Dissertation Second Draft

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Contents

1 Estimating Functions From Observed Data

1.1 How is the Observed Data Related To The Functional Data?

If a statistician wishes to work with functional data they must estimate these functions from their observed data. In order to do this a relationship must be established between the observed data and the functional data. Within FDA, the following relationship is assumed between the observed data and the function underlying it.

$$Y_i = f(t_i) + \epsilon_i \tag{1}$$

where Y_i is the observed value of the variable of interest at time t_i, $f(t_i)$ is the value of the function underlying the data evaluated at time t_i and $\epsilon_i \sim N(0, \sigma^2)$ is some random error in the observations from the function (σ is a constant).

Within this dissertation, it will be assumed that the error in each observation are independent and identically distributed normal random variables with constant variance. There is some literature which attempts to relax these assumptions about the errors in observation (Liu (2016)).

An example is given in Figure 1 of some data generated from an underlying function which fulfills the relationship given in Equation (1).

1.2 Introductory Example: UK Alcohol Mortality Rates

In order to easily introduce the stages of analysis and analytical techniques used in FDA I will use a simple example. In this example, I wish to use FDA to attempt to answer two questions. These questions are:

1. Is there a difference in the number of alcohol related deaths between countries in the United Kingdom (UK)?
2. Is there a correlation between the unemployment rate of a country and it's number of alcohol related deaths?

All of the data I will use to answer these questions is taken from the Office of National Statistics (ONS). The first dataset I will use (Breen and Butt (2022)) contains the "age-standardised alcohol-specific death rates per 100,000 people, in UK constituent countries, for deaths registered between 2001 and 2021". These "age-standardized death rates" are calculated according to the guidance laid out in European Standard Population

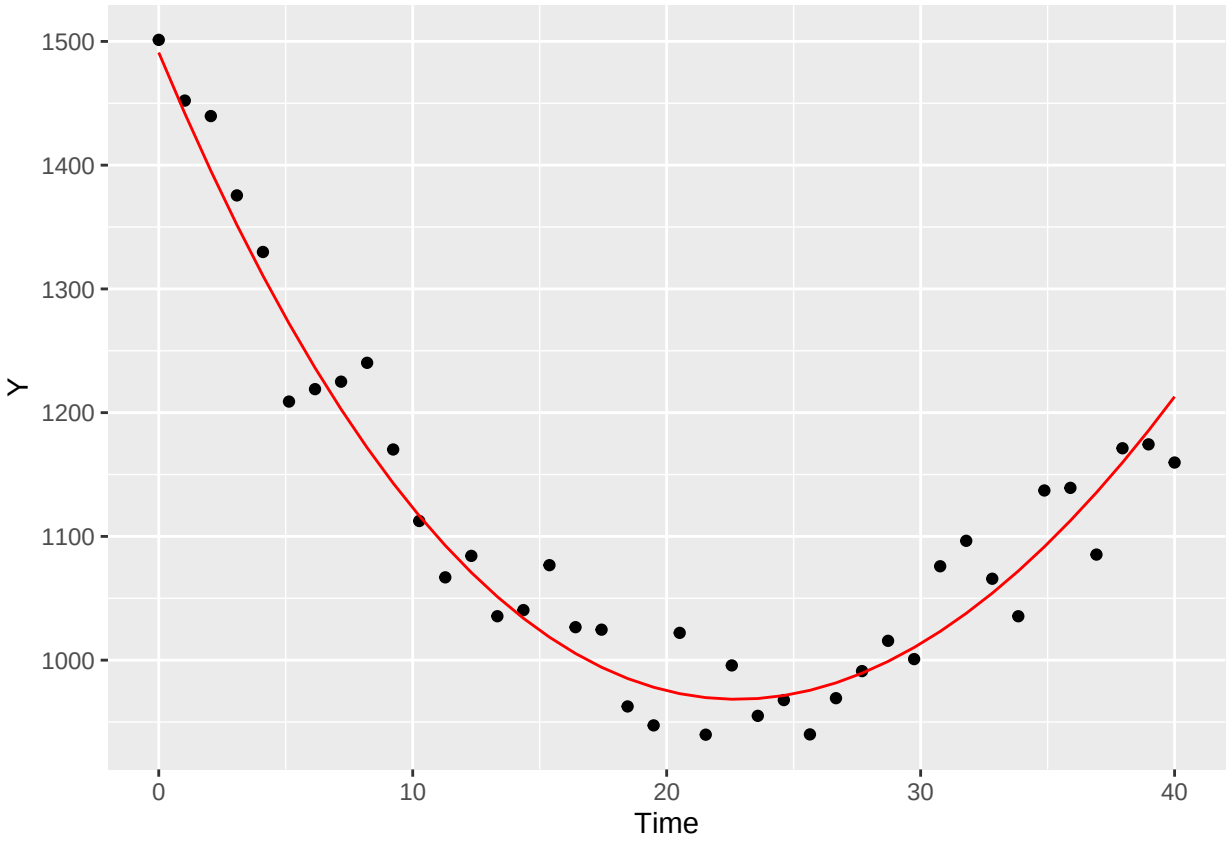


Figure 1: An Example of Data Simulated From a Function According to the Assumptions of FDA. The Red Line Shows the Function Y(t) which Generates the Data ($\sigma^2 = 30$)

2013 (ESP 2013) (Pace M (2013)) and adjust the death rates of a country to avoid over representing larger age categories within the population. An initial plot of this data can be seen in Figure 2 below.

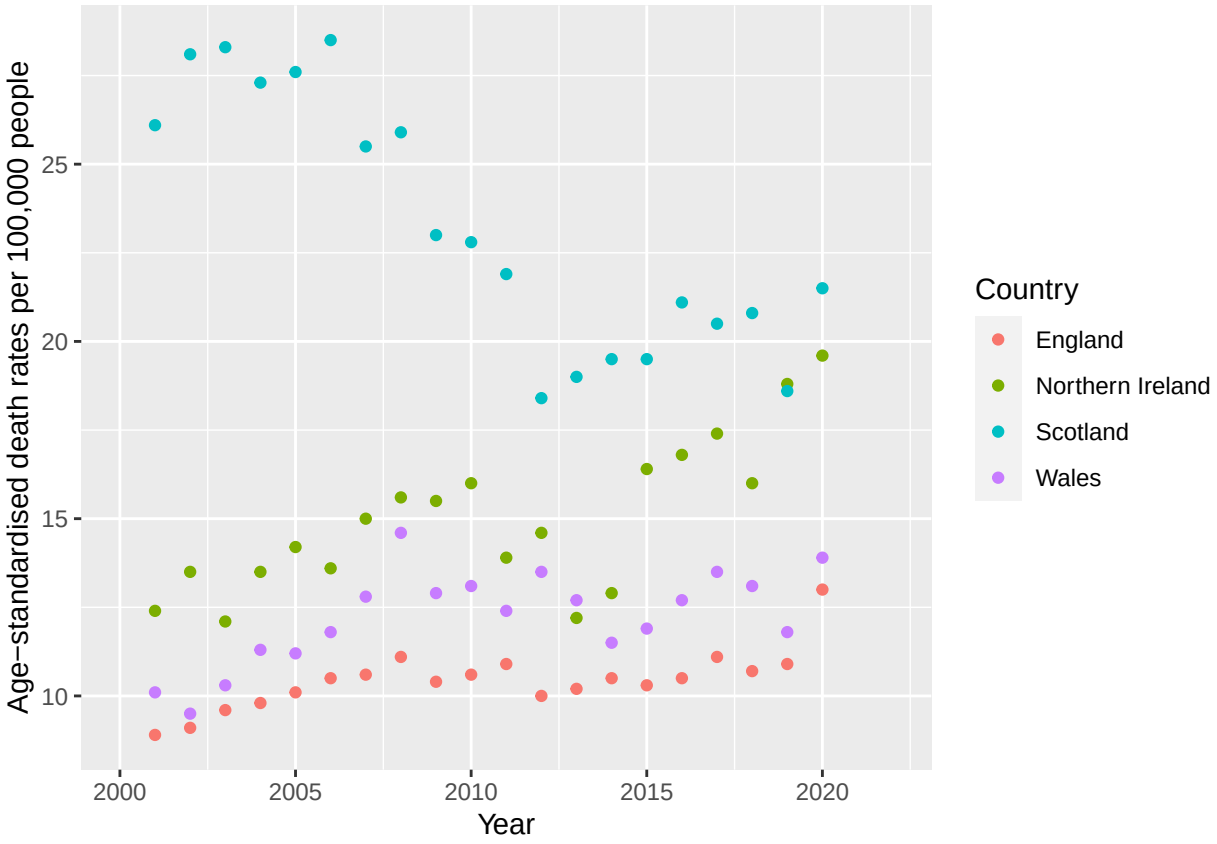


Figure 2: Age Standardised Alcohol-Specific Death Rates For Each Country within the UK from 2001 to 2022

The second dataset I will use is taken from the Labour Force Survey (LFS) ("Labour Market Overview, UK: February 2023" (2023)). This dataset gives the unemployment rate, as estimated using the methodologies laid out within the LFS, as the percentage of the population of a country which is unemployed. This dataset gives the unemployment rate for 1992 to 2022. I will only be using the data from the years 2001 to 2022 as that is the range of years that the alcohol related deaths data covers. An initial plot of the unemployment data can be seen in Figure 3 below.

In order to use FDA methods to analyse this data I have to find the functions which underlie the data as laid out in Equation (1). I will have to estimate a function which underlies the alcohol mortality rate and another function which underlies for the unemployment rate for each country and use these to answer the questions presented. These analytical form of these functions is not known in this example and, therefore, they must be estimated from the observed data. This estimation will be done using basis functions.

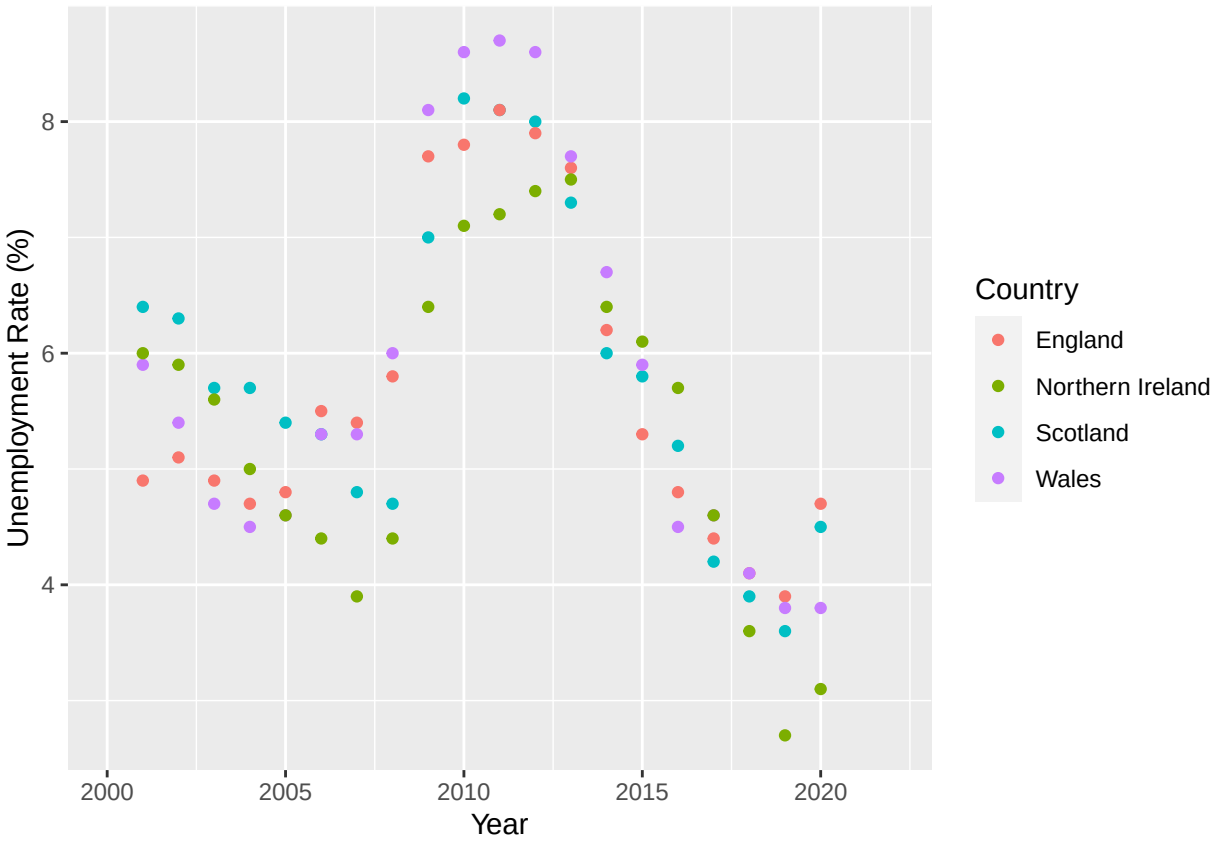


Figure 3: Unemployment Rates for Each Country in The UK From 2001 to 2022

1.3 Basis Functions

The functions which underlie the data we observe are not known when we receive our data. We must estimate them from our observed data. In order to estimate these functions basis functions must be used.

To understand what basis functions are let us first consider a set of three functions Ψ defined below.

$$\Psi = \{1, x, x^2\} \tag{2}$$

The span of these functions, that being the set of functions produced by taking all linear combinations of these 3 functions, is the set of all polynomials of degree 2 (or less) with coefficients in the real numbers, $\mathcal{P}_2(\mathbb{R})$. This implies that the set of functions Ψ is a basis of P_2. Each of the functions within Ψ is called a basis function.

We wish to find a basis which spans a set of functions that the functions we are trying to estimate are contained in. If we can find such a basis then we can estimate our functions by taking a general linear combination of the functions in this basis and estimating the coefficients which provide the best fit based on the observed data.

An arbitary function f can be estimated by a linear combination of a set of basis functions which form a basis Ω for the functional space F with $f \in F$ as shown below.

$$f(t) \approx \sum_{k=1}^{K} c_k \phi_k(t) = \boldsymbol{c'}\boldsymbol{\phi}(t) \tag{3}$$

c_k is the coefficient of the k_{th} basis function $\phi_k(t) \in \Omega$ and there are K functions in Ω. $\boldsymbol{\phi}(t)$ is a K-dimensional vector of all of the basis functions in Ω evaluated at time t and $\boldsymbol{c}$ is a K-dimensional vector of the coefficients of these basis functions. The estimation of the coefficients c_k in $\boldsymbol{c}$. This basis expansion of f is an estimation, not an equality, as the coefficients of the basis functions must be estimated through smoothing techniques (discussed in Smoothing Techniques section of this dissertation) and it is not possible to obtain the actual coefficients without knowledge of the analytical form of f.

There is an infinite number of bases which can be used to estimate our functions. Therefore, we must assume some things about our functions in order to narrow down the basis that we wish to use. There are a few standard sets of basis functions which can be used to estimate functions from data with various different properties. One such example is the Fourier basis, a set of basis functions, defined by their period T, which can be linearly combined to create any T periodic function. The functions which I am trying to estimate in

the alcohol mortality rates example appear to be non-periodic in nature, as shown by their being no obvious repeated patterns in the data over time, and so I must use a set of basis functions which can estimate non-periodic functions. There are several bases which can do this but I will be estimating my functions using a B-Spline basis.

1.4 B-Spline Basis Functions

A B-Spline basis is a set of piece-wise polynomial functions defined by their domain, $[a, b] \subset \mathbb{R}$, their knots/break points and their order/degree. The span of a set of degree n B-Spline basis functions with domain $[a, b]$ is the set of all spline functions of degree n (or less) with domain $[a, b]$. A spline function of degree n is a piecewise continuous curve made of polynomial segments all of degree n or less.

B-Spline basis functions can be linearly combined to estimate functions which are non-periodic in nature. To do this a particular set of B-Spline functions must be chosen to estimate the functions. This means choosing the domain, knots/break points and degree of the B-Spline basis functions to be used.

Choosing the domain of the basis functions is a relatively trivial task as it is often obvious from the data observed. Typically we do not want to define our functions to have a domain that is outside of that of the observed data as any values of the function estimated outside of the domain of the observed data will be based not on an inference but on an extrapolation from the data. Therefore, in almost all cases the domain of the B-Spline functions is chosen to be that of the observed data. In the case of the alcohol mortality rates example, the first year that the death rate is measured in is 2001 and the final year is 2020 so the domain of the B-Spline functions I will be using is $[2001, 2020]$.

Choosing the degree/order of our basis functions is a slightly more challenging task. The degree of a polynomial is the exponent of the highest order term in the polynomial e.g. if $f(x) = x^{24} + x^3 + 6$ then the degree of $f(x)$ is 24. The order of a polynomial is one more than the degree of the polynomial e.g. the order of defined $f(x)$ is $24+1 = 25$. The function we estimate from the observed data will never match the function that underlies the data exactly as we must estimate the coefficients of the basis functions using smoothing. We only need our function to be estimated well enough that it provides the information we need from it. For example, if we wish to use the functions 1st derivative we would need our estimate of the function to be smooth when differentiated once. Therefore, our choice of degree of the B-Spline functions is dependent on what we wish to do with them. It is good practice in these type of situations to fix the order of B-splines used to be two higher than than the highest order of derivative to be used in the analysis (Ramsay J. O. (2009)). In the alcohol mortality rates example, the derivatives of the functions do not need to be used to

answer either of the two questions posed. In the case where no derivatives are to be used often polynomial splines will not suffice in estimating the function and cubic splines should be used in this case, e.g. splines of order 4. I will, therefore, use order 4 basis splines.

The final thing to decide is where to place the knots/break points defining the splines on the domain $[a, b]$. The break points of a B-Spline basis are the points where each of the B-Spline functions in the basis meet. The knots are related to break points such that each break point has at least one knot situated at it. The number of knots placed at a break point indicates the number of derivatives of the function that should appear smooth across that break point with k knots at a point indicating the first $n - k - 1$ derivatives should be smooth. In all of the examples of FDA, I will share within this dissertation I will only place 1 knot at each break point as I will not be using the derivatives of functions. The choice of where break points go can be an incredibly simple task as the optimum break point placement is placing a break point on each point on the domain where there is an observation within the original data. In the alcohol mortality rates example, this is exactly where I will place my break points. However, this is often not computationally feasible. This is because the number of knots that basis is defined by also determines the number of basis functions within that basis. The relation between the two is given below.

$$number\ of\ basis\ functions\ =\ order\ +\ number\ of\ interior\ knots \tag{4}$$

If, for example, our original data consisted of 4000 data points and we placed a knot at each of them then we would have more than 4000 functions within our basis which would mean we would have to estimate more than 4000 coefficients, one for each these basis functions when estimating our function to fit to the data. The question of optimal knot placement for these types of situations will be revisited in the final example fo this dissertation.

Returning to my alcohol mortality rates example, I have chosen the domain, order and break point placements of the B-Spline basis I wish to use to estimate my functions for each country. I can now create this B-Spline basis in R. I will do this using the `create.bspline.basis` function within the `fda` package in R (Ramsay, Graves, and Hooker (2022)). To create a B-Spline basis of functions with domain $[2001, 2022]$, order 4 and a break point at each year I used the following function call.

I now have the basis I will be using to estimate my functions within the alcohol mortality rates example. Referring back to Equation (3), I have my basis functions but I am still yet to find the coefficients of the linear combination of these basis functions which provides the best estimate of the underlying functions. To estimate these coefficients a process called smoothing must be used.

1.5 Smoothing Techniques

1.5.1 What is Smoothing?

1.5.2 Smoothing using a Roughness Penalty

The generally preferred method of finding the coefficients for a functional data object is smoothing using a roughness penalty. This method of smoothing seeks to minimise the sum of squared errors of the fitted function while also penalising the roughness of the function.

Lets first consider the sum of squared errors (SSE) of a function estimated from observed data via smoothing. The SSE of a function gives a measure of the difference between the function and the observed data without regard to the direction of the difference. The SSE of a functional fit can be derived from Equation (1). This derivation is given below.

$$Y_i = f(t_i) + \epsilon_i \tag{5}$$

$$\Rightarrow \epsilon_i = Y_i - f(t_i) \tag{6}$$

$$SSE(f) = \sum_{j=1}^{n} [\epsilon_i]^2 \tag{7}$$

$$\Rightarrow SSE(f) = \sum_{j=1}^{n} [Y_j - f(t_j)]^2 \tag{8}$$

An SSE of 0 implies that the function passes through all of the observed data points. An example is given below in Figure 4 of a function with SSE 0. While an SSE of 0 can initially sound like the function fits perfectly to the data we must bear in mind that one of the main assumptions of FDA is that there is some observation error in the observed data points, as stated in Equation (1). This is why the function with SSE 0, given by the dashed line, in Figure 4 estimates the actual function, given by the red line, so badly.

We do not want our function to interpolate the observed data. We want to penalise the functions roughness so that it cannot have large changes in value over a small range of time in order to fit the observed data. The "roughness" of a function is not a clearly defined concept and is often situational. In this case, we define roughness to be synonymous with the wigglyness of the function e.g. how steep the slopes of the function are. The steepness of the slopes of a function can be examined by looking at derivatives of the function. Within smoothing, many different derivatives of the function can be examined but within this dissertation I will be using the second derivative of the function. The area under the squared second derivative of a function is a

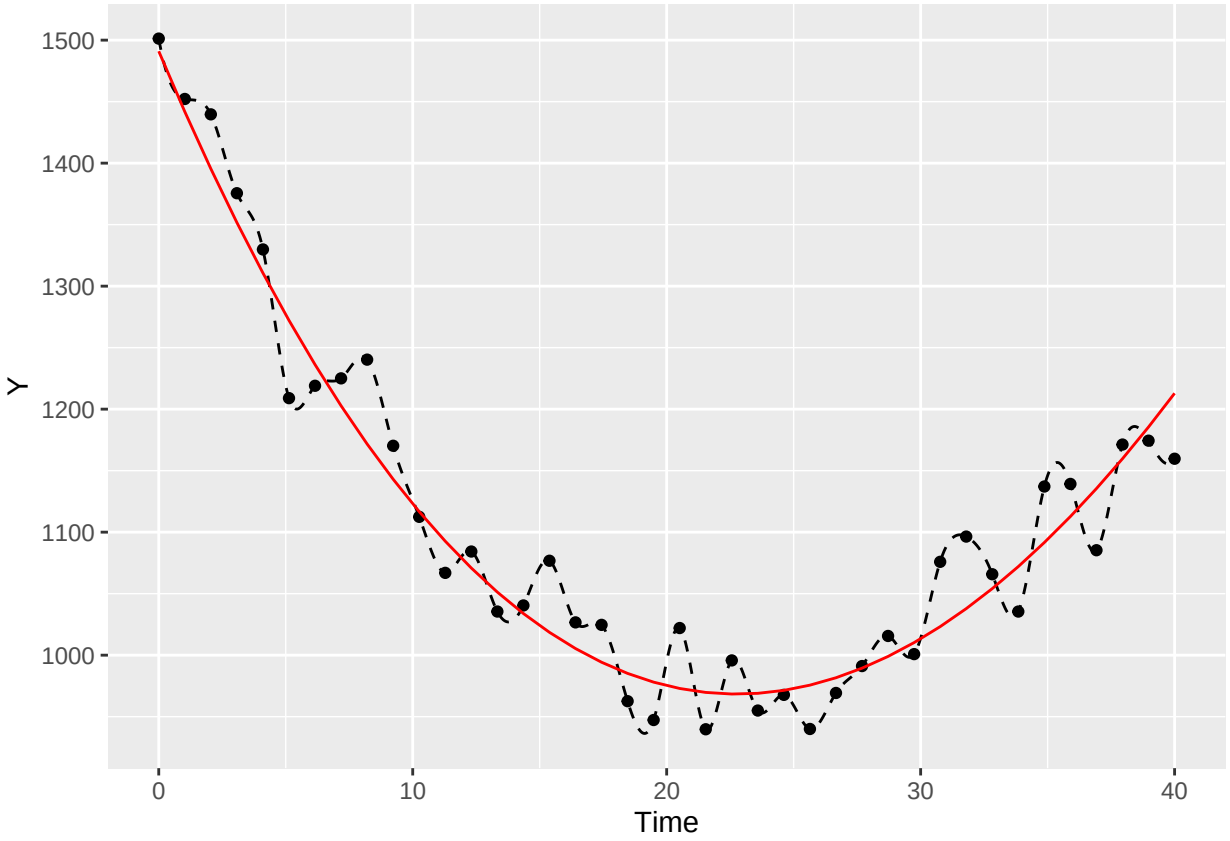
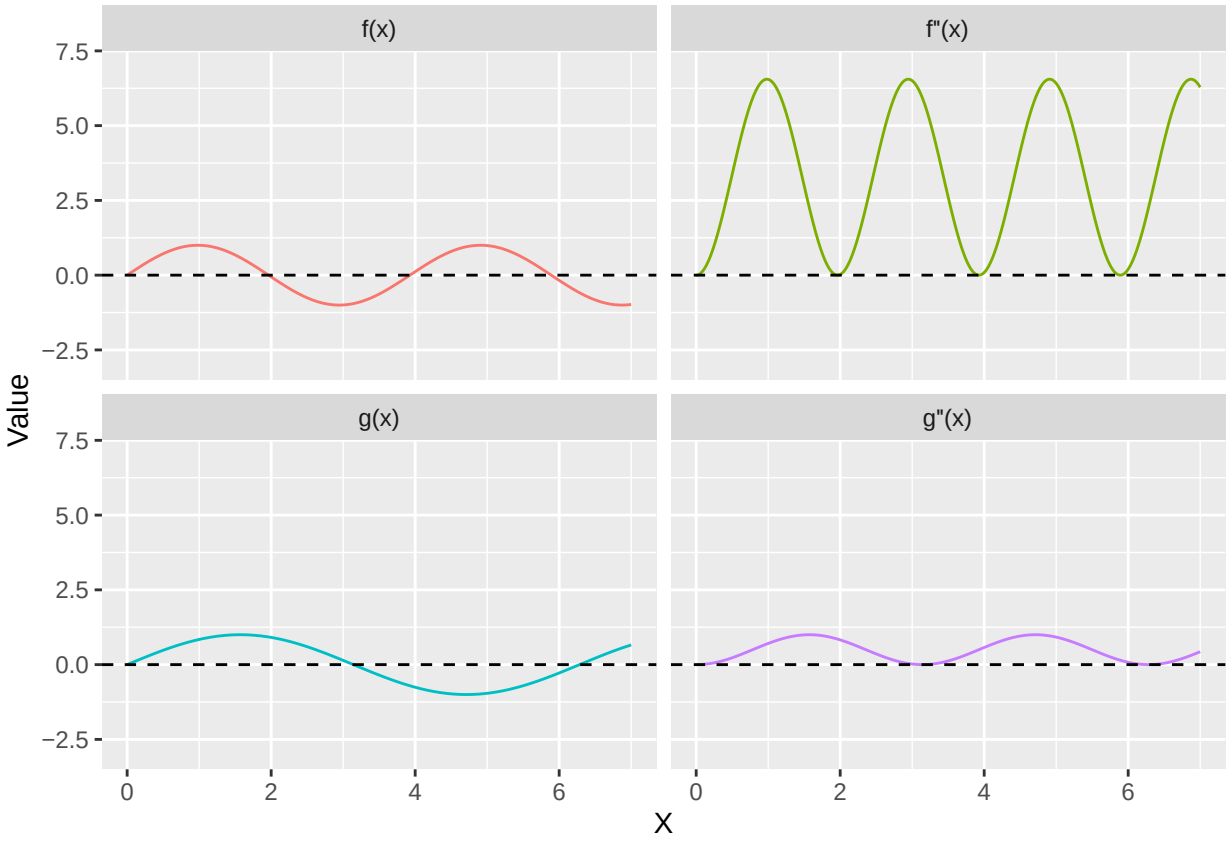


Figure 4: Estimate of Function with SSE=0 (Dashed Line) With True Function (Red Line) and the Data Used to Estimate It Overlayed

good measure of how rough a function is. A straight line would have a squared second derivative of 0 for all values of x. Therefore, the area under the squared second derivative is effectively a measure of how far away a function is from being a straight line. Shown below are two functions $f(x)$ and $g(x)$, their second derivatives and their second derivatives squared. $f(x)$ is clearly "rougher" than $g(x)$. We can see that the area under $(f''(x))^2$ is larger than that of $(g''(x))^2$.



We to find a function which we can minimise to find out coefficients which combines the integral of the squared second derivative, known as the roughness penalty of the smoothing process, and the SSE of the function. We minimise the objective function shown below. It is a linear combination of the SSE and the roughness penalty. The function we are trying to find is also rewritten using it's basis expansion as a reminder that we are trying to find the coefficients which minimise this objective function, not any functional components as these are fixed.

$$F(f) = \sum_j [Y_j - f(t_j)]^2 + \lambda \int_{t_0}^{t_1} [f''(t)]^2 dt \tag{9}$$

$$\Rightarrow F(\boldsymbol{c}) = \sum_j [Y_j - \boldsymbol{c'}\boldsymbol{\phi}(t_j)]^2 + \lambda \boldsymbol{c'} [\int_{t_0}^{t_1} \boldsymbol{\phi}''(t)\boldsymbol{\phi}''(t)^T dt]\boldsymbol{c} \tag{10}$$

The parameter λ featured in Equation (10) is known as the smoothing parameter of the objective function F. λ can be thought of as determining how smooth we want out function to be. If $\lambda = 0$ then the objective function becomes the SSE, therefore, providing no smoothing. As $\lambda \to \infty$ the roughness penalty approaches 0 implying that a straight line is fit to the data.

The ideal λ, e.g. the ideal weighting of the roughness penalty and the SSE, is found using the generalized cross-validation (GCV) criteria as developed by Craven P. and G. Wahba (Craven and Wahba (1978)). This criteria is given below for an arbitrary function f and measures how well a function fits the observed data.

$$GCV(f) = \left(\frac{n}{n - df(f)}\right)\left(\frac{SSE(f)}{n - df(f)}\right) \tag{11}$$

The degrees of freedom of f are as defined in page 65 of Ramsay J. O. (2009).

In order to find the value of the smoothing parameter which minimises this equation many functions are fit, each minimising the objective function with a different smoothing parameter and their GCVs are compared to see which value of the smoothing parameter provides the function with the best fit to the data. The value of the smoothing parameter that gives the lowest GCV is the most preferable.

Now that we know how to find the smoothing parameter we are able to construct our objective function which we will minimise to find our function which best estimates the function which underlies the data.

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