

Generalized Additive Model (GAM)

study group

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General form

- ▶ **Generalized additive model** is a generalized linear model with a linear predictor, involving a sum of smooth functions of covariates.

$$g(u_i) = X_i^* \theta + f_1(x_{1i}) + f_2(x_{2i}) + f_3(x_{3i}, x_{4i}) + \dots$$

(eqn. 3.1)

- ▶ GAM specifies the model with **smooth functions** rather than detailed parametric relationships.

Univariate smooth functions f

$$y_i = f(x_i) + \epsilon_i \text{ (eqn. 3.2)}$$

y_i : response variable

f : **smooth function**

x_i : covariate

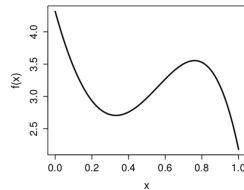
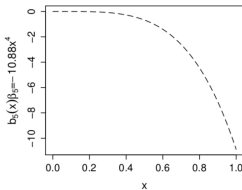
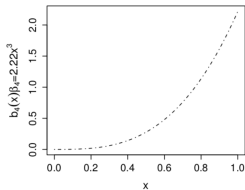
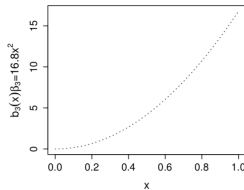
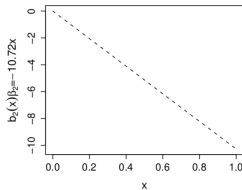
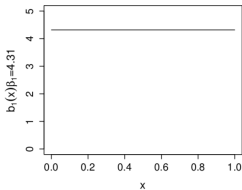
ϵ_i : i.i.d. $N(0, \sigma^2)$ variable (error)

- ▶ Represent the smooth function f in a way that (eqn. 3.2) becomes a linear model.
- ▶ The smooth function f can then be expressed as some *basis functions* (b) with parameter β

$$f(x_i) = \sum_{j=1}^q b_j(x) \beta_j$$

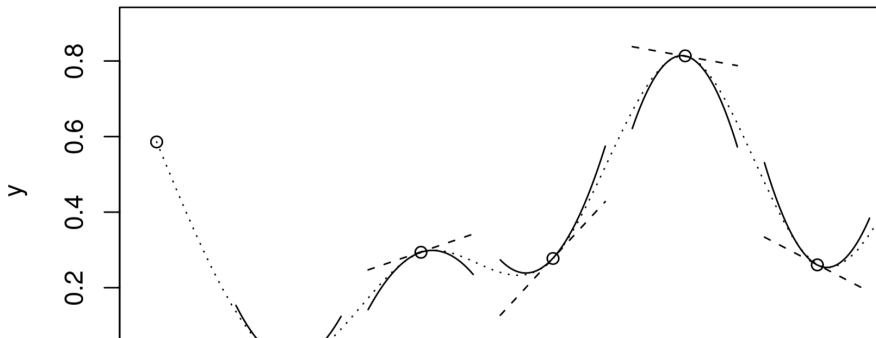
Simple example of smooth function: 4th order polynomial basis

$$f(x) = \beta_1 + x\beta_2 + x^2\beta_3 + x^3\beta_4 + x^4\beta_5$$



Cubic spline basis

- ▶ A univariate function represented using a cubic spline.
- ▶ A cubic spline is a curve, made up of sections of cubic polynomial, joined together so that they are continuous in value as well as first and second derivatives



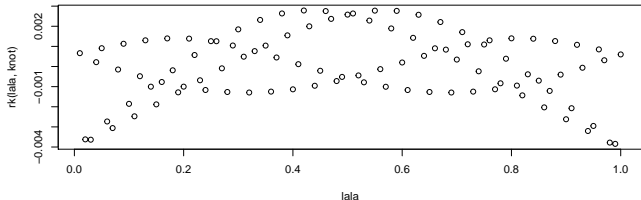
A cubic spline basis can be expressed as...

$$b_1(x) = 1, b_2(x) = x, \dots, b_{i+2}(x, x_k^*)$$

- ▶ Consist of *one constant, one 1st order (linear) term, and k cubic polynomials*
 - ▶ **k is the number of knots**
 - ▶ knots are evenly spaced or at the quantile of distribution of x ($x_i^*; i = 1 \sim k$)
 - ▶ $k + 2$ is the rank of the cubic spline function
- ▶ $b_{i+2}(x, x_k^*)$ is a cubic polynomial written as:

$$R(x, z) = \left[(z - 1/2)^2 - 1/12 \right] \left[(x - 1/2)^2 - 1/12 \right] \\ - \left[(|x - z| - 1/2)^4 - 1/2 (|x - z| - 1/2) \right]$$

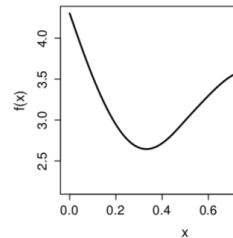
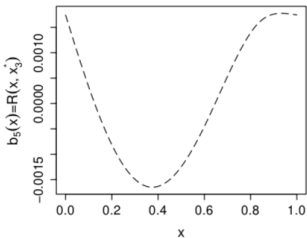
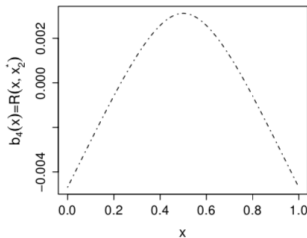
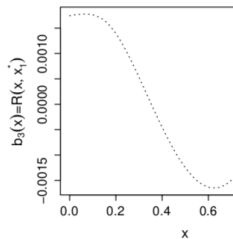
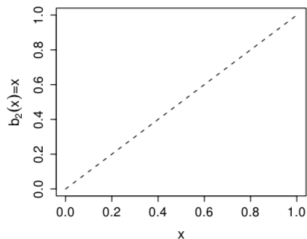
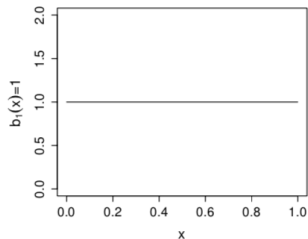
- ▶ Each cubic polynomial will peak at the knot
 - ▶ e.g. The four cubic polynomials when $k = 4$



The peak of the cubic polynomial is *conceptually* the weight when fitting the y

Example of cubic spline bases

rank 5 cubic regression spline basis



Working example

Data

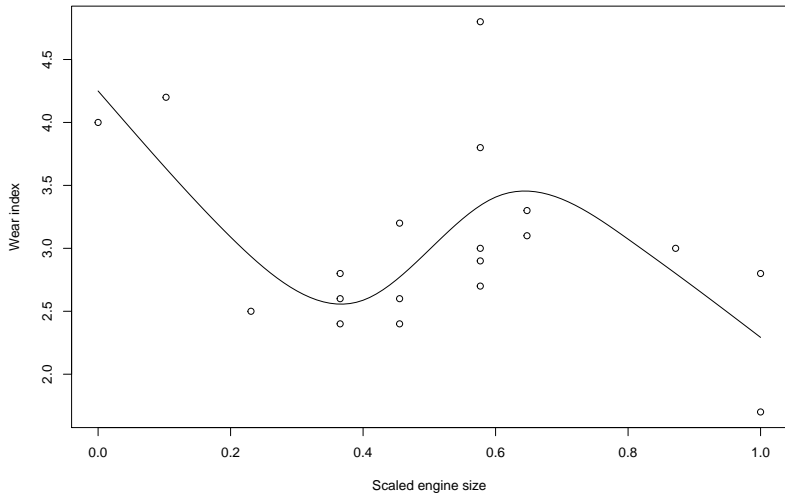
```
size <- c(1.42, 1.58, 1.78, 1.99, 1.99, 1.99, 2.13, 2.13, 2.13)
wear <- c(4.0, 4.2, 2.5, 2.6, 2.8, 2.4, 3.2, 2.4, 2.6)

x <- size - min(size)
x <- x / max(x)
```

Function for generating the model matrix

```
spl.X <- function(x,xk) # set up model matrix
{ q <- length(xk) + 2 # number of parameter
  n <- length(x) # number of data
  X <- matrix(1, n, q) # initialized model
  X[,2] <- x # set second column to x
```

Results...



Knots determine the smoothness

- ▶ How many knots?
- ▶ **Penalized regression splines**

Minimize the

following. . . $\|y - X\beta\| + \lambda \int_0^1 [f''(x)]^2 dx$

High λ penalizes high wiggleness ($\int_0^1 [f''(x)]^2 dx$)

Fig. 3.8

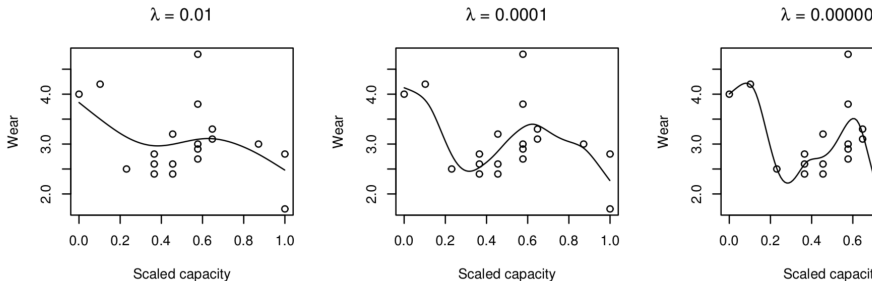
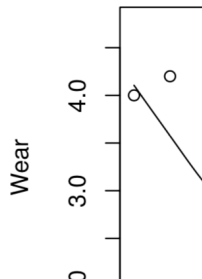
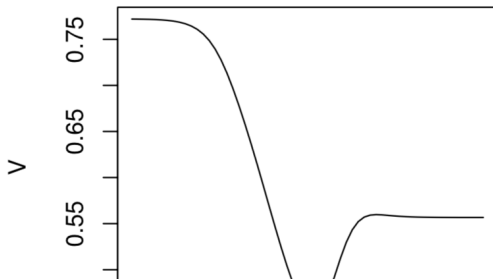


Figure 3.8 *Penalized regression spline fits to the engine wear versus capacity data using*

To determine λ

- ▶ Ordinary cross validation (OCV)
Leave one data point at a time when doing cross validation
- ▶ Generalized cross validation (GCV)
Use *influence matrix* to estimate the deviance when leaving one data point out Fig. 3.10

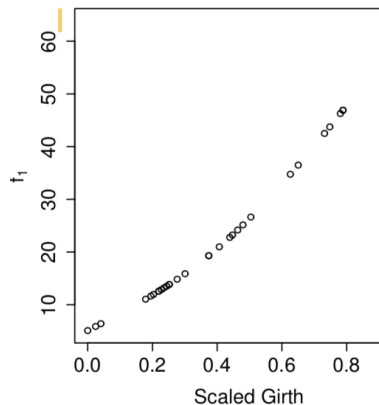
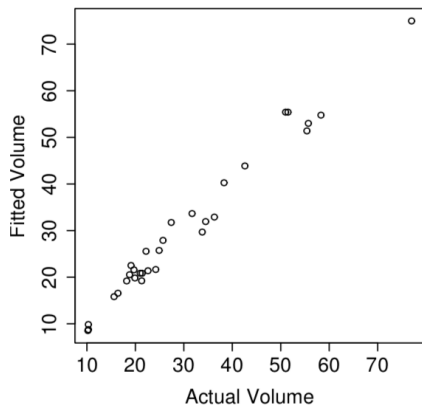
GCV score



Additive model (more than one x)

$$y_i = f_1(x_{1i}) + f_2(x_{2i}) + \epsilon_i$$

All calculations are conceptually the same as mentioned above.



Generalized additive model

Due to the link function, penalized likelihood is being maximized.

In practice, **penalized iteratively re-weighted least square (P-IRLS)** is implemented.