10. Lecture 10

Extension of Trigonometric interpolation. On $[0, \pi]$ use

$$\mathbb{V}_{N-1} = \text{span}\{\sin(jx) \ : \ j = 1, 2, ..., N-1\}$$

so that the interpolation problem reads: find $S_N \in \mathbb{V}_{N-1}$ satisfying

$$S_N(x_j) = f(x_j), \qquad \text{for } j = 1, ..., N-1,$$

with $x_j = \frac{\pi}{N} j = hj$ where $h := \frac{\pi}{N}$.

Remark 10.1 (Existence and Uniqueness). The above interpolation problem has a unique solution. Moreover, computing the coefficients c_j in the interpolating polynomial

$$S_N(x) = \sum_{j=1}^{N-1} c_j \sin(jx)$$

can be done using $FFT's$ of size $2N$.

Remark 10.2 (Spectral Convergence). This sine approximation also exhibits spectral convergence as in Theorem 8.2.

On $[0, \pi]$ one can also use

$$\mathbb{V}_{N+1} = \text{span}\{\cos(jx) \ : \ j = 0, 1, ..., N\}.$$

In this case, $x_j = hj$ for $j = 0, ..., N$ and the interpolation problem consists in finding $C_{N+1} \in \mathbb{V}_{N+1}$ such that

$$C_{N+1}(x_j) = f(x_j), \qquad j = 0, ..., N.$$

As in the sine case, similar remarks holds.

Numerical Differentiation

We start with the simplest example: use the difference quotient from the definition of the derivative, i.e.

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}, \qquad h > 0. \tag{6}$$

This is called a forward difference. Similarly,

$$f'(x) \approx \frac{f(x) - f(x-h)}{h}, \qquad h > 0. \tag{7}$$

is called a backward difference.

Error estimates. The Taylor series around x reads

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(\xi)$$

for some $\xi \in (x, x+h)$. Whence,

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \underbrace{\frac{h}{2} f''(\xi)}_{O(h)}.$$

This implies that error due to the approximation (6) is $O(h)$ or first order!

The same property holds for (7) since

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2} f''(\xi)$$

for some $\xi \in (x-h, x)$ and so

$$f'(x) = \frac{f(x) - f(x-h)}{h} + \underbrace{\frac{h}{2} f''(\xi)}_{O(h)}.$$

Example 10.1 (Method of Undetermined Coefficients)**.** *We propose to find an approximation of the derivative of highest possible order of the form*

$$f'(x) \approx af(x) + bf(x-h) + cf(x-2h).$$

To do this, we use the method of undetermined coefficients. *We write the Taylor's series around x and expand $f(x-h)$ and $f(x-2h)$*

$$\begin{aligned} f(x) &= f(x) \\ f(x-h) &= f(x) - hf'(x) + \frac{h^2}{2} f''(x) + ... \\ f(x-2h) &= f(x) - 2hf'(x) + 2h^2 f''(x) + ... \end{aligned}$$

Now, use these expression to expand $af(x) + bf(x-h) + cf(x-2h)$ and regroups terms with the same power of h

$$af(x)+bf(x-h)+cf(x-2h) = (a+b+c)f(x) - (b+2c)hf'(x) + \frac{h^2}{2}(b+4c)f''(x) - \frac{h^3}{6}(b+8c)f'''(x) + ...$$

We want this to equal $f'(x) + O(h^r)$ for r as large as possible. To do this, we constraint the coefficients to satisfy

$$\begin{aligned} a + b + c &= 0 \\ -(b+2c)h &= 1 \\ b + 4c &= 0. \end{aligned}$$

This has a unique solution. Indeed, it is equivalent to (upon multiplying the second constraint by $-1/h$)

$$\underbrace{\begin{pmatrix} 1 & 1 & 1 \\ 0 & 1 & 2 \\ 0 & 1 & 4 \end{pmatrix}}_{=:A} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} 0 \\ -1/h \\ 0 \end{pmatrix}.$$

We compute $\det(A) = 1. \det \begin{pmatrix} 1 & 2 \\ 1 & 4 \end{pmatrix} = 2 \neq 0$. *This implies that the system has a unique solution and we cannot get rid of higher order terms. The solution is given by $a = \frac{3}{2h}$, $b = -\frac{2}{h}$ and $c = \frac{1}{2h}$ so that the desired approximation is*

$$f'(x) \approx \frac{\frac{3}{2} f(x) - 2f(x-h) + \frac{1}{2} f(x-2h)}{h}.$$

To derive an expression of the error, we use Taylor series with remainder (at the lowest remaining term), i.e.

$$\begin{aligned} f(x) &= f(x) \\ f(x-h) &= f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f'''(\xi_1), \qquad \xi_1 \in (x-h,x) \\ f(x-2h) &= f(x) - 2hf'(x) + 2h^2 f''(x) - \frac{8h^3}{6}f'''(\xi_2), \qquad \xi_2 \in (x-2h,x). \end{aligned}$$

Then, we compute

$$\frac{\frac{3}{2}f(x) - 2f(x-h) + \frac{1}{2}f(x-2h)}{h} = f'(x) - \frac{h^3}{6}\left(-\frac{2}{h}f''(\xi_1) + \frac{8}{2h}f'''(\xi_2)\right) = f'(x) + O(h^2).$$

This is the highest order method of this form and its order is 2.

Example 10.2 (Second Derivatives)**.** *We use the method of undetermined coefficients to get a difference approximation to*

$$-f''(x) \approx af(x-h) + bf(x) + cf(x+h)$$

of highest possible order. We have

$$\begin{aligned} f(x) &= f(x) \\ f(x \pm h) &= f(x) \pm f'(x) + \frac{h^2}{2}f''(x) \pm \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(x) \pm ... \end{aligned}$$

Hence,

$$\begin{aligned} af(x-h) + bf(x) + cf(x+h) =& (a+b+c)f(x) + h(c-a)f'(x) + \frac{h^2}{2}(c+a)f''(x) \\ &+ \frac{h^3}{6}(c-a)f'''(x) + \frac{h^4}{24}(c+a)f^{(4)}(x) + ... \end{aligned}$$

To have this expression agree with $-f''(x)$ to highest order we set

$$\begin{aligned} a+b+c &= 0 \\ c-a &= 0 \\ \frac{h^2}{2}(c+a) &= -1. \end{aligned}$$

This is probably as far as we can go and leads to the system

$$\underbrace{\begin{pmatrix} 1 & 1 & 1 \\ -1 & 0 & 1 \\ 1 & 0 & 1 \end{pmatrix}}_{=:A} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ -2/h^2 \end{pmatrix}.$$

We compute $\det(A) = -1 \det \begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix} = 2 \neq 0$. *The unique solution is given by* $a = -\frac{1}{h^2}$, $b = \frac{2}{h^2}$ *and* $c = -\frac{1}{h^2}$ *so that the desired approximation is Note that* $c = a$ *implies that the leading error term is the one involving* $f^{(4)}$. *The Taylor series with remainder (at that term) are*

$$f(x \pm h) = f(x) \pm f'(x) + \frac{h^2}{2}f''(x) \pm \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(\xi_\pm),$$

where $\xi_+ \in (x, x+h)$ *and* $\xi_- \in (x-h, x)$. *Thus,*

$$\frac{-f(x-h)+2f(x)-f(x+h)}{h^2} = -f''(x) - \frac{h^2}{24}\left(f^{(4)}(\xi_+)+f^{(4)}(\xi_-)\right).$$

The approximation is second order but requires $f \in C^4[x-h, x+h]$.

11. Lecture 11

11.1. **Differentiation via Polynomial Interpolation.** Suppose we want a differentiation formula of the form

$$f'(x) = \sum_{i=0}^{n} \alpha_i f(x_i),$$

with $\{x_0, ..., x_n\}$ distinct in $[a, b]$.

Let $p \in \mathbb{P}^n$ be the polynomial interpolating f at $x_0, ..., x_n$, i.e.

$$p(x) = \sum_{i=0}^{n} l_i(x) f(x_i),$$

where $l_i(x)$ are the Lagrange polynomials (see Section 3.2). Then $p'(x) = \sum_{i=0}^{n} l_i'(x) f(x_i)$ should approximate $f'(x)$. This is indeed the case at $x = x_i$, $i = 0, ..., n$ but it is less clear what happen when x is not an interpolation point.

Theorem 11.1. *Assume that* $f \in C^{n+1}[a, b]$, $\{x_0, ..., x_n\}$ *distinct in* $[a, b]$ *and* $p \in \mathbb{P}^n$ *interpolates* f *at* $x_0, ..., x_n$. *Then, there exists* $\xi_j \in [a, b]$ *such that*

$$f'(x_j) - p'(x_j) = \frac{f^{(n+1)}(\xi_j)}{(n+1)!} \prod_{l \neq j} (x_j - x_l).$$

Proof. For $x \notin \{x_0, ..., x_n\}$, define

$$\Theta(x) := \frac{f(x) - p(x)}{\prod_{i=0}^{n} (x - x_i)} (n+1)! \qquad .$$

Note that Theorem 4.1 guarantees that

$$f(x) - p(x) = \frac{f^{(n+1)}(\xi_x)}{(n+1)!} \prod_{i=0}^{n} (x - x_i)$$

so

$$\Theta(x) = f^{(n+1)}(\xi_x)$$

Since we do not know what happens to ξ_x when $x \to x_j$, we cannot use this representation further but it shows that

$$\Theta(x) \in \text{Range}(f^{(n+1)}), \qquad \text{for } x \in [a, b].$$

Instead, we evaluate

$$\lim_{x \to x_j} \Theta(x) = \lim_{x \to x_j} \frac{(f(x) - p(x))(n+1)!}{\prod_{i=0}^{n} (x - x_i)}.$$

This is a 0/0 type of indetermination so we can use L'Hospital's rule

$$\lim_{x \to x_j} \Theta(x) = \lim_{x \to x_j} \frac{(f'(x) - p'(x))(n+1)!}{\left(\prod_{i=0}^{n} (x - x_i)\right)'}.$$

We now compute the denominator

$$\left(\prod_{i=0}^{n} (x - x_i) \right)' = \sum_{i=0}^{n} \prod_{l \neq i} (x - x_l).$$

Each term of the above sum has a factor $(x - x_j)$ except when $i = j$ and so the only one that is not vanishing when $x \to x_j$ is the *ith* factor. This implies that

$$\lim_{x \to x_j} \left(\prod_{i=0}^{n} (x - x_i) \right)' = \prod_{l \neq j} (x_j - x_l)$$

and thus

$$\lim_{x \to x_j} \Theta(x) = \frac{(f'(x_j) - p'(x_j))(n+1)!}{\prod_{l \neq j}(x_j - x_l)}.$$

Now, $f^{(n+1)}$ is continuous on $[a, b]$ by assumption and we have already seen that

$$\Theta(x) \in \text{Range}(f^{(n+1)}), \qquad \text{for } x \in [a, b].$$

In particular,

$$\lim_{x \to x_j} \Theta(x) \in \text{Range}(f^{(n+1)})$$

or, there exists $\xi_j \in [a, b]$ with

$$\lim_{x \to x_j} \Theta(x) = \xi_j.$$

Thus

$$f^{(n+1)}(\xi_j) = \frac{(f'(x_j) - p'(x_j))(n+1)!}{\prod_{l \neq j}(x_j - x_l)},$$

which is the desired estimate after simple algebraic manipulations. □

Remark 11.1 (Continuity of ξ_x). Within the proof of the above theorem, we actually showed that the function

$$x \mapsto f^{(n+1)}(\xi_x)$$

is continuous on $[a, b]$ provided $f \in C^{(n+1)}[a, b]$. This fact will be used later.

Example 11.1 (3 points differentiation scheme). *Use polynomial interpolation to derive an approximation to the derivative of the form*

$$f'(x) \approx af(x) + bf(x-h) + cf(x-2h).$$

We first compute the lagrange basis for the interpolation points $\{x, x-h, x-2h\}$ *(we use t for the variable for a fixed x)*

$$\begin{aligned}
l_0(t) &= \frac{(t-(x-h))(t-(x-2h))}{(x-(x-h))(x-(x-2h))} = \frac{t^2 - (2x-3h)t + (x-h)(x-2h)}{2h^2}; \\
l_1(t) &= \frac{(t-x)(t-(x-2h))}{((x-h)-x)((x-h)-(x-2h))} = \frac{t^2 - (2x-2h)t + x(x-2h)}{-h^2}; \\
l_2(t) &= \frac{(t-x)(t-(x-h))}{(x-2h-x)(x-2h-(x-h))} = \frac{t^2 - (2x-h)t + x(x-h)}{2h^2}.
\end{aligned}$$

The associated interpolant is

$$p(t) = l_0(t)f(x) + l_1(t)f(x-h) + l_2(t)f(x-2h)$$

so that

$$f'(x) \approx l_0'(x)f(x) + l_1'(x)f(x-h) + l_2'(x)f(x-2h).$$

This means

$$\begin{aligned} f'(x) \approx& \frac{2x-(2x-3h)}{2h^2}f(x) + \frac{2x-(2x-2h)}{-h^2}f(x-h) + \frac{2x-(2x-h)}{2h^2}f(x-2h) \\ =& \frac{3}{2h}f(x) - \frac{2}{h}f(x-h) + \frac{1}{2h}f(x-2h). \end{aligned}$$

The error term is

$$\begin{aligned} f'(x) - \left(\frac{3}{2h}f(x) - \frac{2}{h}f(x-h) + \frac{1}{2h}f(x-2h)\right) &= \frac{f'''(\xi_0)}{6}(x-(x-h))(x-(x-2h)) \\ &= \frac{f'''(\xi_0)}{3}h^2. \end{aligned}$$