Mathematical Tripos Part IB: Easter 2001

Numerical Analysis – Lecture 12[1]

8.3 Numerical differentiation

Consider the interpolating formulae for numerical differentiation

$$\ell(f) = f^{(k)}(x) \approx \sum_{i=0}^{n} a_i f(x_i), \qquad a_i = \ell(L_i) = L_i^{(k)}(x),$$

which are exact on the polynomials of degree n. The simplest ones are with $n = k$, i.e., $f^{(k)}(x) \approx p^{(k)}(x)$ where p is the interpolating polynomial of degree k. But $p^{(k)}(x)$ is $k!$ times the leading coefficient of p, i.e., $k!f[x_0, \dots, x_k]$, and we obtain the simplest rules $f^{(k)}(x) \approx k!f[x_0, \dots, x_k]$.

Examples.

the forward difference:	$\boxed{f'(x) \approx f[x, x+h] = \frac{f(x+h)-f(x)}{h}}$	2-point, exact on linear f-ns
the central difference:	$\boxed{f'(x) \approx f[x-h, x+h] = \frac{f(x+h)-f(x-h)}{2h}}$	2-point, of higher accuracy, exact on quadratics
the 2-nd central difference:	$\boxed{f''(x) \approx 2f[x-h, x, x+h] = \frac{f(x-h)-2f(x)+f(x-h)}{h^2}}$	3-point, of higher accuracy, exact on cubics

Example. $2 = n > k = 1$, $[a, b] = [-1, 1]$. (Of course, one can transform any formula to any interval.)

$$f'(0) \approx -\tfrac{3}{2} f(0) + 2f(1) - \tfrac{1}{2} f(2) \tag{8.2}$$

Example. A general formula has the form $\ell(f) \approx \sum_{i=0}^{n} a_i \ell_i(f)$, where ℓ_i can be any fixed functionals, e.g.,

$$f(x+2h) \approx f(x+h) + h[\tfrac{3}{2} f'(x+h) - \tfrac{1}{2} f'(x)]$$

9 Error of approximation

Given an approximation $\ell(f) \approx \sum_{i=0}^{n} a_i f(x_i)$, we are interested of course in its error

$$e(f) := \ell(f) - \sum_{i=0}^{n} a_i f(x_i).$$

If ℓ acts on C^{n+1}, then it is natural to seek an estimate in terms of $f^{(n+1)}$. For the interpolating formulae we obtain

$$e(f) := \ell(f) - \ell(p) = \ell(f - p), \qquad e(f) = 0 \quad \forall f \in \mathbb{P}_n.$$

9.1 The Peano kernel theorem

Our point of departure is the *Taylor formula with an integral remainder term*,

$$f(x) = \sum_{j=0}^{n} \frac{(x-a)^j}{j!} f^{(j)}(a) + \frac{1}{n!} \int_a^x (x-\theta)^k f^{(n+1)}(\theta)\, \mathrm{d}\theta, \tag{9.1}$$

where the sum is the *Taylor polynomial* to f (at the point a). One can can verify (9.1) by integration by parts. It is standard to write the remainder in the slightly different form,

$$r(x) = \frac{1}{n!} \int_a^b (x-\theta)_+^k f^{(n+1)}(\theta)\, \mathrm{d}\theta, \quad \text{where } (x-\theta)_+^k = [\max(x-\theta, 0)]^k,$$

which makes the range of integration independent of x. Let L be a linear functional on C^{n+1} which vanishes on $\mathbb{P}_n$. Then $L(f) = L(r) = \frac{1}{n!} L\left(\int_a^b (x-\theta)_+^k f^{(n+1)}(\theta)\, \mathrm{d}\theta\right)$. Set $g_\theta(x) := (x-\theta)_+^k$, and $K(\theta) := L[g_\theta] := L[(x-\theta)_+^k]$. The function K is called the *Peano kernel* of L.

[1]Corrections and suggestions to these notes should be emailed to `a.shadrin@damtp.cam.ac.uk`. All handouts are available on the WWW at the URL `http://www.damtp.cam.ac.uk/user/na/PartIB/Handouts.html`.

The Peano kernel theorem. *With L and K as above,*

$$L(f) = \tfrac{1}{n!}\int_a^b K(\theta) f^{(n+1)}(\theta)\,\mathrm{d}\theta \tag{9.2}$$

provided that the exchange of L with the integration sign is valid. □

Remark. Typically, forming L involves differentiation, integration and linear combination of function values. In these cases the exchange is justified.

Example 1 (*Formula* (8.2)). The error can be expressed as

$$e(f) = f'(0) - [-\tfrac{3}{2}f(0) + 2f(1) - \tfrac{1}{2}f(2)] = \tfrac{1}{2!}\int_0^2 K(\theta) f'''(\theta)\,\mathrm{d}\theta$$

where with $g_\theta(x) := (x-\theta)_+^2$

$$K(\theta) = e(g_\theta) = 2(0-\theta)_+ - \big[-\tfrac{3}{2}(0-\theta)_+^2 + 2(1-\theta)_+^2 - \tfrac{1}{2}(2-\theta)_+^2\big] = \begin{cases} 2\theta - \frac{3}{2}\theta^2, & \theta \in [0,1], \\ \frac{1}{2}(2-\theta)^2, & \theta \in [1,2]. \end{cases} \tag{9.3}$$

Example 2 (*The midpoint rule*). The error can be expressed as

$$e(f) = \int_{-1}^1 f(x)\,\mathrm{d}x - 2f(0) = \int_{-1}^1 K(\theta) f''(\theta)\,\mathrm{d}\theta$$

where with $g_\theta(x) := (x-\theta)_+^1$

$$K(\theta) = e(g_\theta) = \int_{-1}^1 (x-\theta)_+^1\,\mathrm{d}x - 2(0-\theta)_+^1 = \begin{cases} \frac{1}{2}(1+\theta)^2, & \theta \in [-1,0], \\ \frac{1}{2}(1-\theta)^2, & \theta \in [0,1]. \end{cases} \tag{9.4}$$

Theorem. *Suppose that K doesn't change sign in (a,b) and that $f \in \mathrm{C}^{n+1}[a,b]$. Then*

$$L(f) = \Big(\tfrac{1}{n!}\int_a^b K(\theta)\,\mathrm{d}\theta\Big)\, f^{(n+1)}(\xi) \quad \textit{for some} \quad \xi \in (a,b). \tag{9.5}$$

Proof. Let $K \ge 0$. Then, letting $c(K) := \frac{1}{n!}\int_a^b K(\theta)\,\mathrm{d}\theta$, we obtain

$$c(K)\min_{x\in[a,b]} f^{(n+1)}(x) \le \underbrace{\tfrac{1}{n!}\int_a^b K(\theta) f^{(n+1)}(\theta)\,\mathrm{d}\theta}_{L(f)} \le c(K)\max_{x\in[a,b]} f^{(n+1)}(x),$$

so that, by the intermediate value theorem, there is a $\xi \in [a,b]$ s.t. $c(K)f^{(n+1)}(\xi) = L(f)$. □

Examples 1-2 (*again*). In both cases $K \ge 0$, so that calculating the integrals in (9.3)-(9.4) we obtain

1) $e(f) = \frac{1}{2!}\cdot\frac{2}{3}\cdot f'''(\xi) = \frac{1}{3}f'''(\xi)$ for the formula (8.2) 2) $e(f) = \frac{1}{3}\cdot f''(\xi)$ for the midpoint rule.

Corollary. *Let $\ell(f) = f^{(k)}(x)$ and let a formula $f^{(k)}(x) \approx \sum_{i=0}^n a_i f(x_i)$ be exact on $\mathbb{P}_n$. If the Peano kernel K for the error functional $e(\cdot)$ does not change its sign, then, for some $\xi \in (a,b)$,*

$$e(f) = \tfrac{1}{(n+1)!}\omega^{(k)}(x) f^{(n+1)}(\xi), \qquad \omega(x) = \textstyle\prod_{i=0}^n (x - x_i) \tag{9.6}$$

Proof. We need to prove that $\int_a^b K(\theta)\,\mathrm{d}\theta = \frac{1}{n+1}\omega^{(k)}(x)$. Substitute $f(x) = \omega(x)$ into (9.2). Since $f(x_i) = 0$, the left-hand side becomes $e(f) = f^{(k)}(x) = \omega^{(k)}(x)$. And because $f^{(n+1)}(x) \equiv (n+1)!$, the right-hand side will be $\frac{1}{n!}\int_a^b K(\theta) f^{(n+1)}(\theta)\,\mathrm{d}\theta = (n+1)\int_a^b K(\theta)\,\mathrm{d}\theta$. □

Example 1 (*again and again*). Since $K \ge 0$, and $\omega(x) = x(x-1)(x-2)$, it follows that $e(f) = \frac{1}{3!}\omega'(0)f'''(\xi) = \frac{1}{3}f'''(\xi)$, in accordance with previous calculations.

For any formula $f^{(k)}(x) \approx p^{(k)}(x) = \sum_{i=0}^n a_i f(x_i)$, there is a complete description (in terms of (x_i)) of those points $x \in [a,b]$ for which the Peano kernel of the error functional does not change its sign. In particular, these are the end-points of $[a,b]$ (again in accordance with the Example).

Function norms: The value $f^{(n+1)}(\xi)$, say in (9.5)-(9.6), with *some* $\xi \in [a,b]$ is useless. One uses instead the bounds for the so-called L_p-*norms* $\|g\|_p$ which for $p = 1, 2, \infty$ are

$$\|g\|_1 = \int_a^b |f(x)|\,\mathrm{d}x, \qquad \|g\|_2 = \{\int_a^b [g(x)]^2\,\mathrm{d}x\}^{1/2}, \qquad \|g\|_\infty = \max_{x\in[a,b]} |g(x)|.$$

The equality $e(f) = \frac{1}{3}f'''(\xi)$ is being rewritten then as $|e(f)| \le \frac{1}{3}\|f'''\|_\infty$.

Likewise we can easily deduce from $\big|\int_a^b f(x)g(x)\,\mathrm{d}x\big| \le \|g\|_\infty \|f\|_1$ that

$$|L(f)| \le \tfrac{1}{n!}\|K\|_1 \|f^{(n+1)}\|_\infty \qquad \text{and} \qquad |L(f)| \le \tfrac{1}{n!}\|K\|_\infty \|f^{(n+1)}\|_1,$$

what is valid also when K changes sign.