

# Introduction to Statistical Learning *with applications in Python*

*Based on "Introduction to Statistical Learning, with applications in R" by Gareth James, Daniela Witten, Trevor Hastie, Robert Tibshirani*

## Beyond Linearity

*Polynomial Regression, Basis Functions, Splines, Generalised Additive Models*

Kurt Rinnert

Physics Without Frontiers



The Abdus Salam  
International Centre  
for Theoretical Physics



UNIVERSITY OF  
LIVERPOOL

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Kurt Rinnert <kurt.rinnert@cern.ch>, Kate Shaw <kshaw@ictp.it>

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# Abstract

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Linear models are often applicable and easy to interpret. However, as we have stressed several times, the *true* functional relationships are rarely linear.

In this lecture we will explore several ways to drop the assumption of linearity.

# Overview

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- Polynomial Regression
- Basis Functions
- Splines
- Smoothing Splines
- Generalised Linear Models (GLMs)

**We'll see again that model flexibility is related to the bias-variance trade-off.**

# Polynomial Regression

- We have already seen some ways to extend linear regression to include non-linear terms.
- In particular we have fitted and interpreted polynomial models:

$$y_i = \beta_0 + \beta_1 X_1 + \beta_2 X_1^2 + \beta_3 X_1^3 + \epsilon_i$$

- Or models with interaction terms:

$$y_i = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1 X_2 + \epsilon_i$$

- We will not go through all this again, but some exercises will still refer to these ideas.

**In this lecture we will explore more powerful concepts to move beyond linearity.**

# Basis Functions

- The idea is quite simple: we don't limit ourselves to polynomials or interactions.
- Instead we allow arbitrary functions of the predictors:

$$y_i = \beta_0 + \beta_1 b_1(x_i) + \beta_2 b_2(x_i) + \cdots + \beta_K b_K(x_i) + \epsilon_i$$

- We can think of this as a linear model with predictors

$$b_1(x_i), b_2(x_i), \dots, b_K(x_i)$$

- This means we can use the regression methods we learned about to estimate the parameters  $\beta$ .

**All techniques for evaluating performance and model selection are still applicable.**

# Piecewise Polynomials

- Fitting high-degree polynomials is not ideal as it can lead to severe over-fitting.
- We can instead fit lower-degree *piecewise polynomials*, for example:

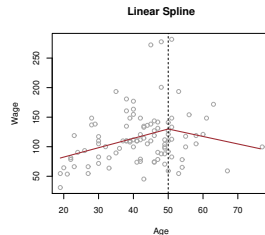
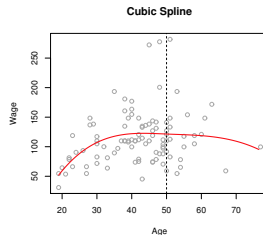
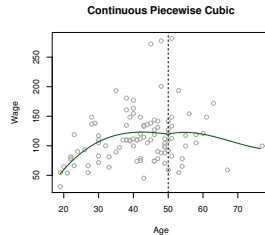
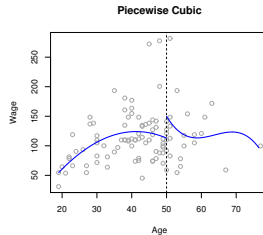
$$y_i = \begin{cases} \beta_{01} + \beta_{11}x_i + \beta_{21}x_i^2 + \beta_{31}x_i^3 + \epsilon_i & \text{if } x_i < c \\ \beta_{02} + \beta_{12}x_i + \beta_{22}x_i^2 + \beta_{32}x_i^3 + \epsilon_i & \text{if } x_i \geq c \end{cases}$$

- Keeping the degree low mitigates the chance of over-fitting.
- In this example the piecewise polynomial has one *knot* at  $x_i = c$ .
- We can increase the flexibility by introducing more knots.

Here, and in the following we assume on single predictor  $X$ .

# Piecewise Polynomials

- The piecewise polynomial has a discontinuity at  $c$  (age = 50).
- This can be removed by requiring *continuity*.
- That still leaves us with a kink.
- The situation is further improved by requiring the derivatives to be continuous.



Putting constraints on the knots of piecewise polynomials leads to splines.

# Constraints and Splines

- To construct a *cubic spline* we start from a piecewise polynomial of degree 3 and impose the following constraints.

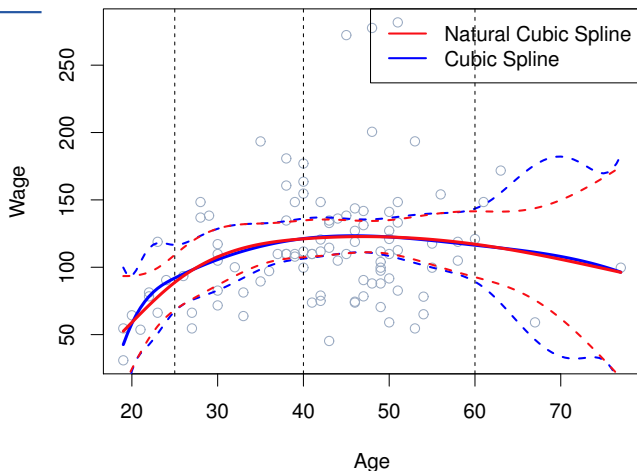
constraint	continuity
$b(x_i)$	value
$b'(x_i)$	slope
$b''(x_i)$	curvature

- Each constraint frees up one degree of freedom.
- In general, cubic splines with  $K$  knots use  $K + 4$  degrees of freedom.

**We do not concern ourselves with the details involved in imposing the constraints.**



# Natural Splines

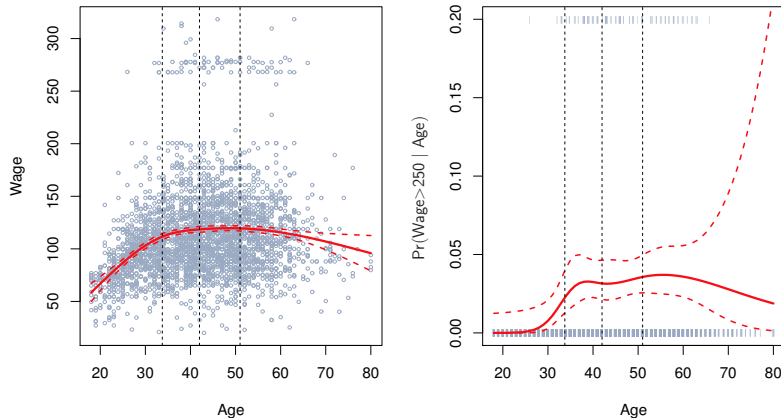


- Splines can have large variance at the outer range of the predictors.
- *Natural splines* are constrained to be linear at the boundaries.

**Note that the confidence interval for the natural spline is narrower.**

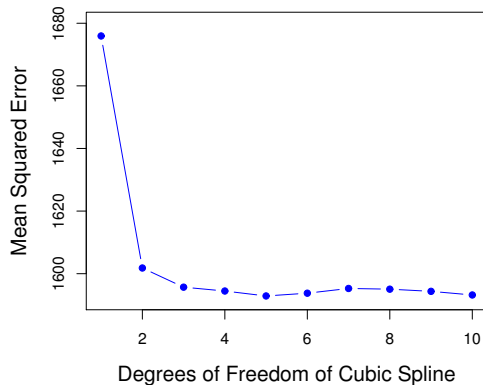
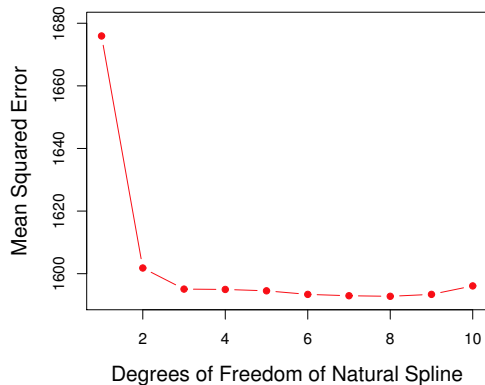
# Choosing $K$ & Knot Positions

## Natural Cubic Spline



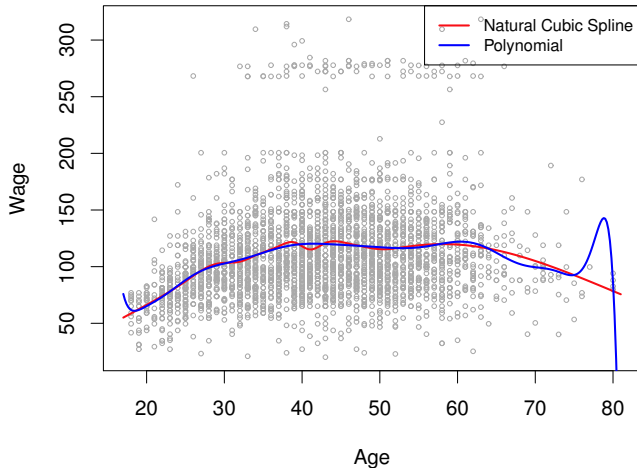
We usually specify the degrees of freedom and place the knots uniformly over quantiles .

# Choosing $K$ & Knot Positions



In practice – you guessed it – we use cross-validation.

# Splines versus Polynomial Regression



High degree polynomials tend to behave badly at the boundaries.

# Smoothing Splines

- *Smoothing splines* are a different approach to fitting splines.
- We want to find some *smooth* function  $g(x)$  that fits the data well, that is

$$\text{RSS} = \sum_{i=1}^n (y_i - g(x_i))^2$$

is small.

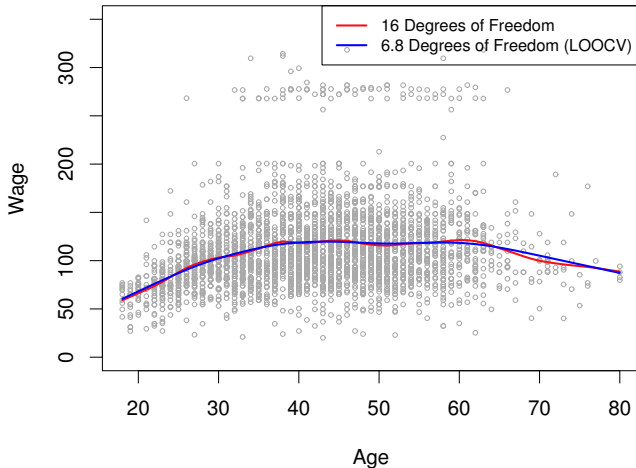
- The smoothness can be imposed by minimising

$$\underbrace{\sum_{i=1}^n (y_i - g(x_i))^2}_{\text{loss}} + \lambda \underbrace{\int g''(t)^2 dt}_{\text{penalty}}$$

The *loss + penalty* approach is very common in machine learning practice.

# Choosing the $\lambda$ Parameter

## Smoothing Spline



The  $\lambda$  parameter is continuous, leading to the concept of *effective degrees of freedom*.

# Generalised Additive Models

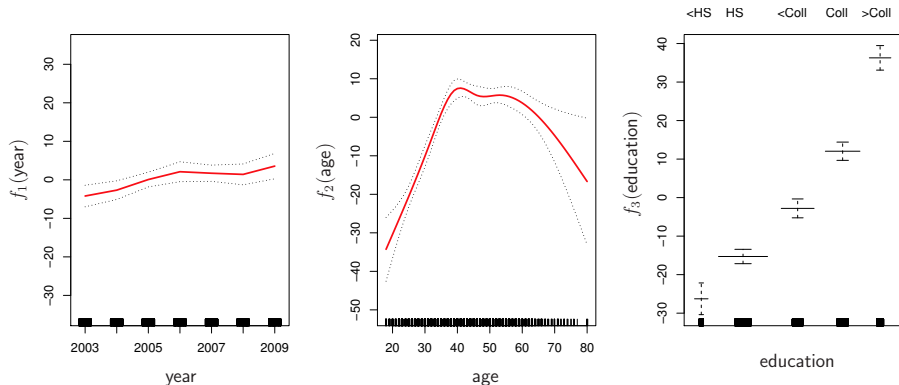
- We now release the condition of having a single predictor in the model.
- This leads to the concept of *generalised additive models* (GAMs).
- This is analogous of moving from simple linear regression to multiple linear regression.
- That is, the models can now take the form

$$\begin{aligned}y_i &= \beta_0 + \sum_{j=1}^p f_j(x_{ij}) + \epsilon_i \\ &= \beta_0 + f_1(x_{i1}) + f_2(x_{i2}) + \cdots + f_p(x_{ip}) + \epsilon_i\end{aligned}$$

with *smooth* functions  $f_j$ .

The model still *additive* because we *add* separate  $f_j$  for each  $X_j$ .

# Generalised Additive Models

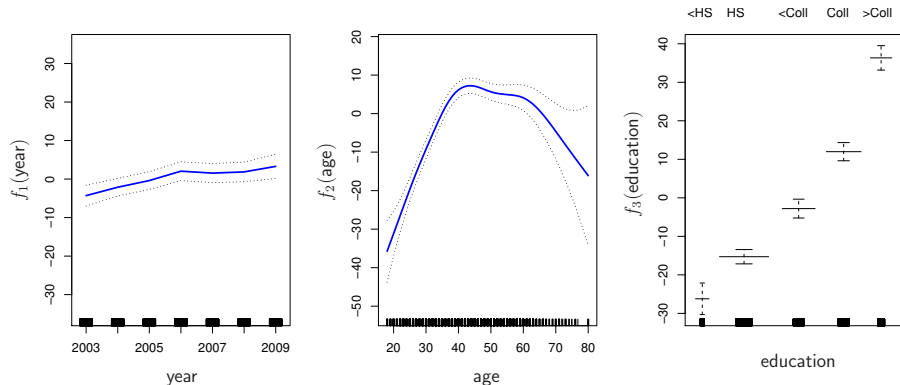


$$\text{wage} = \beta_0 + f_1(\text{year}) + f_2(\text{age}) + f_3(\text{education}) + \epsilon$$

A GAM model on the Wage data set with two cubic splines and a qualitative variable.



# Generalised Additive Models



$$\text{wage} = \beta_0 + f_1(\text{year}) + f_2(\text{age}) + f_3(\text{education}) + \epsilon$$

A GAM model on the Wage data set with two smoothing splines and a qualitative variable.

# GAMs for Classification

- GAMs can also be used for classification.
- Just like with ordinary linear models, we use logistic regression in this scenario:

$$\log\left(\frac{p(X)}{1-p(X)}\right) = \beta_0 + f_1(x_{i1}) + f_2(x_{i2}) + \cdots + f_p(x_{ip}) + \epsilon_i$$

- For example:

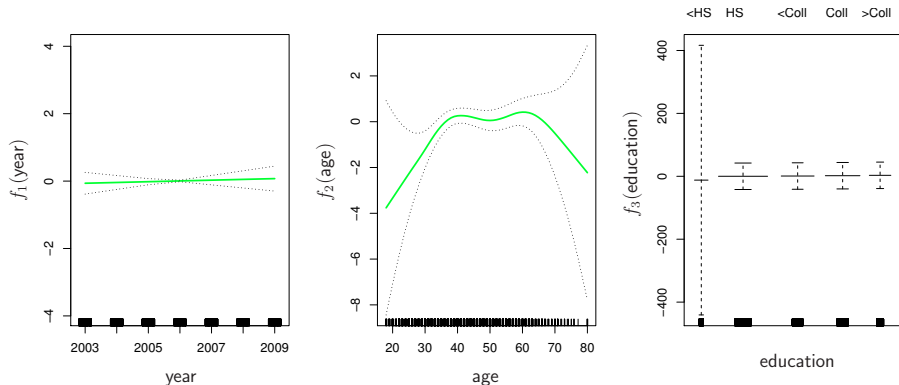
$$\log\left(\frac{p(X)}{1-p(X)}\right) = \beta_0 + \beta_1 \times \text{year} + f_2(\text{age}) + f_3(\text{education})$$

where

$$p(X) = P(\text{wage} > 250 | \text{year}, \text{age}, \text{education})$$

**That is, we want to predict whether the yearly income is greater than \$250,000.**

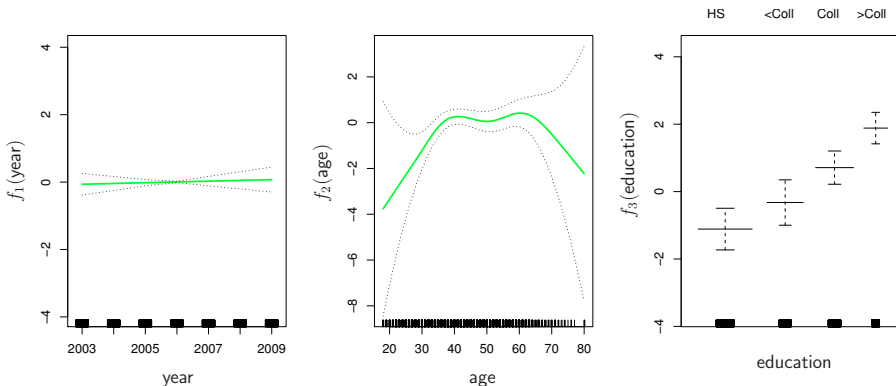
# GAMs for Classification



$$p(X) = P(\text{wage} > 250 | \text{year}, \text{age}, \text{education})$$

There seems to be a problem with the qualitative variable.

# GAMs for Classification



$$p(X) = P(\text{wage} > 250 | \text{year, age, education})$$

It turns out high school drop-outs never earn more than \$250,000/year.