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Splines: A theoretical and computational study

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Abstract

The purpose of this paper is to fit a curve $f(x)$ to a set of points $(x_1, y_1), \ldots, (x_n, y_n)$. We want this function to be such that the error $f(x_i) - y_i,\ i = 1, \ldots, n$ is small, but at the same time we want $f(x)$ to be reasonably smooth. We will do this by considering smoothing splines, which are minimizers of a particular functional. An interpolation coefficient denoted λ, that is included within the functional, captures the trade-off between smoothness and interpolation (the deviation of $f(x)$ from the points). We will use simple theory of optimization in vector spaces to derive this function $f(x)$. We will also show an example on how the behaviour of $f(x)$ will vary depending on the choice of λ.

Contents

1 Introduction

The purpose of this paper is to fit a curve $f(x)$, to some points $(x_1, \alpha_1), ..., (x_n, \alpha_n)$, that can for example be interpreted as experimental measurements, where x_i are points in an interval (a, b) with $x_1 < x_2 < \ldots < x_n$, and α_i are some real numbers. We want the function $f(x)$ to be such that it is relatively smooth and the error $f(x_i) - \alpha_i$ is small in some sense. One way to fit a curve to some points is to consider smoothing splines, which are minimizers of the functional:

$$\mathcal{E}(f) = \int_a^b (f''(x))^2 dx + \lambda \sum_{i=1}^{n} (f(x_i) - \alpha_i)^2, \quad \lambda > 0$$

This is a problem of optimization in function spaces. All definitions and theorems that will be used are stated in section 2. We have chosen to omit the proof of these theorems since they can be quite complicated and will not really increase one's understanding in the actual matter. In section 3 we apply these theorems to the problem. In section 4 we derive certain properties of the minimizer using elementary calculus and basic linear algebra. In the references we have given two examples of books concerning these matters.

In the equation above you can interpret λ as a parameter that captures the trade-off between the smoothness and interpolation (deviation of $f(x)$ from the points $(x_1, \alpha_1), \ldots, (x_n, \alpha_n)$). We will refer to λ as the interpolation coefficient. The two criteria of smoothness and interpolation don't walk hand in hand. A smoother curve will be flatter, thus the most deviant measurement values will play less part when "constructing" the function. The higher value on λ the more the function will focus on going through the points $(x_1, \alpha_1), ..., (x_n, \alpha_n)$. You can see that by looking at the second part of the functional which will be large if you don't make the gap between $f(x_i)$ and α_i small. In section 5 we will consider an example on the impact of choosing different values of λ.

Another application besides fitting a curve to experimental measurements is when you have a function, say $g(x)$ whose function values are really hard to compute. In this case you could settle for calculating the function values of $g(x)$ in some points and then use smoothing splines to approximate this function. If these smoothing splines approximates the complicated function well, then they could be used to calculate other values of $g(x)$ in a much simpler way. In this case you obviously would choose a large interpolation coefficient λ.

2 Necessary definitions and theorems

In this section we will define all notions as well as state all theorems needed in order to solve the problem of minimizing $\mathcal{E}(f)$. All definitions and theorems that we have used, as well as the proofs of the theorems can be found in [1] in the references. We will hovewer state the necessary theorems and definitions here as well. First, have a look at the following theorem:

Theorem 1. *Let X be a normed space and $I : X \longrightarrow \mathbb{R}$ differentiable. Suppose that I is convex. If $x_0 \in X$ is such that $(DI)(x_0) = 0$, then I has a global minimum at x_0. Moreover, if I is strictly convex, the global minimum is unique.*

This is, as you may have noticed, a generalization of the well-known theorem concerning optimization of functions from $\mathbb{R}$ to $\mathbb{R}$. This powerful theorem is pretty much everything we need in order to solve the problem of minimizing $\mathcal{E}(f)$. Before applying this theorem to our problem, let us first have a closer look at all the notions involved so that we fully understand their meaning. In the text below, we will give the definition of normed spaces; continuity, convexity and differentiation among functions from $X \longrightarrow Y$, where X and Y are vector spaces.

Definition 1. *A vector space over $\mathbb{R}$ is a set X together with two functions: $+ : X \times X \longrightarrow X$, called vector addition and $\cdot : \mathbb{R} \times X \longrightarrow X$, called scalar multiplication that satisfy the following:*

V1 For all $x_1, x_2, x_3 \in X, x_1 + (x_2 + x_3) = (x_1 + x_2) + x_3$

V2 There exists an element, denoted by 0 (called the zero vector) such that for all $x \in X, \quad x + 0 = 0 + x = x$

V3 For every $x \in X$, there exists an element, denoted by $-x$, such that $x + (-x) = (-x) + x = 0$

V4 For all $x_1, x_2 \in X$, $x_1 + x_2 = x_2 + x_1$

V5 For all $x \in X$, $1 \cdot x = x$

V6 For all $x \in X$, and all $\alpha, \beta \in \mathbb{R}$, $\alpha \cdot (\beta \cdot x) = (\alpha\beta) \cdot x$

V7 For all $x \in X$, and all $\alpha, \beta \in \mathbb{R}$, $(\alpha + \beta) \cdot x = \alpha \cdot x + \beta \cdot x$

V8 For all $x_1, x_2 \in X$, and all $\alpha \in \mathbb{R}$, $\alpha \cdot (x_1 + x_2) = \alpha \cdot x_1 + \alpha \cdot x_2$

Definition 2. *Let X be a vector space over $\mathbb{R}$. A norm on X is a function $\| \cdot \| : X \longrightarrow [0, +\infty)$ such that:*

N1 (Positive definiteness) For all $x \in X, \|x\| \geq 0$. If $x \in X$, then $\|x\| = 0$ iff $x = 0$

N2 For all $\alpha \in \mathbb{R}$ and for all $x \in X$ $\|\alpha x\| = |\alpha|\|x\|$

N3 (Triangle inequality) For all $x, y \in X$, $\|x + y\| \leq \|x\| + \|y\|$.

A vector space equipped with a norm is called a normed space. The concept of a normed space is an important one. Let us explain what a normed space is in a more intuitive way so that one can get a better picture of what it actually is. Consider for example two elements x and y in some vector space X. A norm $\|x - y\|$ is a measure of distance between these two elements, where the elements can be for example vectors or functions. Obviously $\|x\| = \|x - 0\|$, is a measure of the distance between x and the 0-element. What we mean with distance between two functions is not very straightforward. You can measure a distance between two functions in many different ways (use different kinds of norms), depending on what you are interested in looking for. But you must then keep in mind that a normed space consisting of a vector space V with a norm n_1 is different from the normed space consisting of the same vector space V with another norm n_2. We look at some examples to clear things up even more.

In $\mathbb{R}$ which is a one dimensional space, the only norm is the absolute value $|x_2 - x_1| = \sqrt{(x_2 - x_1)^2}$, where $x_1, x_2 \in \mathbb{R}$. This is the distance between the two numbers x_2 and x_1. In $\mathbb{R}^2$ where we have a two dimensional vector space with real valued vectors, for any two vectors $(x_1, y_1), (x_2, y_2) \in \mathbb{R}^2$ the standard norm is defined as $\|(x_1, y_1) - (x_2, y_2)\| = \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2}$, which is a measure of the distance between two vectors in a two dimensional vector space. In the same way the standard norm is defined in higher dimensional vectorspaces over $\mathbb{R}$.

But it gets more complicated when we want to measure the distance between functions. For example when we deal with a function $x(t) \in C[0,1]$ where $C[0,1]$ is the set of all continuous functions on the interval $[0,1]$ you can define the norm$\|x\|_\infty$ as $\max|x(t)|$ for $t \in [0,1]$ if you are interested in how much the function is diverging from the t-axis on the interval [0,1] at most. So if your function is $x(t) = e^t$, the norm $\|x\|_\infty$ will be e since e^t assumes the greatest value at $t = 1$.

Let us now give the definition of what is meant by a continuous function between normed spaces as well as a continuous linear transformation.

Definition 3. *Let X and Y be normed spaces over $\mathbb{R}$ and $x_0 \in X$. A map f: $X \longrightarrow Y$ is said to be continuous at x_0 if*
$\forall \epsilon > 0$, $\exists \delta > 0$ *such that for all $x \in X$ satisfying $\|x - x_0\| < \delta$, one has $\|f(x) - f(x_0)\| < \epsilon$.*
The map f: $X \longrightarrow Y$ is called continuous if for all $x_0 \in X$, f is continuous at x_0.

Definition 4. *Let X,Y be vector spaces over $\mathbb{R}$. A map T:$X \longrightarrow Y$ is called a linear transformation if it satisfies the following conditions:*

L1. For all x_1,$x_2 \in X$, $T(x_1 + x_2) = T(x_1) + T(x_2)$.

L2. For all $x \in X$ and all $\alpha \in \mathbb{R}$, $T(\alpha \cdot x) = \alpha \cdot T(x)$.

A map that is both continuous and linear is called a continuous linear transformation.

The definition of a continuous function is rather abstract and not very efficient to use when investigating whether a function is continuous or not. The following theorem will however give us an easy method to use when checking for continuity.

Theorem 2. *Let X and Y be normed spaces over $\mathbb{R}$. Let T:$X \longrightarrow Y$ be a linear transformation. Then the following properties of T are equivalent:*
1. T is continuous.
2. T is continuous at 0.
3. There exists a number M such that for all $x \in X$, $\|Tx\| \leq M\|x\|$.

Now we have everything needed to be able to define what is meant by the derivative of a function between two normed spaces.

Definition 5. *Let X and Y be normed spaces. Let F:$X \longrightarrow Y$ be a map and $x_0 \in X$, then F is said to be differentiable at x_0 if there exists a continuous linear transformation L such that:*
$\forall \epsilon > 0$, $\exists \delta > 0$ *such that* $\forall x \in X \setminus \{x_0\}$ *satisfying* $\| x - x_0 \| < \delta$,

$$\frac{\|F(x) - F(x_0) - L(x - x_0)\|}{\|x - x_0\|} < \epsilon.$$

The operator L is called the derivative of F at x_0. If F is differentiable at every point $x \in X$, then it is simply said to be differentiable.

Now all that is left is to define what is meant by a convex function, then we have everything needed to be able to use Theorem 1.

Definition 6. *Let X be a normed space. A function I: $X \longrightarrow \mathbb{R}$ is said to be convex if for all x_1, $x_2 \in X$ and $\alpha \in [0,1]$,*

$$I(\alpha x_1 + (1-\alpha)x_2) \leq \alpha I(x_1) + (1-\alpha)I(x_2)$$

Moreover, a function is said to be strictly convex if for all x_1, $x_2 \in X$ such that $x_1 \neq x_2$ and $\alpha \in (0,1)$,

$$I(\alpha x_1 + (1-\alpha)x_2) < \alpha I(x_1) + (1-\alpha)I(x_2)$$

Now we are ready to apply Theorem 1 on $\mathcal{E}(f)$ and start solving the problem of finding a minimizer.

3 Calculating the derivative and checking for convexity

3.1 Choosing a proper norm for f

Before we start the calculations of our derivative we need to decide what normed space to use. We know that $\mathcal{E}$ is a functional defined from $C^2[a,b] \longrightarrow \mathbb{R}$. Let $x \in C^2[a,b]$, we define the norm of $x \in C^2[a,b]$ as the following one:

$$\begin{aligned} \|x\| &:= \max_{t\in[a,b]} |x(t)| + \max_{t\in[a,b]} |\frac{dx}{dt}(t)| + \max_{t\in[a,b]} |\frac{d^2x}{dt^2}(t)| \\ &= \|x\|_\infty + \|x'\|_\infty + \|x''\|_\infty \end{aligned}$$

Let us quickly check that this choice of norm is valid. Recall from the definition of the norm the following three conditions:

N1.

This condition holds since

$$\|x\| = \underbrace{\max_{t\in[a,b]} |x(t)|}_{\geq 0} + \underbrace{\max_{t\in[a,b]} |\frac{dx}{dt}(t)|}_{\geq 0} + \underbrace{\max_{t\in[a,b]} |\frac{d^2x}{dt^2}(t)|}_{\geq 0} \geq 0$$

$$\|x\| = 0 \Longleftrightarrow \max_{t\in[a,b]} |x(t)| + \max_{t\in[a,b]} |\frac{dx}{dt}(t)| + \max_{t\in[a,b]} |\frac{d^2x}{dt^2}(t)| = 0 \Longleftrightarrow x(t) = 0$$

since $|x(t)|, |\frac{dx}{dt}(t)|$ and $|\frac{d^2x}{dt^2}(t)| \geq 0$ on the interval $[a,b]$

N2.

$$\begin{aligned} \|\alpha x\| &= \|\alpha x\|_\infty + \|\alpha x'\|_\infty + \|\alpha x''\|_\infty \\ &= |\alpha|\|x\|_\infty + |\alpha|\|x'\|_\infty + |\alpha|\|x''\|_\infty \\ &= |\alpha|(\|x\|_\infty + \|x'\|_\infty + \|x''\|_\infty) \\ &= |\alpha|\|x\| \end{aligned}$$

N3.

$$\begin{aligned}\|x+y\| &= \|x+y\|_\infty + \|x'+y'\|_\infty + \|x''+y''\|_\infty \\ &\leq \|x\|_\infty + \|y\|_\infty + \|x'\|_\infty + \|y'\|_\infty + \|x''\|_\infty + \|y''\|_\infty \\ &= \|x\| + \|y\|\end{aligned}$$

Thus our choice of norm is valid. Now we may go on and calculate the derivative of $\mathcal{E}(f)$.

3.2 Calculating the derivative of $\mathcal{E}(f)$

We want to differentiate the functional

$$\mathcal{E}(f) = \int_a^b (f''(x))^2 dx + \lambda \sum_{i=1}^{n} (f(x_i) - \alpha_i)^2$$

with respect to f, where f is a function of a variable x. First of all, let us split this expression into two parts which will be treated separately. This will give us a better overview of the calculations. Let

$$\mathcal{E}_1(f) = \int_a^b (f''(x))^2 dx$$

$$\mathcal{E}_2(f) = \lambda \sum_{i=1}^{n} (f(x_i) - \alpha_i)^2$$

After we have differentiated the functions $\mathcal{E}_1(f)$ and $\mathcal{E}_2(f)$ respectively, we simply use the summation rule for derivatives to obtain the derivative of $\mathcal{E}(f)$.

3.2.1 Calculating the derivative of $\mathcal{E}_1$

Calculating the derivative of a function of the type we are considering is far more complicated than an ordinary function from $\mathbb{R} \longrightarrow \mathbb{R}$. It is not very clear from the definition of the derivative how one proceeds in order to calculate it. We will give a brief explanation to every step in the calculations to make things more clear.

First, recall the definition of the derivative. This basically means that for each $\epsilon > 0$ we should be able to produce a δ such that if f satisfies $\|f - f_0\| < \delta$, then

$$\frac{\|\mathcal{E}_1(f) - \mathcal{E}_1(f_0) - L_1(f - f_0)\|}{\|f - f_0\|} < \epsilon$$

Thus our L_1 must be such that the numerator of the above expression must be small in some sense compared to the denominator. Another way of putting it is to let

$$\begin{aligned}\mathcal{E}_1(f) - \mathcal{E}_1(f_0) - L_1(f - f_0) = \mathit{error} \Longleftrightarrow \\ \mathcal{E}_1(f) - \mathcal{E}_1(f_0) = L_1(f - f_0) + \mathit{error}\end{aligned} \tag{1}$$

where the *error* is some small bounded term that will be small enough for the derivative expression to hold. Our goal is to express L_1 as a function of $f - f_0$ by studying the left hand side of (1) and then simply insert this L_1 into to derivative expression and see if it holds up. Let us now have a closer look at the left hand side of (1):

$$\begin{aligned}
\mathcal{E}_1(f) - \mathcal{E}_1(f_0) &= \int_a^b (f''(x))^2 dx - \int_a^b (f_0''(x))^2 dx \\
&= \int_a^b ((f''(x))^2 - (f_0''(x))^2) dx \\
&= \int_a^b (f''(x) - f_0''(x))(f''(x) + f_0''(x)) dx \\
&= \int_a^b (f - f_0)''(x)(f + f_0)''(x) dx.
\end{aligned}$$

We now have one factor that involves $f - f_0$ which is what we wanted. The other factor however, involves $f + f_0$ which is not what we wanted. Thus by letting $f \longrightarrow f_0$ we get:

$$\mathcal{E}_1(f) - \mathcal{E}_1(f_0) \approx \int_a^b (f - f_0)''(x) \cdot 2f_0''(x) dx = L_1(f - f_0)$$

We now have a transformation L_1 which is our candidate for the derivative. Notice that we have not yet in any way shown that this actually is the derivative, so let us do that now. The first step is to check whether L_1 is linear or not. It will be easier to follow these calculations if we express L_1 as a function of h, rather than $f - f_0$:

$$L_1(h) = \int_a^b h''(x) \cdot 2f_0''(x) dx.$$

Recall from the previous chapter that the following conditions must be satisfied in order for L_1 to be linear:

L1.

$$\begin{aligned}
L_1(h_1 + h_2) &= \int_a^b (h_1 + h_2)''(x) \cdot 2f_0''(x) dx \\
&= \int_a^b (h_1''(x) \cdot 2f_0''(x) + h_2''(x) \cdot 2f_0''(x)) dx \\
&= \int_a^b h_1''(x) \cdot 2f_0''(x) dx + \int_a^b h_2''(x) \cdot 2f_0''(x) dx \\
&= L_1(h_1) + L_1(h_2)
\end{aligned}$$

L2.

$$\begin{aligned}
L_1(\alpha h) &= \int_a^b (\alpha h)''(x) \cdot 2f_0''(x) dx \\
&= \int_a^b \alpha h''(x) \cdot 2f_0''(x) dx \\
&= \alpha \int_a^b h''(x) \cdot 2f_0''(x) dx \\
&= \alpha L_1(h)
\end{aligned}$$

We see that both L1 and L2 are satisfied, thus L_1 is a linear transformation.

Next we check whether L_1 is a continuous transformation. Since L_1 is a linear transformation we may use Theorem 2 to show that it is continuous:

$$\begin{aligned}
|L_1 h| &= |\int_a^b h''(x) \cdot 2f_0''(x)dx| \\
&\leq \int_a^b |h''(x)| \cdot |2f_0''(x)|dx \\
&\leq \int_a^b \|h\| \cdot |2f_0''(x)|dx \\
&= \|h\| \underbrace{\int_a^b |2f_0''(x)|dx}_{=M}
\end{aligned}$$

Notice that f_0 is some fixed function, thus $\int_a^b |2f_0''(x)|dx$ is some fixed number. By letting M be equal to this number, all conditions for Theorem 2 are satisfied, thus L_1 is a continuous transformation.

We have shown that L_1 is indeed a continuous linear transformation. Now we need to insert this L_1 into the definition of the derivative and see if it satisfies all conditions required.

First, let us approximate the numerator in the definition of the derivative

$$\begin{aligned}
|\mathcal{E}_1(f) - \mathcal{E}_1(f_0) - L_1(f - f_0)| &= |\int_a^b (f''(x))^2 dx - \int_a^b (f_0''(x))^2 dx - \int_a^b (f - f_0)''(x) \cdot 2f_0''(x)dx| \\
&= |\int_a^b ((f''(x))^2 - (f_0''(x))^2 - (f - f_0)''(x) \cdot 2f_0''(x))dx| \\
&= |\int_a^b (f''(x) - f_0''(x))(f''(x) + f_0''(x)) - (f - f_0)''(x) \cdot 2f_0''(x))dx| \\
&= |\int_a^b (f - f_0)''(x)(f''(x) + f_0''(x) - 2f_0''(x))dx| \\
&= |\int_a^b ((f - f_0)''(x))^2 dx| \\
&= \int_a^b |(f - f_0)''(x)|^2 dx \\
&\leq \int_a^b \|f - f_0\|^2 dx \\
&= \|f - f_0\|^2 (b - a)
\end{aligned}$$

By inserting the calculations from above into the definition of the derivative we get the following expression:

$$\frac{|\mathcal{E}_1(f) - \mathcal{E}_1(f_0) - L(f - f_0)|}{\|f - f_0\|} \leq \frac{\|f - f_0\|^2 (b - a)}{\|f - f_0\|} = \|f - f_0\|(b - a) < \delta(b - a)$$

The last inequality follows from the fact that $\|f - f_o\| < \delta$. By choosing $\delta = \frac{\epsilon}{(b-a)}$ we see that our L_1 is indeed the derivative of $\mathcal{E}_1$ at f_0.

3.2.2 Calculating the derivative of $\mathcal{E}_2$

Let us now move on with $\mathcal{E}_2$ and proceed in the same way as we did with $\mathcal{E}_1$.
We start by looking at $\mathcal{E}_2(f) - \mathcal{E}_2(f_0)$ to see if we can conclude what the derivative of $\mathcal{E}_2$ ought to be.

$$\begin{aligned}
\mathcal{E}_2(f) - \mathcal{E}_2(f_0) &= \lambda \sum_{i=1}^{n} (f(x_i) - \alpha_i)^2 - \lambda \sum_{i=1}^{n} (f_0(x_i) - \alpha_i)^2 \\
&= \lambda \sum_{i=1}^{n} \big((f(x_i))^2 - 2f(x_i)\alpha_i + (\alpha_i)^2\big) - \lambda \sum_{i=1}^{n} \big((f_0(x_i))^2 - 2f_0(x_i)\alpha_i + (\alpha_i)^2\big) \\
&= \lambda \sum_{i=1}^{n} \big((f(x_i))^2 - 2f(x_i)\alpha_i + (\alpha_i)^2 - ((f_0(x_i))^2 - 2f_0(x_i)\alpha_i + (\alpha_i)^2)\big) \\
&= \lambda \sum_{i=1}^{n} \big((f(x_i))^2 - 2f(x_i)\alpha_i + (\alpha_i)^2 - (f_0(x_i))^2 + 2f_0(x_i)\alpha_i - (\alpha_i)^2\big) \\
&= \lambda \sum_{i=1}^{n} \big((f(x_i))^2 - (f_0(x_i))^2 + 2f_0(x_i)\alpha_i - 2f(x_i)\alpha_i\big) \\
&= \lambda \sum_{i=1}^{n} \big((f(x_i) - f_0(x_i))(f(x_i) + f_0(x_i)) + 2f_0(x_i)\alpha_i - 2f(x_i)\alpha_i\big) \\
&= \lambda \sum_{i=1}^{n} \big((f - f_0)(x_i)(f + f_0)(x_i) - 2(f - f_0)(x_i) \cdot \alpha_i\big)
\end{aligned}$$

We now see that $f - f_0$ occurs twice in $\mathcal{E}_2(f) - \mathcal{E}_2(f_0)$ which is the variable we are looking for. We also see that $f + f_0$ occurs which is not what we wanted. Thus by letting $f \longrightarrow f_0$ we end up with

$$\begin{aligned}
\mathcal{E}_2(f) - \mathcal{E}_2(f_0) &\approx \lambda \sum_{i=1}^{n} \big((f - f_0)(x_i) 2f_0(x_i) - 2(f - f_0)(x_i) \cdot \alpha_i\big) \\
&= 2\lambda \sum_{i=1}^{n} \big((f - f_0)(x_i)(f_0(x_i) - \alpha_i)\big) = L_2(f - f_0)
\end{aligned}$$

Let us first rewrite L_2 as a transformation of h rather than $f - f_0$, this will make the later calculations easier to follow. Thus we get

$$L_2(h) = 2\lambda \sum_{i=1}^{n} h(x_i)(f_0(x_i) - \alpha_i)$$

The next step is to check whether L_2 is linear. Recall from the definition of linearity that the following conditions must be satisfied:

L1.

$$\begin{aligned}
L_2(h_1 + h_2) &= 2\lambda \sum_{i=1}^{n} \big((h_1 + h_2)(x_i) f_0(x_i) - (h_1 + h_2)(x_i)\alpha_i\big) \\
&= 2\lambda \sum_{i=1}^{n} \big(h_1(x_i) f_0(x_i) + h_2(x_i) f_0(x_i) - (h_1(x_i)\alpha_i + h_2(x_i)\alpha_i)\big) \\
&= 2\lambda \sum_{i=1}^{n} \big(h_1(x_i) f_0(x_i) - h_1(x_i)\alpha_i + h_2(x_i) f_0(x_i) - h_2(x_i)\alpha_i\big) \\
&= 2\lambda \Big(\sum_{i=1}^{n} (h_1(x_i) f_0(x_i) - h_1(x_i)\alpha_i) + \sum_{i=1}^{n} (h_2(x_i) f_0(x_i) - h_2(x_i)\alpha_i) \Big) \\
&= 2\lambda \sum_{i=1}^{n} (h_1(x_i) f_0(x_i) - h_1(x_i)\alpha_i) + 2\lambda \sum_{i=1}^{n} (h_2(x_i) f_0(x_i) - h_2(x_i)\alpha_i) \\
&= L_2(h_1) + L_2(h_2)
\end{aligned}$$

L2.

$$\begin{aligned}
L_2(\beta \cdot h) &= 2\lambda \sum_{i=1}^{n} \big((\beta \cdot h)(x_i) f_0(x_i) - (\beta \cdot h)(x_i)\alpha_i\big) \\
&= 2\lambda \sum_{i=1}^{n} \big(\beta \cdot h(x_i) f_0(x_i) - \beta \cdot h(x_i)\alpha_i\big) \\
&= 2\lambda \sum_{i=1}^{n} \beta \cdot \big(h(x_i) f_0(x_i) - h(x_i)\alpha_i\big) \\
&= \beta \cdot 2\lambda \sum_{i=1}^{n} \big(h(x_i) f_0(x_i) - h(x_i)\alpha_i\big) \\
&= \beta L_2(h)
\end{aligned}$$

Both conditions are satisfied, thus L_2 is a linear transformation.

We now investigate the continuity of the function. Because of the linearity of $L_2(h)$ we once again are able to use Theorem 2 for this matter.

$$
\begin{aligned}
|L_2 h| &= |2\lambda \sum_{i=1}^{n} (h(x_i) f_0(x_i) - h(x_i)\alpha_i)| \\
&= |2\lambda| \cdot \Big| \sum_{i=1}^{n} h(x_i) \cdot (f_0(x_i) - \alpha_i) \Big| \\
&\leq |2\lambda| \sum_{i=1}^{n} |h(x_i) \cdot (f_0(x_i) - \alpha_i)| \\
&\leq |2\lambda| \sum_{i=1}^{n} |h(x_i)| \cdot |(f_0(x_i) - \alpha_i)| \\
&\leq |2\lambda| \sum_{i=1}^{n} \|h\| \cdot |(f_0(x_i) - \alpha_i)| \\
&= \|h\| \cdot \underbrace{n \cdot |2\lambda| \sum_{i=1}^{n} |(f_0(x_i) - \alpha_i)|}_{=M}
\end{aligned}
$$

Notice that f_0 is some fixed function, thus $n \cdot |2\lambda| \cdot \sum_{i=1}^{n} |(f_0(x_i) - \alpha_i)|$ some fixed number. By letting this number be equal to M, all conditions for Theorem 2 are satisfied meaning that L_2 is continuous. We have shown that L_2 is a continuous linear transformation. Now it only remains to see if L_2 really is the derivative of $\mathcal{E}_2(f)$. We start off by approximating the numerator of the derivative expression:

$$
\begin{aligned}
&|\mathcal{E}_2(f) - \mathcal{E}_2(f_0) - L_2(f - f_0)| = \\
&|\lambda \sum_{i=1}^{n} (f(x_i) - \alpha_i)^2 - \lambda \sum_{i=1}^{n} (f_0(x_i) - \alpha_i)^2 - 2\lambda \sum_{i=1}^{n} (f - f_0)(x_i)(f_0(x_i) - \alpha_i)| = \\
&|\lambda| \cdot \Big| \sum_{i=1}^{n} (f(x_i) - \alpha_i)^2 - \sum_{i=1}^{n} (f_0(x_i) - \alpha_i)^2 - 2 \sum_{i=1}^{n} (f - f_0)(x_i)(f_0(x_i) - \alpha_i) \Big|
\end{aligned}
$$

after expanding the quadratics and canceling of the α^2 term we get

$$
\begin{aligned}
&|\lambda| \cdot \Big|\sum_{i=1}^{n} \big((f(x_i))^2 - (f_0(x_i))^2 + 2f_0(x_i)\alpha_i - 2f(x_i)\alpha_i\big) \\
&\qquad - 2\sum_{i=1}^{n}(f(x_i)f_0(x_i) - (f_0(x_i))^2 - f(x_i)\alpha_i + f_0(x_i)\alpha_i\big)\Big| \\
=&|\lambda| \cdot \Big|\sum_{i=1}^{n} \big((f(x_i))^2 - (f_0(x_i))^2 + 2f_0(x_i)\alpha_i \\
&\quad - 2f(x_i)\alpha_i - 2f(x_i)f_0(x_i) + 2(f_0(x_i))^2 + 2f(x_i)\alpha_i - 2f_0(x_i)\alpha_i\big)\Big| \\
=&|\lambda| \cdot \Big|\sum_{i=1}^{n} \big((f(x_i))^2 + (f_0(x_i))^2 - 2f(x_i)f_0(x_i)\big)\Big| \\
=&|\lambda| \cdot \Big|\sum_{i=1}^{n} \big(f(x_i) - f_0(x_i)\big)^2\Big| \\
=&|\lambda| \cdot \sum_{i=1}^{n} |((f - f_0)(x_i))^2| \\
\leq&|\lambda| \cdot \sum_{i=1}^{n} \|(f - f_0)\|^2 \\
=&|\lambda| n \cdot \|(f - f_0)\|^2
\end{aligned}
$$

When we insert this into the definition of the derivative we get:

$$
\frac{\|\mathcal{E}_2(f) - \mathcal{E}_2(f_0) - L_2(f - f_0)\|}{\|f - f_0\|} \leq \frac{n\lambda \cdot \|f - f_0\|^2}{\|f - f_0\|} = n\lambda \cdot \|f - f_0\| < n\lambda\delta
$$

The last inequality follows from the fact that $0 < \|f - f_0\| < \delta$. If we now choose $\delta = \frac{\epsilon}{n\lambda}$ we have shown that the derivative of $\mathcal{E}_2$ at a point f_0 is given by the continuous linear transformation:

$$
L_2(h) = 2\lambda \sum_{i=1}^{n} h(x_i)(f_0(x_i) - \alpha_i)
$$

3.3 Check for convexity of $\mathcal{E}(f)$

Let us now make sure that $\mathcal{E}(f)$ is convex. Notice first that if two functions $f(x)$ and $g(x)$ are convex then so is their sum $f(x) + g(x)$, furthermore if one of the functions $f(x)$ or $g(x)$ is strictly convex, then their sum is strictly convex, this follows directly from the definition of strict convexity. In our case, we are interested in showing that the functional $\mathcal{E}(f)$ is strictly convex, since then, if we can find a function f_0 such that $\mathcal{E}'(f_0) = 0$, the minimizer f_0 will be unique. Let $\mathcal{E}_1$ and $\mathcal{E}_2$ be the same functionals as in previous subsection. We will now show that their sum is strictly convex.

First, let us look at the simple function $g(y) = y^2$, $y \in \mathbb{R}$. Since $g''(y) = 2 > 0$ we know from ordinary calculus that this function is strictly convex. According to the definition of strict convexity stated in the previous section we also know that: $\forall \alpha \in (0, 1)$ and $y_1 \neq y_2$ we have $g(\alpha y_1 + (1 - \alpha)y_2) < \alpha g(y_1) + (1 - \alpha)g(y_2)$. Let us use this knowledge when we look at

$\mathcal{E}_1$. Let $\alpha \in (0,1)$ and $f_1, f_2 \in C^2[a,b]$ be such that $f_1 \neq f_2$.

$$\begin{aligned}
\mathcal{E}_1(\alpha f_1 + (1-\alpha)f_2) &= \int_a^b ((\alpha f_1(x) + (1-\alpha)f_2(x))'')^2 dx \\
&= \int_a^b (\alpha f_1''(x) + (1-\alpha)f_2''(x))^2 dx \\
&\leq \int_a^b (\alpha(f_1''(x))^2 + (1-\alpha)(f_2''(x))^2) dx \\
&= \alpha \int_a^b (f_1''(x))^2 dx + (1-\alpha) \int_a^b (f_2''(x))^2 dx \\
&= \alpha \mathcal{E}_1(f_1) + (1-\alpha)\mathcal{E}_1(f_2)
\end{aligned} \tag{2}$$

If $f_1''(x) = f_2''(x)$ for all $x \in [a,b]$ then the inequality from the calculations above will be an equality. Otherwise it will be a strict inequality.

Let us now have a look at $\mathcal{E}_2$. Consider the following simple function: $h(y) = (y-b)^2$, obviously this is strictly convex since $h''(y) = 2 > 0$. Thus $\forall \beta \in (0,1)$ and $y_1 \neq y_2$ we have $h(y_1\beta + (1-\beta)y_2) < \beta h(y_1) + (1-\beta)h(y_2)$. Let us apply this to $\mathcal{E}_2$. Let $\beta \in (0,1)$, $f_1, f_2 \in C^2[a,b]$ be such that $f_1 \neq f_2$.

$$\begin{aligned}
\mathcal{E}_2(\beta f_1 + (1-\beta)f_2) &= \lambda \sum_{i=1}^{n} ((\beta f_1 + (1-\beta)f_2)(x_i) - \alpha_i)^2 \\
&= \lambda \sum_{i=1}^{n} (\beta f_1(x_i) + (1-\beta)f_2(x_i) - \alpha_i)^2 \\
&\leq \lambda \sum_{i=1}^{n} (\beta(f_1(x_i) - \alpha_i)^2 + (1-\beta)(f_2(x_i) - \alpha_i)^2) \\
&= \lambda \sum_{i=1}^{n} \beta(f_1(x_i) - \alpha_i)^2 + \lambda \sum_{i=1}^{n} (1-\beta)(f_2(x_i) - \alpha_i)^2 \\
&= \beta\lambda \sum_{i=1}^{n} (f_1(x_i) - \alpha_i)^2 + (1-\beta)\lambda \sum_{i=1}^{n} (f_2(x_i) - \alpha_i)^2 \\
&= \beta \mathcal{E}_2(f_1) + (1-\beta)\mathcal{E}_2(f_2)
\end{aligned} \tag{3}$$

If $f_1(x_i) = f_2(x_i)$ for $i = 1, \ldots, n$ then the inequality in the calculations above will be an equality. Otherwise it will be a strict inequality.

We will now show that the two equalitys $f_1''(x) = f_2''(x)$ for all $x \in [a,b]$ and $f_1(x_i) = f_2(x_i)$ for $i = 1, \ldots, n$ cannot both be true at the same time if $f_1 \neq f_2$. This means that we will have strict inequality in at least one of the two equations (2) and (3) and thus the sum $\mathcal{E}_1(f) + \mathcal{E}_2(f) = \mathcal{E}(f)$ is a strictly convex functional.

Suppose $f_1''(x) = f_2''(x)$ for all $x \in [a,b]$ and $f_1(x_i) = f_2(x_i)$ for $i = 1, \ldots, n$ are both true at the same time, then

$$f_1''(x) = f_2''(x) \Longleftrightarrow f_1'(x) = f_2'(x) + c.$$

Where c is some constant. We now look at two cases.

$\underline{c = 0} \Longrightarrow f_1(x) = f_2(x) + d$, for some constant d. Since we have the condition $f_1(x_i) = f_2(x_i)$, it follows that $d = 0$. This implies that $f_1(x) = f_2(x)$ and thus contradicts our choice of f_1 and f_2. This means that $c \neq 0$ must hold.

$\underline{c \neq 0.}$ Suppose $c > 0$ ($c < 0$ is shown in a similar way). We have $f_1'(x) = f_2'(x) + c$, i.e. $\overline{f_1'(x)} > f_2'(x)\ \forall x \in [a, b]$. Let us use this condition together with $f_1(x_i) = f_2(x_i)$ for $i = 1, \ldots, n$. Suppose $f_1(x_1) = f_2(x_1)$, since $f_1'(x) > f_2'(x)$ we have that for a point $x_2 > x_1$, $f_1(x_2)$ cannot be equal to $f_2(x_2)$ and thus contradicts the condition that $f_1(x_i) = f_2(x_i)$ for $i = 1, \ldots, n$, and so the two equalitys cannot both hold at the same time. Thus we have shown that at least one of the inequalitys in (2) and (3) must be a strict inequality and it follows that the sum of $\mathcal{E}_1$ and $\mathcal{E}_2$ is strictly convex.

However, you may have noticed that we assumed that we had at least two points that we were trying to approximate with a function. The argumentation from above does not hold if there is just one point. Consider for example the following case involving only one point x_1: Suppose $f_1(x) = (x - x_1)$ and $f_2(x) = (1 - d) \cdot (x - x_1)$ then we get $f_1(x_1) = f_2(x_1)$ and $f_1'(x) = f_2'(x) + d \Longleftrightarrow f_1''(x) = f_2''(x)$. And thus the two equalitys are satisfied at the same time meaning that $\mathcal{E}$ is not strictly convex. One could also notice this by considering that any straight line passing through a single point would be a minimizer of $\mathcal{E}$ (since $\mathcal{E} = 0$), thus it has infinitely many minimizers so $\mathcal{E}$ is not strictly convex. This is however a somewhat ridiculous case since what would be the point of trying to approximate a function to a single point.

3.4 Summary

In the previous two subsections we calculated the derivative of $\mathcal{E}_1(f)$ and $\mathcal{E}_2(f)$. Adding these two together we find that the derivative of $\mathcal{E}(f)$ at f_0 to be

$$2\int_a^b f''(x) \cdot f_0''(x)dx + 2\lambda \sum_{i=1}^n f(x_i)(f_0(x_i) - \alpha_i).$$

We have also shown that $\mathcal{E}(f)$ is strictly convex. We now have everything needed to be able to use Theorem 1 and solve the problem of finding a minimizer f_0 of $\mathcal{E}(f)$. This will be done in the next section.

4 Finding the minimizer f_0 of $\mathcal{E}(f)$

By inserting the derivative of $\mathcal{E}$ into Theorem 1 we get the following expression:

$$\int_a^b h''(x) \cdot f_0''(x)dx + \lambda \sum_{i=1}^n h(x_i)(f_0(x_i) - \alpha_i) = 0 \qquad \forall h \in C^2[a, b]$$

where f_0 is the minimizer of $\mathcal{E}(f)$. Notice that we have changed the general function f to h in order to avoid confusion later on. We have also made the quite obvious assumption that f_0 must be at least a C^1 function. One can see that by looking at $\mathcal{E}(f)$, which contains a second derivative of f that would not exist if f_0' wouldn't be continuous.

The above expression must hold for every choice of $h \in C^2[a,b]$. By choosing a different function h depending on the situation we will be able to discover several different properties of our minimizer f_0 which will eventually lead us to an exact function that must be the minimizer. We start by looking at an arbitrary interval between some x_k and x_{k+1}, $1 \leq k \leq n-1$, and try to derive some properties about f_0 in this particular interval. This is a natural way of studying the function f_0 since it may consist of different adjoining functions on the interval $[a,b]$.

4.1 Behaviour of f_0 on the interval between x_k and x_{k+1}

Since the equation should hold for any choice of $h \in C^2[a,b]$ we can in particular choose an $h(x)$ with the following properties: $h(x_i) = 0$, $h'(x_i) = 0$ for $i = 1, \ldots, n$ and $h(x) = 0$ outside the interval $[x_k, x_{k+1}]$.
The sum $\lambda \sum_{i=1}^n h(x_i)(f_0(x_i) - \alpha_i)$ is now 0 with this choice of $h(x)$. If we use integration by parts on the remaining part of $\mathcal{E}'(f_0)$ we get:

$$\begin{aligned}\int_{x_k}^{x_{k+1}} h''(x) f_0''(x)dx &= [h'(x)f_0''(x)]_{x_k}^{x_{k+1}} - \int_{x_k}^{x_{k+1}} h'(x) f_0^{(3)}(x)dx \\ &= \underbrace{[h'(x)f_0''(x)]_{x_k}^{x_{k+1}}}_{=0} - \underbrace{[h(x)f_0^{(3)}(x)]_{x_k}^{x_{k+1}}}_{=0} + \int_{x_k}^{x_{k+1}} h(x) f_0^{(4)}(x)dx \\ &= \int_{x_k}^{x_{k+1}} h(x) f_0^{(4)}(x)dx\end{aligned}$$

The first two terms in the second to last step are equal to zero since we have chosen a function $h(x)$ that is zero in each x_i and also $h'(x)$ is zero in each x_i. Also notice that we have assumed that f_0 is four times differentiable on the interval (x_k, x_{k+1}). Later on, in section 4.4, we will show that this assumption is valid, but for now we just assume that it is in fact true.

$$\because \int_{x_k}^{x_{k+1}} h(x) f_0^{(4)}(x)dx = 0$$

We now have three options
1)$h(x) = 0 \ \forall x \in [x_k, x_{k+1}]$
2) $h(x)f_0^{(4)}(x)$ is a function that has the same amount of area over and under the x-axis and the integral is therefore 0 on the interval $[x_k, x_{k+1}]$
3) $f_0^{(4)}(x) = 0 \ \forall x \in [x_k, x_{k+1}]$

We can conclude that option 3) is the correct one since $\int_{x_k}^{x_{k+1}} h(x) f_0^{(4)}(x)dx = 0$ must hold for all functions h with just the restriction that $h(x_i) = 0$, $h'(x_i) = 0$ for $i = 1, \ldots, n$ and $h(x) = 0$ outside the interval $[x_k, x_{k+1}]$(as we assumed). In particular option 1) is incorrect since we are allowed to choose h in any way we want in (x_k, x_{k+1}) and especially such that it doesn't meet the requirement that $h(x) = 0 \ \forall x \in [x_k, x_{k+1}]$. For option 2), consider for example $h(x) = f_0^{(4)}(x)$ on the interval (x_k, x_{k+1}) (along with the previous assumptions on $h(x)$), this is a function that cannot have any area under the x-axis which means that the integral is only satisfied when $f_0^{(4)}(x) = 0$. So if $f_0^{(4)}(x) \neq 0$ option 2) will not hold.

We have now shown that $f_0^{(4)}(x) = 0$ in $[x_k, x_{k+1}]$ this means that $f_0(x)$ is a polynomial of third degree, say $f_0(x) = Ax^3 + Bx^2 + Cx + D$ on the interval $[x_k, x_{k+1}]$. We can choose k arbitrary, and thus we have shown that $\mathcal{E}(f)$ consists of different (in general) third degree polynomials on each interval (x_i, x_{i+1}) $i = 1, \ldots, n$. Notice that we cannot say anything, yet, about the behaviour of f_0 in the points x_i.

4.2 Behaviour of f_0 on the first and last interval

Since we only have one point to fit the curve to in the first and the last interval we can always choose a straight line that have the same value and slope as $f_0(x)$ in the points x_1 and x_n respectively. This must be the optimal choice in these intervals since no other function than a first degree polynomial would yield a smaller value in $\mathcal{E}(f)$ (the second derivative is zero and thus the integral part of $\mathcal{E}(f)$ is zero in these intervals).

4.3 Behaviour of f_0 at the points x_i

In section 4.1 we let $h(x)$ be a function that behaved in a certain way in the points $x_1, x_2, \ldots, x_n$. If we loosen up this criterion and have no restrictions of $h(x)$ we again take a look at the derivative. If we divide the interval [a,b] into subintervals and integrate over each subinterval $[a, x_1]$, $[x_1, x_2]$, $[x_2, x_3], \ldots, [x_n, b]$ we can write the derivative as

$$\int_a^{x_1} h''(x) f_0''(x) dx + \sum_{i=1}^{n-1} \int_{x_i}^{x_{i+1}} h''(x) f_0''(x) dx +$$
$$\int_{x_n}^{b} h''(x) f_0''(x) dx + \lambda \sum_{i=1}^{n} h(x_i)(f_0(x_i) - \alpha_i) = 0$$

If we do the same integration by parts as in section 4.1 on the integrals, we get the expression

$$\begin{aligned} &[h'(x) f_0''(x)]_a^{x_1} - [h(x) f_0^{(3)}(x)]_a^{x_1} + \sum_{i=1}^{n-1} \left([h'(x) f_0''(x)]_{x_i}^{x_{i+1}} - [h(x) f_0^{(3)}(x)]_{x_i}^{x_{i+1}} \right) + \\ &[h'(x) f_0''(x)]_{x_n}^{b} - [h(x) f_0^{(3)}(x)]_{x_n}^{b} + \underbrace{\int_{x_1}^{x_2} h(x) f_0^{(4)}(x) dx}_{=0} + \lambda \sum_{i=1}^{n} h(x_i)(f_0(x_i) - \alpha_i) = 0 \end{aligned} \quad (4)$$

The third term on the last line is equal to zero since we concluded in section 4.1 that $f_0^{(4)} = 0$ on the intervals. We also know that in the points x_i, $f_0(x)$ and $f_0'(x)$ are continuous, otherwise the function $\mathcal{E}(f)$ would not be meaningful since $f_0'(x)$ would not have a derivative. But we can't say anything about the second derivative just by looking at $\mathcal{E}(f)$ since we could still integrate a discontinuous function by dividing the integral into sub intervals and integrating them one by one. But with a bit of calculation (following below) we can show that $f_0''(x)$ is continuous in each point x_i hence $f_0(x)$ is a C^2 function in [a,b].
(4) should hold for all $h(x)$. We can choose $h(x)$ to be zero in each x_i. Then we get

$$[h'(x) f_0''(x)]_a^{x_1} + \sum_{i=1}^{n-1} [h'(x) f_0''(x)]_{x_i}^{x_i+1} + [h'(x) f_0''(x)]_{x_n}^{b} = 0$$

Since we don't know (yet) how $f_0''(x)$ behave near the points x_i we introduce ϵ as a limit variable which tends to 0^+. We know that $f_0(x)$ is a polynomial of first degree on the intervals $[a, x_1]$ and $[x_n, b]$, hence $f''(x)$ is zero in the points $a, x_1 - \epsilon, x_n + \epsilon$ and b. But we will keep $x_1 - \epsilon, x_n + \epsilon$ so we can rewrite the equation as

$$\lim_{\epsilon \to 0} \sum_{i=1}^{n} h'(x)(f_0''(x_i - \epsilon) - f_0''(x_i + \epsilon)) = 0$$

If we now make another restriction of $h(x)$ by saying that its derivative should be zero in each x_i except for one point which we denote x_k, in this point we set the derivative to 1. Then what we have left is

$$\lim_{\epsilon \to 0} \left(f_0''(x_k - \epsilon) - f_0''(x_k + \epsilon) \right) = 0$$

which says that $f_0''(x)$ is continuous in x_k. We can then let k be any number $1, 2, \ldots, n$, and so the second derivative of our function is continuous in each point x_i.

$\because$ $f_0(x)$ is a C^2-function in $[a, b]$.

We have now concluded that f_0 is a C^2-function and if we look at the derivative again with no restrictions on $h(x)$ we see that every term involving $f''(x)$ vanishes since they cancel each other out. But we still don't know anything about the third derivative in the points x_i (doesn't need to be continuous), we will therefore do similar calculations when we calculate the relation of the third derivatives as we did with the second derivative. Once again we use ϵ as a limit-variable that tends to 0^+. We also have that $f^{(2)}$ and $f^{(3)}$ is zero in a and b. So what actually remains of our derivative is

$$\begin{aligned} &\lim_{\epsilon \to 0} \big(- h(x_1) f_0^{(3)}(x_1 - \epsilon) - h(x_n) f_0^{(3)}(x_n + \epsilon) - \\ &\quad \sum_{i=1}^{n-1} (h(x_{i+1}) f_0^{(3)}(x_{i+1} - \epsilon) - h(x_i) f_0^{(3)}(x_i + \epsilon)) + \\ &\quad \lambda \sum_{i=1}^{n} h(x_i)(f_0(x_i) - \alpha_i) \big) = 0 \end{aligned}$$

We would once more like to stress that $f_0^{(3)}$ doesn't need to be continuous and hence $f_0^{(3)}(x_k - \epsilon)$ will in general not have the same limit value as $f_0^{(3)}(x_k + \epsilon)$. We now do a bit of rearranging in the expression. First of all we insert the two first terms into the sum and once we have done that the index changes to running from 1 to n. Secondly we change the sign in front of all the terms. This gives the much more convenient expression

$$\lambda \sum_{i=1}^{n} h(x_i)(f_0(x_i) - \alpha_i) + \sum_{i=1}^{n} h(x_i)(f_0^{(3)}(x_i + \epsilon) - f_0^{(3)}(x_i - \epsilon)) = 0.$$

Since we are looking at different third-degree polynomials on each interval x_i to x_{i+1} we change notation of the optimal function $f_0(x)$ to $p_i(x)$, where $p_i(x)$ denotes the optimal polynomial between the points x_i and x_{i+1}. This is more practical since the actual optimal function consists of several different adjoining polynomials. In the preceding step, note that $f_0(x_k) = p_k(x_k) = p_{k-1}(x_k)$.
The expression we ended up with should hold for all functions $h(x) \in C^2[a, b]$. If we once

again consider a special function $h(x)$ that is zero in each point x_i except for one, say when i=k. Then

$$\lim_{\epsilon \to 0} \lambda(p_k(x_k) - \alpha_k) - p_{k-1}^{(3)}(x_k - \epsilon) + p_k^{(3)}(x_k + \epsilon) = 0$$

is what is left of the expression. This says that the third derivatives in the points $x_1, x_2, \ldots, x_n$ have a special relation, namely

$$p_{k-1}^{(3)}(x_k) = p_k^{(3)}(x_k) + \lambda(p_k(x_k) - \alpha_k).$$

We also have that the function we are working with is a $C^2[a,b]$ function and hence $p_{i-1}(x_i) = p_i(x_i)$ and $p'_{i-1}(x_i) = p'_i(x_i)$ and $p''_{i-1}(x_i) = p''_i(x_i)$. This is just as many equations as we need in one point, since a third degree polynomial has four coefficients.

4.4 Validating the minimizer f_0

When we tried to find the minimizer f_0, we assumed without proof in section 4.1 that it was four times differentiable on the intervals (x_i, x_{i+1}). With this assumption we derived certain properties, for example that it was a C^2 function on the entire interval and that the third derivatives between two neighbouring polynomials had a special linear relation. We will now show that $\mathcal{E}'(f_0) = 0$. Thus our assumption that f_0 was four times differentiable on the intervals (x_i, x_{i+1}) was in fact a valid one, since we will show that f_0 is indeed the unique minimizer of $\mathcal{E}(f)$. Recall that our derivative in f_0 is

$$\mathcal{E}'(f_0)(h) = \int_a^b h''(x) f_0''(x) dx + \lambda \sum_{i=1}^{n} h(x_i)(f_0(x_i) - \alpha_i) \qquad \forall h \in C^2[a,b].$$

We now look at the first part of $\mathcal{E}'(f_0)$. We will use the same calculations as before but this time with the knowledge that $f_0(x)$ consists of several adjoining third degree polynomials except for the first and last interval, where it consists of a first degree polynomial. We now use the same notation for the (in general) different polynomials as before, namely, let p_i be the optimal polynomial on the interval $[x_i, x_{i+1}]$, p_0 the optimal polynomial on $[a, x_1]$ and p_n the optimal polynomial on $[x_n, b]$. If we split up the integral and do the same integration by parts, we get

$$\begin{aligned}\int_a^b h''(x) f_0''(x) dx = & \underbrace{[h'(x)p_0''(x)]_a^{x_1} + \sum_{i=1}^{n-1} [h'(x)p_i''(x)]_{x_i}^{x_{i+1}} + [h'(x)p_n''(x)]_{x_n}^b}_{(1)} \\ & \underbrace{-[h(x)p_0^{(3)}(x)]_a^{x_1} - \sum_{i=1}^{n-1} [h(x)p_i^{(3)}(x)]_{x_i}^{x_{i+1}} - [h(x)p_n^{(3)}(x)]_{x_n}^b}_{(2)} \\ & + \underbrace{\int_a^{x+1} h(x)p_0^{(4)}(x)dx + \sum_{i=1}^{n-1} \int_{x_i}^{x_{i+1}} h(x)p_i^{(4)}(x)dx + \int_{x_n}^b h(x)p_n^{(4)}(x)dx}_{(3)}\end{aligned}$$

We know that (1) will sum to 0 since $f_0(x)$ is a C^2 function over $[a,b]$, moreover we also know that (3) is equal to zero since $p_i^{(4)}(x) = 0 \quad \forall i = 0, \dots, n$. Thus, the only remaining part of the above expression is (2). Using this fact, we can now rewrite $\mathcal{E}'(f_0)$ as

$$\mathcal{E}'(f_0)(h) = -[h(x)p_0^{(3)}(x)]_a^{x_1} - \sum_{i=1}^{n-1}[h(x)p_i^{(3)}(x)]_{x_i}^{x_{i+1}} - [h(x)p_n^{(3)}(x)]_{x_n}^{b} + \lambda \sum_{i=1}^{n} h(x_i)(p_i(x_i) - \alpha_i)$$
$$= \underbrace{h(a)p_0^{(3)}(a)}_{(i)} - h(x_1)p_0^{(3)}(x_1) + h(x_n)p_n^{(3)}(x_n) - \underbrace{h(b)p_n^{(3)}(b)}_{(ii)}$$
$$+ \sum_{i=1}^{n-1}(h(x_i)p_i^{(3)}(x_i) - h(x_{i+1})p_i^{(3)}(x_{i+1})) + \lambda \sum_{i=1}^{n} h(x_i)(f_0(x_i) - \alpha_i)$$

where (i) and (ii) are equal to zero since we know that f_0 is a polynomial of first degree order on the intervals $[a, x_1]$ and $[x_n, b]$, hence $p_0''(x) = 0$ and $p_n''(x) = 0$. The above equation becomes

$$-h(x_1)p_0^{(3)}(x_1) + h(x_n)p_n^{(3)}(x_n) + \sum_{i=1}^{n-1}(h(x_i)p_i^{(3)}(x_i) - h(x_{i+1})p_i^{(3)}(x_{i+1})) + \lambda \sum_{i=1}^{n} h(x_i)(f_0(x_i) - \alpha_i) =$$
$$\underbrace{-h(x_1)p_0^{(3)}(x_1)}_{I} + \underbrace{h(x_n)p_n^{(3)}(x_n)}_{II} + \underbrace{\sum_{i=1}^{n-1} h(x_i)p_i^{(3)}(x_i)}_{III} - \underbrace{\sum_{i=1}^{n-1} h(x_{i+1})p_i^{(3)}(x_{i+1})}_{IV} + \lambda \sum_{i=1}^{n} h(x_i)(f_0(x_i) - \alpha_i)$$

If we change the summation index on IV to go from 2 to n, we can then let I be e a part of IV and thus the index will go from 1 to n. We also include II into III and thus the index will change to go from 1 to n. We now end up with the expression

$$\sum_{i=1}^{n} h(x_i)p_i^{(3)}(x_i) - \sum_{i=1}^{n} h(x_i)p_{i-1}^{(3)}(x_i) + \lambda \sum_{i=1}^{n} h(x_i)(f_0(x_i) - \alpha_i).$$

If we use the fact that $p_{i-1}^{(3)}(x_i) = p_i^{(3)}(x_i) + \lambda(p_i(x_i) - \alpha_i)$ we can rewrite the second sum and we get

$$\sum_{i=1}^{n} h(x_i)p_i^{(3)}(x_i) - \sum_{i=1}^{n} h(x_i)(p_i^{(3)}(x_i) + \lambda(p_i(x_i) - \alpha_i)) + \lambda \sum_{i=1}^{n} h(x_i)(f_0(x_i) - \alpha_i) =$$
$$\sum_{i=1}^{n} h(x_i)p_i^{(3)}(x_i) - \sum_{i=1}^{n} h(x_i)p_i^{(3)}(x_i) - \lambda \sum_{i=1}^{n} h(x_i)(p_i(x_i) - \alpha_i) + \lambda \sum_{i=1}^{n} h(x_i)(f_0(x_i) - \alpha_i) = 0$$

Where we have used the equality $p_i(x_i) = f_0(x_i)$ for $i = 1, \dots, n$

Now we have shown that $\mathcal{E}'(f_0)$ is indeed 0, thus f_0 the (unique) minimizer of $\mathcal{E}$. In the above calculations we assumed that $h(x)$ was a C^2 function on the interval $[a,b]$. These calculations will still hold if $h(x)$ is only a C^1 function. Thus we have that our minimizer is still the unique minimum in an even greater set of functions.

4.5 Solving the system of equations

We now have four conditions which yield a uniquely solvable system of equations. In the following section we will use these conditions to set up this system of equations. As you may have noticed, each new point will yield four new unknown variables and four new equations, thus the system will become very large after just a few points. It will be very cumbersome solving by hand and so we must turn to the computer.

Let $p_k(x) = A_k(x - x_k)^3 + B_k(x - x_k)^2 + C_k(x - x_k) + D_k$ be the optimal polynomial in the interval $[x_k, x_{k+1}]$. Notice that we write it in this manner in order for the calculations, done by the computer, to be more numerically stable. Recall from the previous section that we have the following four conditions

$$\begin{cases} p_{k-1}(x_k) = p_k(x_k) \\ p'_{k-1}(x_k) = p'_k(x_k) \\ p''_{k-1}(x_k) = p''_k(x_k) \\ p^{(3)}_{k-1}(x_k) = \lambda(p_k(x_k) - \alpha_k) + p^{(3)}_k(x_k) \end{cases}$$

Lets us first calculate the necessary derivatives of $p_k(x) = A_k(x - x_k)^3 + B_k(x - x_k)^2 + C_k(x - x_k) + D_k$

$$\begin{cases} p_k(x) = A_k(x - x_k)^3 + B_k(x - x_k)^2 + C_k(x - x_k) + D_k \\ p'_k(x) = 3A_k(x - x_k)^2 + 2B_k(x - x_k) + C_k \\ p''_k(x) = 6A_k(x - x_k) + 2B_k \\ p^{(3)}_k(x) = 6A_k \end{cases}$$

We now insert these derivatives into the four conditions from above

$$\begin{cases} A_{k-1}(x_k - x_{k-1})^3 + B_{k-1}(x_k - x_{k-1})x^2 + C_{k-1}(x_k - x_{k-1}) + D_{k-1} = D_k \\ 3A_{k-1}(x_k - x_{k-1})^2 + 2B_{k-1}(x_k - x_{k-1}) + C_{k-1} = C_k \\ 6A_{k-1}(x_k - x_{k-1}) + 2B_{k-1} = 2B_k \\ 6A_{k-1} = \lambda(D_k - \alpha_k) + 6A_k \end{cases}$$

Let us rewrite this to get a better overview

$$\begin{cases} A_{k-1}(x_k - x_{k-1})^3 + B_{k-1}(x_k - x_{k-1})x^2 + C_{k-1}(x_k - x_{k-1}) + D_{k-1} - D_k = 0 \\ 3A_{k-1}(x_k - x_{k-1})^2 + 2B_{k-1}(x_k - x_{k-1}) + C_{k-1} - C_k = 0 \\ 3A_{k-1}(x_k - x_{k-1}) + B_{k-1} - B_k = 0 \\ -6A_{k-1} + 6A_k + \lambda D_k = \lambda\alpha_k \end{cases} \tag{1}$$

The easiest way to solve this system of equations is by writing it in matrix form. Since the system of equation follows a nice pattern we will write it as several block matrices inside a big matrix. Let $a_k(p_{k-1})$ and $a_k(p_k)$ be block matrices that describe the polynomials p_{k-1} and p_k in the point x_k. Since we have a first degree polynomial in the first and last interval the block matrices in the points x_1 and x_n will look a bit different, so lets write them separately. Recall that a and b denotes the start of the first interval and the end of the last interval. The block matrices needed will be the following

$$a_1(p_0) = \begin{pmatrix} x_1 - a & 1 \\ 1 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} \quad a_1(p_1) = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 6 & 0 & 0 & \lambda \end{pmatrix}$$

$$a_k(p_{k-1}) = \begin{pmatrix} (x_k - x_{k-1})^3 & (x_k - x_{k-1})^2 & (x_k - x_{k-1}) & 1 \\ 3(x_k - x_{k-1})^2 & 2(x_k - x_{k-1}) & 1 & 0 \\ 3(x_k - x_{k-1}) & 1 & 0 & 0 \\ -6 & 0 & 0 & 0 \end{pmatrix}$$

$$a_k(p_k) = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ 6 & 0 & 0 & \lambda \end{pmatrix}$$

$$a_n(p_{n-1}) = \begin{pmatrix} (x_n - x_{n-1})^3 & (x_n - x_{n-1})^2 & (x_n - x_{n-1}) & 1 \\ 3(x_n - x_{n-1})^2 & 2(x_n - x_{n-1}) & 1 & 0 \\ 3(x_n - x_{n-1}) & 1 & 0 & 0 \\ -6 & 0 & 0 & 0 \end{pmatrix} \quad a_n(p_n) = \begin{pmatrix} 0 & -1 \\ -1 & 0 \\ 0 & 0 \\ 0 & \lambda \end{pmatrix}$$

We then insert these block matrices into a big matrix, let us denote this matrix by A. Then A will then describe the relations in the left hand side of (1). It will have the following structure

$$A = \begin{pmatrix} a_1(p_0) & a_1(p_1) & 0 & . & . & . & . & 0 \\ 0 & a_2(p_1) & a_2(p_2) & 0 & . & . & . & 0 \\ . & & & & & & & \\ . & & & & & & & \\ 0 & . & a_k(p_{k-1}) & a_k(p_k) & 0 & . & . & 0 \\ 0 & . & 0 & a_{k+1}(p_k) & a_{k+1}(p_{k-1}) & 0 & . & 0 \\ . & & & & & & & \\ . & & & & & & & \\ 0 & . & . & . & 0 & a_{n-1}(p_{n-2}) & a_{n-1}(p_{n-1}) & 0 \\ 0 & . & . & . & . & 0 & a_n(p_{n-1}) & a_n(p_n) \end{pmatrix}$$

Let B be the matrix containing all coefficients of (1), and let C be the matrix containing the right hand side of (1). They will look like this

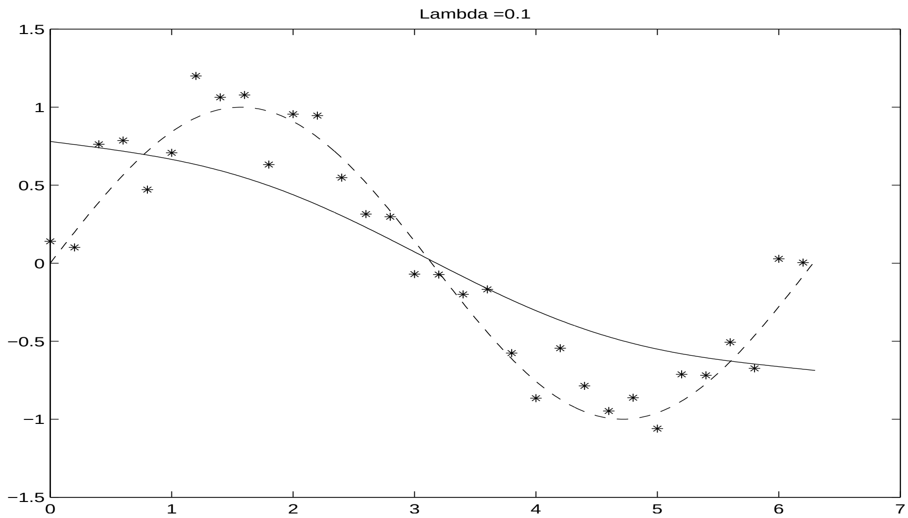
$$B = \begin{pmatrix} C_0 \\ D_0 \\ A_1 \\ B_1 \\ C_1 \\ D_1 \\ . \\ . \\ . \\ A_{n-1} \\ B_{n-1} \\ C_{n-1} \\ D_{n-1} \\ C_n \\ D_n \end{pmatrix} \qquad C = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \alpha_1\lambda \\ 0 \\ 0 \\ 0 \\ \alpha_2\lambda \\ . \\ . \\ \alpha_{n-1}\lambda \\ 0 \\ 0 \\ 0 \\ \alpha_n\lambda \end{pmatrix}$$

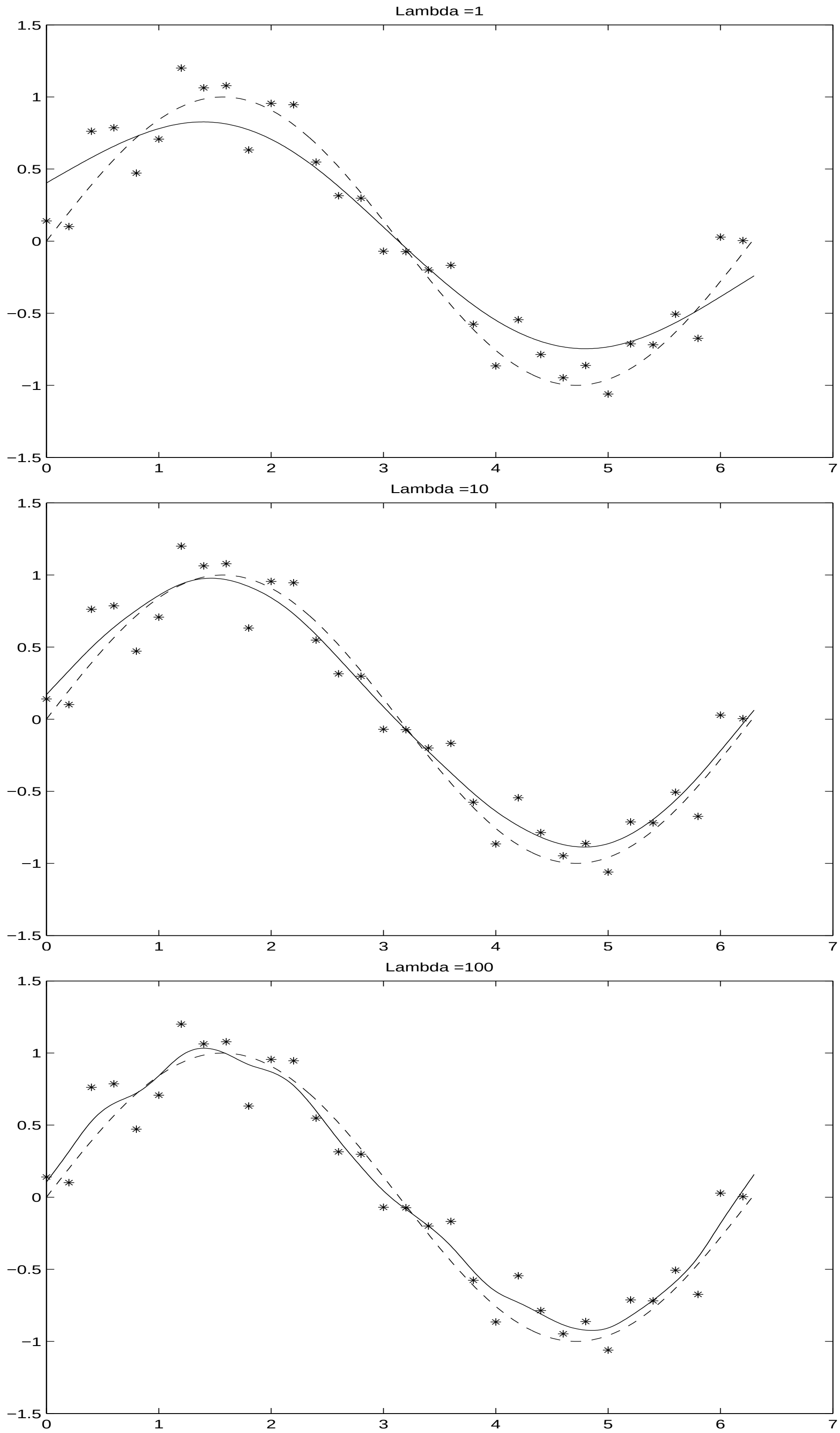
The matrix equation will then look like $A \cdot B = C$. If we multiply this equation with A^{-1} from the left we get $B = A^{-1}C$ which will yield a value to each coefficient in every polynomial. We have solved this matrix equation by using a program called Matlab. In the appendix we will give the code for our program.

5 Investigating the interpolation coefficient λ

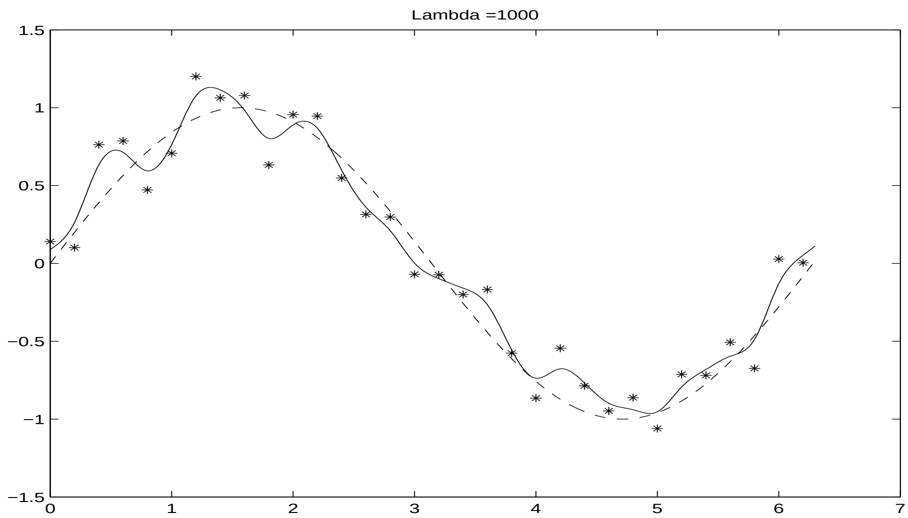
The purpose of this section is to show that the choice of the interpolation coefficient λ plays a crucial part when trying to approximate a curve $f_0(x)$ to a set of points (x_1, α_1),$(x_2, \alpha_2), \dots$, (x_n, α_n). Given a set of points, which for example can be measurements from an experiment, it is natural to believe that these are generated by some underlying function with some certain random error to each measurement. It is also natural to assume that these errors follows some kind of distribution, in our example we will consider a normal distribution. The risk of choosing λ too low is that the generated function f_0 may not reflect the properties of the underlying function very well. Choosing λ too low will make the curve too flat since little effort will be put into approximating the points $(x_1, \alpha_1), (x_2, \alpha_2), \dots, (x_n, \alpha_n)$. However, if we choose λ too high the error terms will play too much of a part when trying to approximate the underlying function. Thus choosing λ too high will cause the function to oscillate too much and not describe the underlying function very well. The following example will illustrate the impact of different choices of λ.

We start off by generating a set of points that follows the sine function, but with a random error to each term. We let this error term follow a normal distribution with mean value 0 and standard deviation 0.20. We generate these points on an interval between 0 and 6.3 ($\approx 2\pi$), with a distance of 0.2 between each x_j. The following plots show the generated function $f_0(x)$ for various choices of λ. The dashed line is the actual sine function, we will refer to this curve as $\sin(x)$. The stars are the generated points $(x_1, \alpha_1), (x_2, \alpha_2), \dots, (x_n, \alpha_n)$. The solid line is the function $f_0(x)$ that approximates the points $(x_1, \alpha_1), \dots, (x_n, \alpha_n)$.





Lambda =1
Lambda =10
Lambda =100



Let us now try to answer the question of which of the above choices of λ seems to give the best approximation of the sine function. The following table will provide us with some useful information. In column 1 we have the various λ values. In column 2 we have the average value of $|f_0(x) - \sin(x)|$, taken in a large set of evenly distributed points between 0 and 6.3. In column 3 we have the average deviation of $f(x)$ from α_i in the points $(x_1, \alpha_1), (x_2, \alpha_2), \ldots, (x_n, \alpha_n)$. In column 4 we have the value of the integral of $(f_0''(x))^2$ over the interval $[0, 6.3]$.

λ	$\lvert f_0(x) - \sin(x)\rvert$	$\lvert f_0(x_i) - \alpha_i\rvert$	$\int_0^{6.3} (f_0''(x))^2 dx.$
0.1	0.3402	0.3058	0.0810
1	0.1585	0.1799	1.1948
10	0.0763	0.1343	2.6837
100	0.0761	0.1206	10.4191
1000	0.1011	0.0853	168.6220

First of all, have a look at column 2. If this value is small, we have an indication that $f_0(x)$ approximates $\sin(x)$ closely. In column 4 we have the integral of $(f_0''(x))^2$, which is a measure of the smoothness of the curve. We don't want this value to be too low, a value of zero would be a straight line. Neither do we want this value to be too high since then the curve would be oscillating a lot. We can see from the table above that for our choices of λ, we have the lowest deviation of $f_0(x)$ from $\sin(x)$ when $\lambda = 100$. Does this necessarily mean that $\lambda = 100$ gives the best approximation of $\sin(x)$? No, not necessarily. We can for example see that for $\lambda = 10$ we have a slightly higher deviation from $\sin(x)$ but the curve's fluctuations seem to resemble that of $\sin(x)$ in a better way. Nonetheless, we can say that for $\lambda = 0.1$ and $\lambda = 1000$, $f_0(x)$ does not seem to be a good approximation of $\sin(x)$.

In the example above we assumed that we knew the underlying function. However, when given some points $(x_1, \alpha_1), (x_2, \alpha_2), \ldots, (x_n, \alpha_n)$, it is more natural not knowing what kind of underlying function they are following. In this case column 2 from our table above would not exist. If we look at column 4 we see that as smoothness decreases as the deviation of $f(x)$ from the points $(x_1, \alpha_1), (x_2, \alpha_2), \ldots, (x_n, \alpha_n)$ decreases. Thus finding the optimal choice of λ becomes much harder, in fact different kinds of λ may be optimal for the same set of points depending on what kind of a problem you are looking at. Any general guidelines on how to choose λ is beyond the scope of this paper.

References

[1] Amol Sasane , Mathematical economics, chapter 1 and 2, lecture notes, Stockholm University.

[2] Anders Tengstrand, Linjär algebra med vektorgeometri, second edition, chapter 1 and 2, Studentlitteratur, 2005.

[3] Persson, Böiers, Analys i en variabel, Chapter 5 and 6,second edition, studentlitteratur, 2001.

6 Appendix

The following code can be used for Matlab in order to solve the system of equations described in section 4.4.

```
%The following program will solve the matrix equation A*koeff = B, where:
%koeff is the vector containing the coefficients that we are looking for.
%A is the n x n matrix containing the equations.
%B is vector which determines the value of each row in A.
%a graph will also be plotted for the final answer

function interpolation(lambda,x,alpha)
m=size(x);
n=4*m(1,2); %number of coefficients
koeff = zeros(n,1); % the coefficients we are looking for

%The B vector is constructed here
B=zeros(n,1);

for i = 1:n
    if mod(i,4) == 0
        B(i,1) = alpha(1,(1/4)*i)*lambda;
    else
        B(i,1) = 0;
    end
end

A = zeros(n);

%These varibles will be used in the construction of A.
c=2;
r=0;
k=5;

%The following section will contruct row 5 to n-4 in the A matrix, the
%first and last 4 rows will be done seperatley later on.
for i=5:(n-4)
           r = mod(i,4);

            if r==3
             A(i,(k-2)) = 3*(x(c)-x(c-1));
             A(i,k-1) = 1;
             A(i,(k+3)) = -1;

            end

            if r==2
             A(i,(k-2)) = 3*((x(c)-x(c-1))^2);
             A(i,(k-1)) = 2*(x(c)-x(c-1));
             A(i,k) = 1;
```

```
            A(i,(k+4)) = -1;

           end

           if r==1
            A(i,(k-2)) = (x(c)-x(c-1))^3;
            A(i,(k-1)) = (x(c)-x(c-1))^2;
            A(i,k) = x(c)-x(c-1);
            A(i,(k+1)) = 1;
            A(i,(k+5)) = -1;

           end

           if r==0
            A(i,(k-2)) = -6;
            A(i,(k+5)) = lambda;
            A(i,(k+2)) = 6;
          end

       if r==0
            k=k+4;
            c=c+1;
       end
end

%This section makes sure that the first and last interval will be of the
%same length as the mean value of the length of the other intervals.
 hh=1;
 jj = m(1,2);
 kk = 0;
 for hh = 1:(jj-1);
        kk = kk + x(1,hh+1) - x(1,hh);
 end
mm = kk/(jj-1); %this denotes the mean value of the length of the intervals

%The first 4 rows are contrcuted here
A(4,3) = 6;
A(4,6) = lambda;
A(3,4) = 1;
A(2,1) = -1;
A(2,5) = 1;
A(1,1) = mm;
A(1,2) = 1;
A(1,6) = -1;

%The last 4 rows are contructed here
p=m(1,2);
A((n),(n-5)) =-6;
A((n),n) =lambda;
A((n-1),(n-5)) =3*(x(p)-x(p-1));
```

```
A((n-1),(n-4)) =1;
A((n-2),(n-5)) =3*((x(p)-x(p-1))^2);
A((n-2),(n-4)) =2*(x(p)-x(p-1));
A((n-2),(n-3)) =1;
A((n-2),(n-1)) =-1;
A(n-3,(n-5)) =((x(p)-x(p-1))^3);
A(n-3,(n-4)) =((x(p)-x(p-1))^2);
A(n-3,(n-3)) =x(p)-x(p-1);
A(n-3,(n-2)) =1;
A(n-3,n) = -1;

%The calculation of the coefficients is done here
koeff = A\B;

%The coeff vector consists of (C_0, D_0, A_1, B_1, C_1, D_1, ... ,A_(n-1),
%%B_(n-1), C_(n-1), D_(n-1), C_n, D_n)'

%We now rewrite the koeff vector so that we can use the command mkpp:
q = [0;0;koeff(1:n-2);0;0;koeff(n-1:n)];
g = size(q);
% The new 4 x n matrix with the the coefficients of polynomial k on row k
% is constructed here.
ko = reshape(q,4,g(1,1)*0.25)';
tt = size(ko);

breaks = [(x(1,1)-mm), x(1:n*0.25),(x(1,(n*0.25))+mm)]; %all x-values, including a and b.

%The plot is made here.
 pp = mkpp(breaks,ko);
xx1=(x(1,1)-mm):0.01:(x(1,(n*0.25))+mm);
 plot(xx1,ppval(pp,xx1),x,alpha,'o');
```