MATH5824 Generalised Linear and Additive Models

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Weekly schedule

Items will be added here week-by-week and so keep checking when you need up-to-date information on what you should be doing. Note that items specific to MATH5824M will be marked accordingly, otherwise items refer to the material common with MATH3823.

i Week 2 (5 - 9 February)

- Before next Lecture: Please re-read Section 2.1: Overview and Section 2.2: Linear models, and self-study Section 2.3: Types of normal linear model.
- Lecture on Tuesday: We will cover Section 2.4: Matrix representation of linear models and briefly Section 2.5: Model shorthand notation.
- Before next Lecture: Please re-read Sections 2.4 and 2.5 carefully.
- Lecture on Thursday: We will cover Section 2.6: Fitting linear models in R then discuss selected Exercises from Chapters 1 and 2.
- **Before next Lecture:** Please re-read the whole of MATH5824M Chapter 1: Non-parametric Modelling.
- Lecture on Friday: We will cover the whole of MATH5824M Chapter 2: Introducing Splines.
- Weekly feedback: Complete the Chapter 2 Quizzes and complete the Exercises in Section 2.8. Also, complete the MATH5824M Section: 1.4 Exercises.

Week 1 (29 January - 2 February)

- Before first Lecture: Please read the Overview.
- Lecture on Tuesday: We will briefly cover all material in *Chapter: Introduction*.
- Before next Lecture: Please re-read *Chapter 1* carefully, especially any sections not covered in Lectures.
- Lecture on Thursday: Start Chapter 2: Essentials of Normal Linear Models with Section 2.1: Overview & Section 2.2: Linear models.
- Before next Lecture: Please read the MATH5824M Overview.
- Lecture on Friday: We will cover the whole of MATH5824M Chapter 1: Non-parametric Modelling.
- Weekly feedback: Complete the Chapter 1 Quizzes and self-study the Exercises in Section 1.5 solutions to be added during Week 1. If you have time, then also self-study the MATH5824M Exercises in Section 1.4.

i Advanced notice

- Module Assessment: Set on 14 March with submission deadline 23 April (that is after the break). You will be expected to write a short report based on an RStudio practical.
- Computer classes: 27/28 February for Practice and 19/20 March for Assessment check your timetable.
- Generative AI usage within this module: The assessments for this module fall in the red category for using Generative AI which means you must not use Generative AI tools. The purpose and format of the assessments makes it inappropriate or impractical for AI tools to be used.

i Provisional Weekly Lecture Schedule

Week 1	Chapter 1	A11
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Week 2	Chapter 2	All
Week 3	Exercises	Exercises 1, 2
	Chapter 3	Sections 3.1-3.3
Week 4		Sections 3.4-3.5
	Exercises	Exercises 3
Week 5	Chapter 4	Sections 4.1-4.3
Week 6		Sections 4.4-4.5
Week 7	Chapter 5	Sections 5.1-5.3
Week 8		Sections 5.4-5.6
	Exercises	Exercises 4, 5
Easter		
Week 9	Chapter 6	All
Week 10	Exercises	Exercises 6
Week 11	Revision	

Overview

Preface

These lecture notes are produced for the University of Leeds module "MATH5824 - Generalized Linear and Additive Models" for the academic year 2023-24. They are based on the lecture notes used previously for this module and I am grateful to previous module lecturers for their considerable effort: Lanpeng Ji, Amanda Minter, John Kent, Wally Gilks, and Stuart Barber. This year, again, I am using Quarto (a successor to RMarkdown) from RStudio to produce both the html and PDF, and then GitHub to create the website which can be accessed at rgaykroyd.github.io/MATH5824/. Please note that the PDF versions will only be made available on the University of Leeds Minerva system. Although I am a long-term user of RStudio, I am a novice at Quarto/RMarkdown and a complete beginner using Github and hence please be patient if there are hitches along the way.

RG Aykroyd, Leeds, January 22, 2024

Changes since last year

Feedback from the students last year was very positive, but there were consistent comments regarding two issues: (1) a shortage of practice exercises and the opportunity to discuss these in class, and (2) limited RStudio support in preparation for the assessment. For the first of these, additional exercises have been prepared and are included in the learning material. Also, I am trying some short quizzes so that you can check your basic knowledge. Further, I intend to set-aside some lecture time for us to discuss selected exercises. For the second, an additional computer session has been added, in Week 5 (26 February - 1 March), this is 3 weeks before the assessed practice in Week 8 (18 - 22 March). Further, a few new instructional videos will be available addressing some RStudio topics. Together, these represents a considerable about of extra work for me, but I hope that they are helpful and so please give your feedback whenever there is an opportunity.

Generative AI usage within this module

The assessments for this module fall in the red category for using Generative AI which means you must not use Generative AI tools. The purpose and format of the assessments makes it inappropriate or impractical for AI tools to be used.

Warning

Statistical ethics and sensitive data

Please note that from time to time we will be using data sets from situations which some might perceive as sensitive. All such data sets will, however, be derived from real-world studies which appear in textbooks or in scientific journals. The daily work of many statisticians involves applying their professional skills in a wide variety of situations and as such it is important to include a range of commonly encountered examples in this module. Whenever possible, sensitive topics will be signposted in advance. If you feel that any examples may be personally upsetting then, if possible, please contact the module lecturer in advance. If you are significantly effected by any of these situations, then you can seek support from the Student Counselling and Wellbeing service.

Official Module Description

Module summary

Linear regression is a tremendously useful statistical technique but is limited to normally distributed responses. Generalised linear models extend linear regression in many ways - allowing us to analyse more complex data sets. In this module we will see how to combine continuous and categorical predictors, analyse binomial response data and model count data. A further extension is the generalised additive model. Here, we no longer insist on the predictor variables affecting the response via a linear function of the predictors, but allow the response to depend on a more general smooth function of the predictor.

Objectives

On completion of this module, students should be able to:

- carry out regression analysis with generalised linear models including the use of link functions, deviance and overdispersion;
- fit and interpret the special cases of log linear models and logistic regression;
- compare a number of methods for scatterpot smoothing suitable for use in a generalised additive model;
- use a backfitting algorithm to estimate the parameters of a generalised additive model;
- interpret a fitted generalised additive model;
- use a statistical package with real data to fit these models to data and to write a report giving and interpreting the results.

Syllabus

Generalised linear model; probit model; logistic regression; log linear models; scatterplot smoothers; generalised additive model.

University Module Catalogue

For any further details, please see MATH5824 Module Catalogue page

1 Non-parametric Modelling

1.1 Introduction

Here is a short video [3 mins] to introduce the chapter.

In the Level 3 component of this module, we extend the simple linear regression model to the generalised linear model which can cope with non-normally distributed response variables, in particular data following binomial and Poisson distributions. However, we still just use linear functions of the predictor variables. A further extension of the linear model is the generalised additive model. Here, we no longer insist on the predictor variables affecting the response via a linear function of the predictors, but allow the response to depend on a more general smooth function of the predictor. In the Level 5 component of this module, we study splines and their use in interpolating and smoothing the effects of explanatory variables in the generalised linear models of the Level 3 component of this module (see separate Lecture Notes accompanying MATH3823). Towards the end of the material, we will learn that the fitting of generalised additive models is a straightforward extension of what is learnt in MATH3823.

Outline of the additional material in MATH5824 compared to MATH3823:

- 1. Interpolating and smoothing splines.
- 2. Cross-validation and fitting splines to data.
- 3. The generalised additive model.

1.2 Motivation

Table 1.1 reports on the depth of a coal seam determined by drilling bore holes at regular intervals along a line. The depth y at location x = 6 is missing: could we estimate it?

Table 1.1: Coal-seam depths (in metres) below the land surface at intervals of 1 km along a linear transect.

$\overline{\text{Location}, x}$	0	1	2	3	4	5	6	7	8	9	10
Depth, y	-90	-95	-140	-120	-100	-75	NA	-130	-110	-105	-50

Figure 1.1 plots these data, superimposed with predictions from several polynomial regression models.

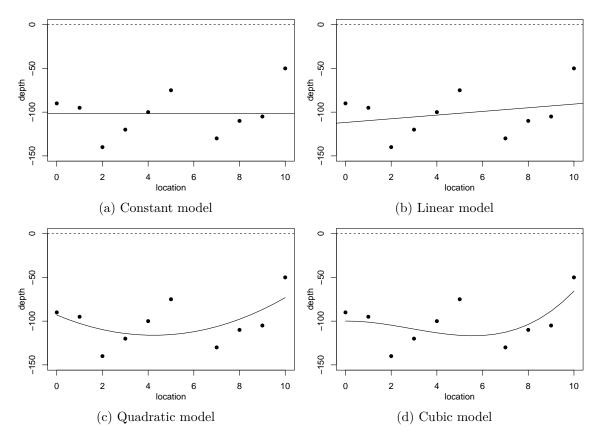


Figure 1.1: The coal-seam data superimposed with predictions from polynomial regression models.

Each of these models would predict a different value for the missing observation y_6 . We do not know the accuracy of the depth measurements, so in principle any of these curves could be correct. Clearly, the residual variance is largest for the constant-depth model in Figure 1.1a, and smallest for the cubic polynomial in Figure 1.1c – the residual sums of squares are: 6252.5, 5773.05, 4489.84, 4242.89. However, none of these models produces a convincingly good fit. Moreover, these models are not particularly believable, since we know that geological pressures exerted over very long periods of time cause the landscape and its underlying layers of rock to undulate and fracture. This suggests we need a different strategy.

Next, consider the simulated example in Figure 1.2. At first look we might be happy with the fitted curves in Figure 1.2a or Figure 1.2b. The data, however, are created with a change-point at x = 0.67 where the relationship changes from linear with slope 0.6 to a constant value of 0.75. This description is completely lost with these two models.

Figure 1.2c shows the result of fitting one linear function to the data below 0.67 and a second linear function above. Clearly, this fits well but it has assumed that the change-

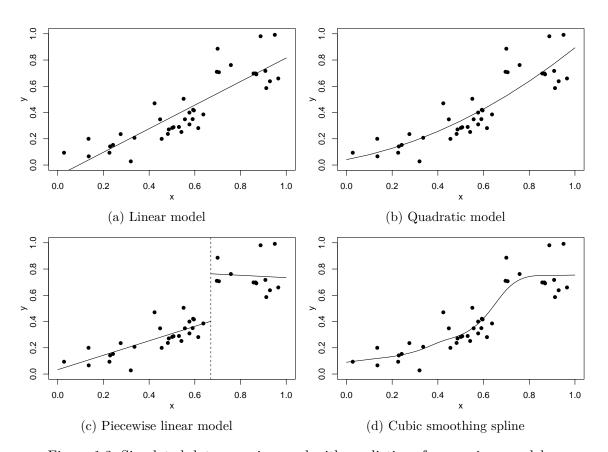


Figure 1.2: Simulated data superimposed with predictions from various models.

point location is known – which is unrealistic. Finally, Figure 1.2d shows a fitted *cubic* smoothing spline to the data – we will studies these models later. This shows an excellent fit and leads to appropriate conclusions. That is, the relationship is approximately linear for small values, then there is a rapid increase, and finally a near constant value for high values. Of course, this is not exactly as the true relationship with a discontinuity at x = 0.67 but it would definitely suggest something extreme occurs between about 0.6 to 0.7. Full details will follow later, but the cubic spline fits local cubic polynomials which are constrained to create a continuous curve.

Now returning to the coal seam data. Figure 1.3 shows the data again, superimposed with predictions from methods which are not constrained to produce such smooth curves.

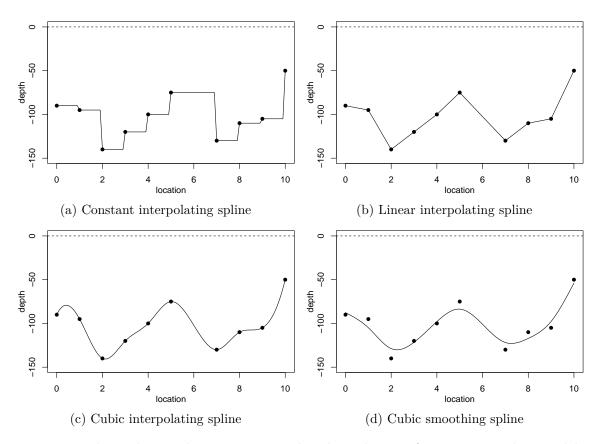


Figure 1.3: The coal-seam data superimposed with predictions from various spline models.

The simplest method, constant-spline interpolation, assumes that the dependent variable remains constant between successive observations, with the result shown in Figure 1.3a. However, the discontinuities in this model make it quite unreliable. A better method, whose results are shown in Figure 1.3b, is linear-spline interpolation, which fits a straight line between successive observations. Even so, this method produces discontinuities in the gradient at each data point. A better method still, shown in Figure 1.3c, is cubic spline interpolation, which fits a cubic polynomial between successive data points such that both the gradient and the curvature at each data point is continuous.

A feature of all these interpolation methods is that they fit the data exactly. Is this a good thing? The final method assumes that there may be some measurement error in the observations, which justifies fitting a smoother cubic spline than the cubic interpolating spline, but as we see in Figure 1.3d which does not reproduce the data points exactly. Is this a bad thing? We will see during this module how to construct and evaluate these curves. Here, the results are presented only for motivation.

Focus on polynomials quiz

Test your knowledge recall and comprehension to reinforce basic ideas about continuity and differentiability.

- 1. Which of the predicted curves in Figure 1.3 are continous?
- (A) None of the models
- (B) Model (a) only
- (C) Models (c) and (d) only
- (D) All models
- 2. Which of the predicted curves in Figure 1.3 have a continous first derivative?
- (A) None of the models
- (B) Model (b) only
- (C) Models (c) and (d) only
- (D) All models
- 3. Which of the predicted curves in Figure 1.3 have a continous second derivative?
- (A) None of the models
- (B) Model (b) only
- (C) Models (c) and (d) only
- (D) All models

- 4. Which of the predicted curves in Figure 1.3 have a continuous third derivative?
- (A) None of the models
- (B) Model (b) only
- (C) Models (c) and (d) only
- (D) All models
- 4. Which of the predicted curves in Figure 1.3 has the highest residual sum of squares?
- (A) None of the models
- (B) Model (a)
- (C) Model (b)
- (D) Model (c)
- (E) Model (d)
- (F) All model

1.3 General modelling approaches

We wish to model the dependence of a response variable y on an explanatory variable x, where y and x are both continuous. We observe y_i at each time x_i , for $i=1,\ldots,n$, where the observation locations are ordered: $x_1 < x_2 < \ldots < x_n$. We imagine that the y's are noisy versions of a smooth function of x, say f(x). That is,

$$y_i = f(x_i) + \epsilon_i, \tag{1.1}$$

where the $\{\epsilon_i\}$ are i.i.d:

$$\epsilon_i \sim \mathcal{N}(0, \sigma^2). \tag{1.2}$$

We suppose we do not know the correct form of function f: how can we estimate it?

It is useful to divide modelling approaches into two broad types: parametric and non-parametric.

Parametric models

By far the most common parametric model is simple linear regression, for example, $f(x) = \alpha + \beta x$, where parameters α and β are to be estimated. This is, of course, the simplest example of the polynomial model family, $f(x) = \alpha + \beta x + \gamma x^2 + \dots + \omega x^p$, where p is the *order* of the polynomial and where all of $\alpha, \beta, \gamma, \dots, \omega$ are to be estimated. This has as special cases: quadratic, cubic, quartic, and quintic polynomials models. Also common are exponential models, for example $f(x) = \alpha e^{-\beta x}$, where α, β are to be estimated – do not confuse this with the exponential probability density function.

Note that the polynomial models are all linear functions of the parameters. They are standard forms in regression modelling, as studied in MATH3714 (Linear regression and Robustness) and MATH3823 (Generalised linear models). The exponential model, however, is an example of a model which is non-linearly in the parameters – it is an example of a non-linear regression model.

Although very many parametric models exist, they are all somewhat inflexible in their description of f. They cannot accommodate arbitrary fluctuations in f(x) over x because they contain only a small number of parameters (degrees-of-freedom).

Non-parametric models

In such models, f is assumed to be a smooth function of x, but otherwise we do not know what f looks like. A smooth function f is such that $f(x_i)$ is close to $f(x_j)$ whenever x_i is close to x_j . To characterise and fit f we will use an approach based on splines. In practice, different approaches to characterizing and fitting smooth f lead to similar fits to the data. The spline approach fits neatly with normal and generalised linear models (NLMs and GLMs), but so do other approaches (for example, kernel smoothing and wavelets). Methods of fitting f based on kernel smoothing and the Nadaraya–Watson estimator are studied in the Level 5 component of MATH5714 (Linear regression, robustness and smoothing) where the choice of bandwidth in kernel methods is analogous to the choice of smoothing parameter value in spline smoothing.

Piecewise polynomial models

A common problem with low-order polynomials is that they can often fit well for part of the data but have unappealing features elsewhere. For example, although none of the models in Figure 1.1 fit the data at all well, we might imagine that three short linear segments might be a good fit to the coal-seam data. Also, the piecewise linear model was a good description of the data in Figure 1.2c. This suggests that local polynomial models might be useful. In some situation, for example when we know that the function f is continuous, jumps in the fitted model, as in Figure 1.2c, are unacceptable. Alternatively, we may require differentiability of f. Such technical issues lead to the use of splines, which is introduced in the next chapter.

1.4 Exercises

1.1 Consider the first three models fitted in Figure 1.1 and let the data be denoted, $\{(x_i, y_i) : i = 1, 2, ..., n\}$. These three models can be written

(a)
$$y = \alpha + \epsilon$$

$$(b) \quad y = \alpha + \beta x + \epsilon$$

(c)
$$y = \alpha + \beta x + \gamma x^2 + \epsilon$$

where ϵ represents normally distributed random error. Use the principle of least squares, or otherwise, to obtain estimates of the model parameters.

Click here to see hints.

For each, start by defining the residual sum of squares (RSS), $RSS = \sum (y_i - \hat{y}_i)^2$ where, in turn (a) $\hat{y}_i = \alpha$, (b) $\hat{y}_i = \alpha + \beta x_i$, (c) $\hat{y}_i = \alpha + \beta x_i + \gamma x_i^2$. Then, find he parameter values which minimise the RSS by (possibly partial) differentiation.

1.2 Discuss possible approaches to fitting an exponential model, $y = \alpha e^{\beta x}$, to data. Note that no actual algebraic derivation, nor numerical coded algorithm is expect.

Click here to see hints.

There is more than one approach. Can least squares be used? Could a simple transformation of the data and the fitted model make solving the problem easier? Is there an algebraic solution? Is there a purely numerical solution?

1.3 In Figure 1.2c, discuss how you might fit a two-part linear model for the case where the change-point is *unknown*. Note that no actual algebraic derivation, nor numerical coded algorithm is expect.

Click here to see hints.

With many similar problems, imaging breaking the problem down into steps. If you know the location of the change-point then what should you do? Can you then try different possible change-point locations?

1.4 Discuss the four fitted models in Figure 1.3. Can you give positive and negative properties of each model? Which do you think is best and which worst? Do you think which is best/worst, depends on the data? Justify your answers.

Click here to see hints.

Don't get too stuck on the data used here, but think of general issues: ease of use, reliability of the data, is there error with the data or is it very reliable? What if the response it discrete?

i Note

Exercise 1 Solutions can be found here.

2 Introducing Splines

Here is a short video [3 mins] to introduce the chapter.

2.1 Basic definitions

Let $t_1 < t_2 < ... < t_m$ be a fixed set of *sites* or *knots* which need not correspond to observation locations, as in Figure 2.1.

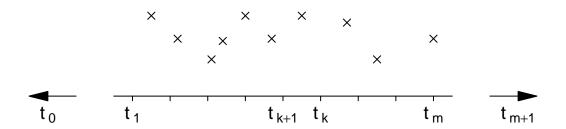


Figure 2.1: Diagram of knots and data points.

Note that we use the symbol t, rather than x, so that we do not confuse knots and observation locations.

A spline of order $p \geq 1$ is a piecewise-polynomial of order p which is (p-1) times differentiable at the knots. Thus there are coefficients $\{a_{k\ell},\ k=0,\ldots,m,\ \ell=0,\ldots,p\}$ such that

$$f(t) = \sum_{\ell=0}^{p} a_{k\ell} t^{\ell}, \quad \text{for } t_k \le t < t_{k+1},$$
 (2.1)

where we take $t_0 = -\infty$ and $t_{m+1} = +\infty$.

If we are using cubic polynomials, (p = 3), then f is given by the following equations:

$$f(t) = a_{00} + a_{01}t + a_{02}t^2 + a_{03}t^3, \quad t_0 \le t < t_1$$

to the left of the first knot,

$$f(t) = a_{10} + a_{11}t + a_{12}t^2 + a_{13}t^3, \quad t_1 \le t < t_2$$

between the first and second knots, and so on until

$$f(t) = a_{m0} + a_{m1}t + a_{m2}t^2 + a_{m3}t^3, \quad t_m \le t < t_{m+1}$$

to the right of the final knot. This is illustrated in Figure 2.2a with m=2.

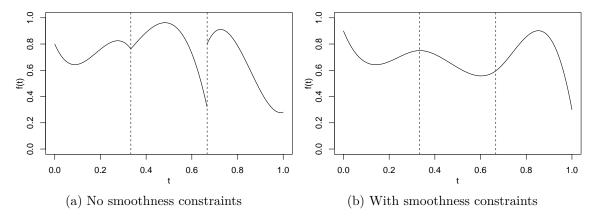


Figure 2.2: Piecewise-cubic functions in three intervals with knot positions indicated with vertical lines.

Focus on splines quiz

Test your knowledge recall and comprehension to reinforce basic ideas about splines.

- 1. Which of the following best describes the relationship between knots and data locations.
- (A) Knots are the response and data locations are the explanatory variable
- (B) There must be fewer knots than data locations
- (C) Knots and data locations are both marked on the x-axis
- (D) Knots and data points are exactly the same
- 2. How many polynomial equations are need to define a cubic spline with four knots?
- (A) 3
- (B) 4

- (C) 5
- (D) 12
- (E) None of the above
- 3. What is the highest power possible in a cubic spline?.
- (A) 0
- (B) 1
- (C) 2
- (D) 3
- (E) None of the above
- 4. How many times can a spline of order 5 be differentiated at the knots?
- (A) Cannot be differentiated
- (B) Twice differentiable
- (C) Four times differentiable
- (D) Infinitly differentiable
- 5. Which of the following is NOT a property of cubic splines?
- (A) Piecewise cubic polynomial
- (B) Twice differentiable
- (C) May contain change-points
- (D) Continuous at the knots

2.2 Imposing smoothness

Because of the use of polynomials, f is smooth *between* each successive pair of knots. At the knots, however, f might not be continuous and it might not be differentiable – in such cases we would say that the function is not smooth.

To ensure that f is also smooth at each of the knots, we impose smoothness constraints which control continuity of the function and its derivatives at the knots.

Let $f^{(\ell)}$ be the ℓ -th order derivative, with $f^{(0)} = f$ being the function itself, $f^{(1)} = f'$ is the first derivative and $f^{(2)} = f''$ the second derivative. Further, let $f^{(\ell)}(t - \epsilon)$ and $f^{(\ell)}(t + \epsilon)$, for $\epsilon \geq 0$, denote evaluation of the function or its derivative at points just below and just above t – we will be interested in their relative values as $\epsilon \to 0$.

To impose smoothness, we require that

$$\lim_{\epsilon \to 0} f^{(\ell)}(t_k - \epsilon) = \lim_{\epsilon \to 0} f^{(\ell)}(t_k + \epsilon), \tag{2.2} \label{eq:2.2}$$

for all $k=1,\ldots,m$ and for $\ell=0,\ldots,(p-1).$

In other words we say that f is smooth if the limits, from below and from above, of the function and its (p-1) derivatives exist and are equal.

The meaning of these smoothness constraints is illustrated in Figure 2.2. In Figure 2.2a, a piecewise cubic function with two knots has been plotted. The first derivative, f', is discontinuous at the first knot and the function itself, f, is discontinuous at the second knot. Figure 2.2b shows a similar shaped cubic spline with two knots. This time, the function f and its first two derivatives are continuous at both knots.

The smoothness conditions in Equation 2.2 induce constraints on the coefficients $\{a_{k\ell}\}$. A polynomial of order p has p+1 coefficients, and there are m+1 intervals when we have m knots. This leads to $(p+1)\times(m+1)$ coefficients but there are p constraints at each of the m knots. Thus the total degrees of freedom of the system is

$$df_{\text{spline}} = (p+1)(m+1) - pm = m+p+1. \tag{2.3}$$

These degrees of freedom provide the necessary flexibility in the spline.

Note that f is infinitely differentiable everywhere, except at the knots where it is p-1 times differentiable. In particular, for p=1, f is a linear spline comprising linear pieces constrained to be continuous at the knots, although the slope of f is discontinuous at the knots. Also, for p=3, f is a cubic spline comprising cubic polynomial pieces continuous at the knots; where the first and second derivatives of f are also continuous, but the third derivative is discontinuous at the knots.

Focus on smoothness quiz

Test your knowledge recall and comprehension to reinforce basic ideas about smoothness.

- 1. Which of the following best describes the motivation for using smooth fitted models?
- (A) Makes model fitting easier
- (B) Calculations are easy to do in R
- (C) It produces nice graphs
- (D) Reduces the effect of measurement error
- (E) None of the above
- 2. Which of the following best describes the motivation for using piecewise polynomial components?
- (A) Can involve change-points
- (B) Well understood and easy to use
- (C) Can model jumps well
- (D) They lead to normally distributed errors
- (E) None of the above
- 3. Is the following a true statement? "The higher the order of the polynomial components the smoother the spline' TRUE / FALSE
- 4. If a model fitted to a particular data set has zero degrees of freedom, then which of the following statements about the solution is most likely to be true?
- (A) Does not fit the data well
- (B) No solution
- (C) Unique solution
- (D) Multiple solutions

- 5. Which of the following best describes spline modeling?
- (A) The only non-parametric method available
- (B) It is a parametric approach
- (C) Requires high-level coding
- (D) A flexible non-parametric approach

2.3 Exercises

2.1 Why is it not sensible to define a smooth function made-up of constant components? Similarly, why is not sensible to create a differentiable function from linear splines?

Click here to see hints.

For each case, think about the number of parameters for each component and the implications of any constraints.

2.2 In the situation illustrated in Figure 2.2b, where p=3 and m=2, clearly identify the $(p+1)\times(m+1)=12$ model parameters and the pm=6 smoothness constraints in terms of the cubic polynomials and their derivatives.

Click here to see hints.

Define a cubic polynomial for each interval and consider continuity and differentiability.

2.3 Further consider the situation illustrated in Figure 2.2b. Suppose now that we require the splines to pass through specified coordinates $(t_1, f(t_1))$ and $(t_2, f(t_2))$. What is the degrees of freedom for this model? How many such cubic splines would satisfy these constraints? Discuss potential additional constraints which would lead to a unique fitted model. Do you think having a unique solution is a positive or negative property?

Click here to see hints.

Think about the degrees of freedom, that is the total number of parameters and the number of constraints, including forcing the spine to pass through two points. Think about the implications of having zero and non-zero degrees of freedom. There are very many (infinitely many?) potential additional constraints, but suggest one or two which sound a good idea.

2.4 For a general problem, what would be the effect of requiring additional constraints of the form of Equation 2.2 but with $\ell=p$? Would this lead to an acceptable fitted cubic spline model? Justify your answer.

Click here to see hints.

Think about the implication of this on the curvature of neighbouring components, and hence on overall curvature.

i Note

Exercise 2 Solutions can be found here.