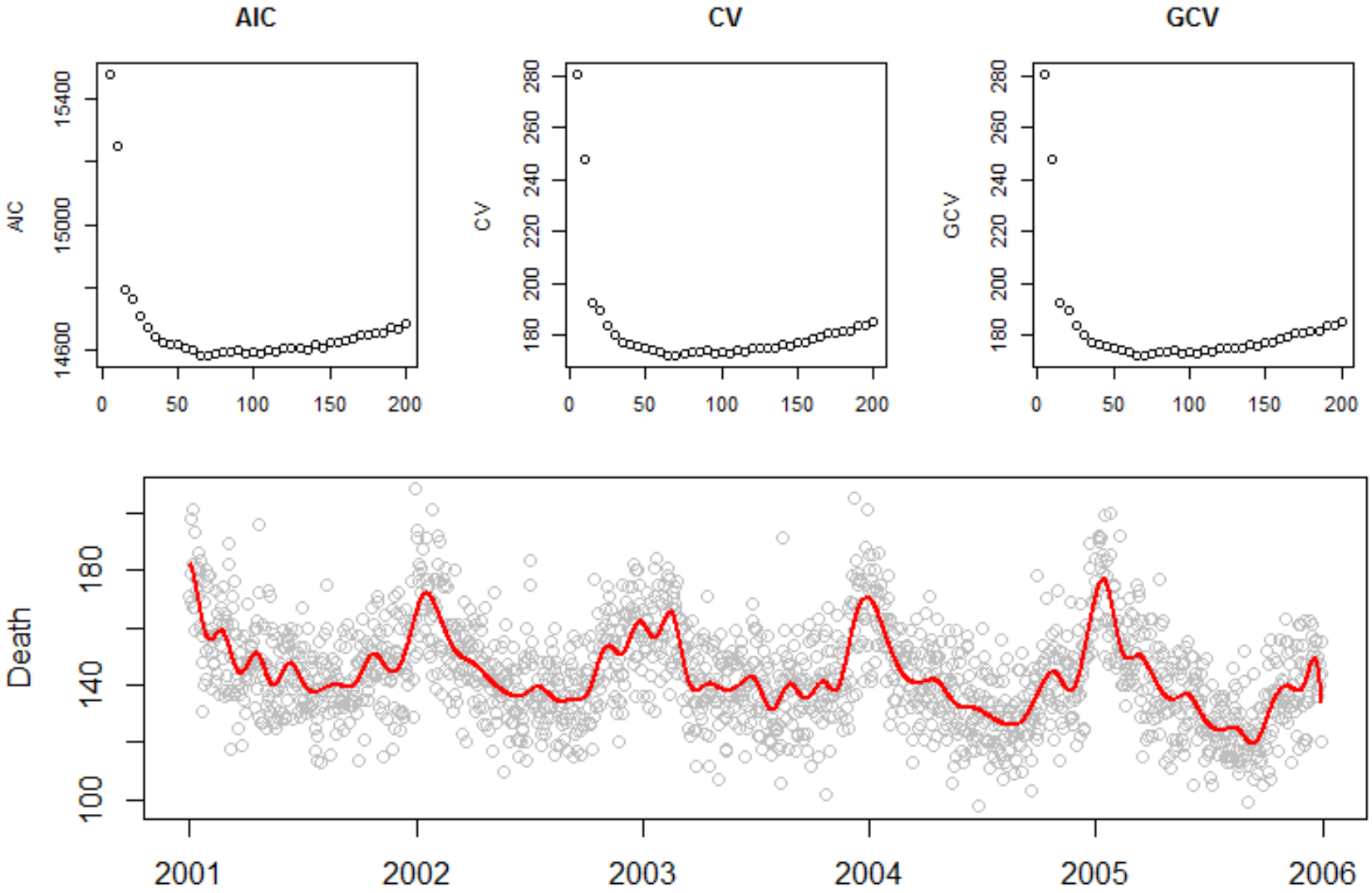
which we wish to minimize also.

Example: Mortality Trends

```
> ### AIC, CV, and GCV calculation examples:

> fit = lm (alldeaths~bs (date, df = 10), data = health)
>
> ##AIC
> AIC (fit)
[1] 15252.54
>

> ##GCV/CV
> H =  hatvalues (fit)

> CV = mean(  (fit$fitted - health$alldeaths)^2 / (1-H)^2 )
> CV
[1] 248.0374

> GCV = mean ((fit$fitted - health$alldeaths)^2) / (1 - mean(H))^2
> GCV
[1] 248.1518
```

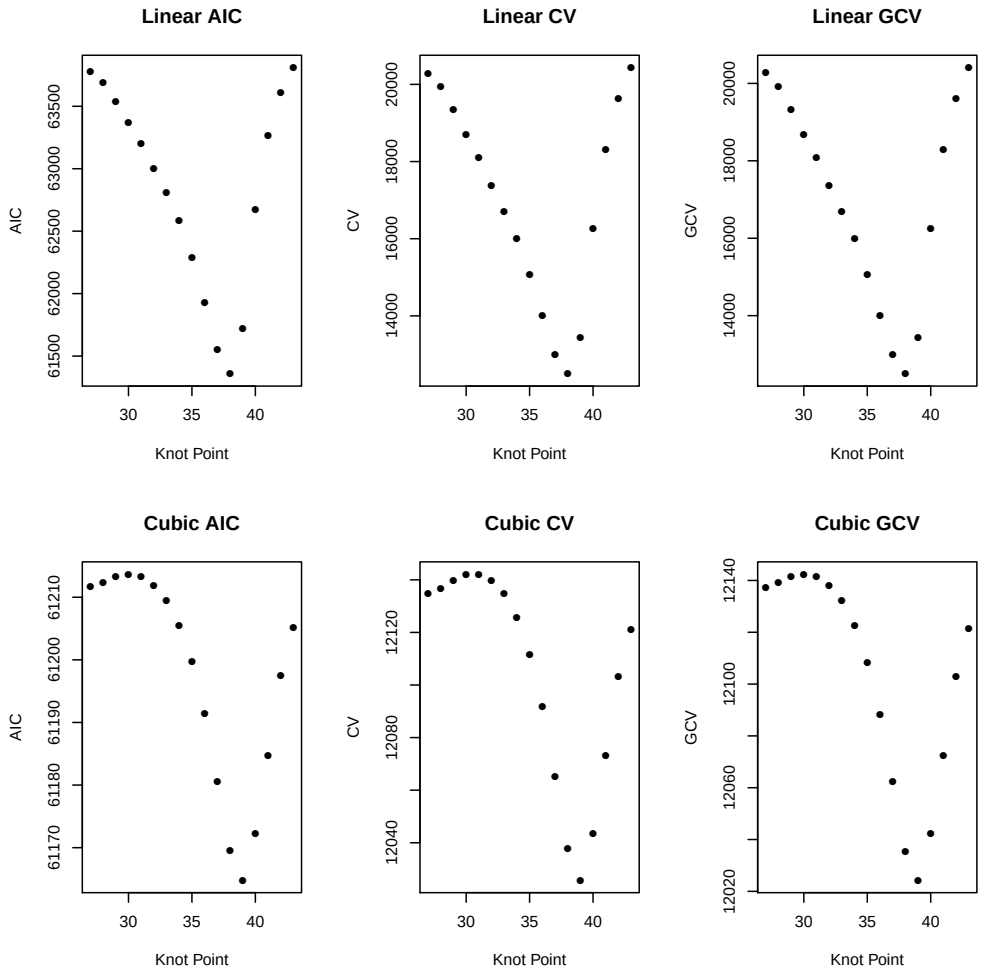
Example: Daily Death Counts in NYC

Optimal = 70 df.



Example: Birth Weight and Pregnancy Length

Linear or cubic splines with 1 knot placed at different locations.



Example: Birth Weight and Pregnancy Length