

Mathematical Tripos Part IB: Lent Term 2024

Numerical Analysis – Lecture 5

5 Error of approximation

Given a linear functional λ and an approximation formula $\lambda(f) \approx \sum_{i=0}^N a_i f(x_i)$, we are interested in the error (which is a linear functional as well)

$$e_\lambda(f) := \lambda(f) - \sum_{i=0}^N a_i f(x_i).$$

If λ acts on $f \in C^{n+1}[a, b]$, then it is natural to seek an estimate in terms of $\|f^{(n+1)}\|_\infty$, i.e.,

$$|e_\lambda(f)| \leq c_\lambda \|f^{(n+1)}\|_\infty, \quad \forall f \in C^{n+1}[a, b]. \quad (5.1)$$

Since $f^{(n+1)} \equiv 0$ on $\mathcal{P}_n$, such an estimate can exist only if

$$e_\lambda(f) = 0 \quad \text{on } \mathcal{P}_n,$$

i.e., the approximation formula *must be exact* on $\mathcal{P}_n$ (e.g., it can be interpolating of degree n).

If (5.1) holds with some c_λ and moreover, for any $\epsilon > 0$, there is an $f_\epsilon \in C^{n+1}[a, b]$ such that

$$|e_\lambda(f_\epsilon)| > (c_\lambda - \epsilon) \|f_\epsilon^{(n+1)}\|_\infty,$$

then the constant c_λ in inequality (5.1) is called *least* or *sharp*. The next section gives a general approach to obtaining *sharp* estimates for the error functionals e_λ that vanish on $\mathcal{P}_n$.

5.1 Peano kernel theorem

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

$$f(x) = \sum_{i=0}^n \frac{1}{i!} (x-a)^i f^{(i)}(a) + \frac{1}{n!} \int_a^x (x-t)^n f^{(n+1)}(t) dt, \quad (5.2)$$

where the sum is the *Taylor polynomial* q_n to f (at the point a). One can verify (5.2) by integration by parts. It is standard to write the remainder R in the slightly different form, which makes the range of integration independent of x :

$$R(x) = \frac{1}{n!} \int_a^b (x-t)_+^n f^{(n+1)}(t) dt, \quad \text{with } (x-t)_+^n := (\max\{x-t, 0\})^n.$$

Let μ be a linear functional on C^{n+1} . Then

$$\mu(f) = \mu(q_n) + \mu(R) = \mu(q_n) + \frac{1}{n!} \mu\left(\int_a^b (x-t)_+^n f^{(n+1)}(t) dt\right). \quad (5.3)$$

Let us formally put μ under the integration sign (that is exchange action of μ and of $\int_a^b$), so that, for any *fixed* value of t , it will act on the function

$$g_t(\bullet) := (\bullet - t)_+^n,$$

a function, say, of x which (for a given t) is defined as $g_t(x) := (x-t)_+^n$, $x \in [a, b]$. To each value $t \in \mathbb{R}$ there corresponds a value $\mu(g_t) \in \mathbb{R}$, thus we have a function

$$K_\mu(t) := \mu(g_t) := \mu((\bullet - t)_+^n), \quad t \in \mathbb{R}.$$

It is called the *Peano kernel* of the functional μ . So, formally, we can rewrite (5.3) as

$$\mu(f) = \mu(q_n) + \frac{1}{n!} \int_a^b K_\mu(t) f^{(n+1)}(t) dt. \quad (5.4)$$

Definition 5.1 Denote by Λ_0 the set of linear functionals which are linear combinations of the functionals of two types

$$1) \mu(f) = f^{(k)}(\bar{x}) \quad (0 \leq k \leq n), \quad \bar{x} \in [a, b], \quad 2) \mu(f) = \int_a^{\bar{x}} f(x) w(x) dx, \quad \bar{x} \in [a, b].$$

Lemma 5.2 (without proof) If $\mu \in \Lambda_0$, then equality (5.4) is valid (i.e., exchange of μ and $\int_a^b$ is justified).

Theorem 5.3 (Peano kernel theorem) Let $\lambda \in \Lambda_0$ and let $\lambda(f) \approx \sum_{i=0}^N a_i f(x_i)$ be an approximation formula which is exact on $\mathcal{P}_n$. Then the error functional e_λ (and any other functional from Λ_0 that vanishes on $\mathcal{P}_n$) has the integral representation

$$e_\lambda(f) = \frac{1}{n!} \int_a^b K_{e_\lambda}(t) f^{(n+1)}(t) dt. \quad (5.5)$$

Proof. The formula follows from (5.4), where we put e_λ instead of μ , and use assumptions $e_\lambda \in \Lambda_0$ and $e_\lambda(q_n) = 0$. $\square$

5.2 Sharp error bounds

Theorem 5.4 Under the assumptions of the previous theorem, for any $f \in C^{n+1}$, we have the sharp inequality

$$|e_\lambda(f)| \leq c_\lambda \|f^{(n+1)}\|_\infty, \quad c_\lambda = \frac{1}{n!} \|K_{e_\lambda}\|_1, \quad (5.6)$$

where $\|K_{e_\lambda}\|_1 := \int_a^b |K_{e_\lambda}(t)| dt$, and $\|f^{(n+1)}\|_\infty := \max_{t \in [a, b]} |f^{(n+1)}(t)|$.

Proof. Applying the inequality

$$\left| \int_a^b g(t) h(t) dt \right| \leq \int_a^b |g(t)| dt \cdot \max_{t \in [a, b]} |h(t)| =: \|g\|_1 \|h\|_\infty \quad (5.7)$$

to the right-hand side of (5.5), we obtain (5.6).

Let us show that the constant c_λ in (5.6) is *sharp* (the least possible). In (5.7), equality occurs if we take $h(t) = \operatorname{sgn} g(t)$. Therefore, we get equality in (5.6) taking f_0 with $f_0^{(n+1)}(t) = \operatorname{sgn} K_{e_\lambda}(t)$. $\square$

Remark 5.5 A minor problem in the above proof of sharpness of c_λ is that the sign-function $f_0^{(n+1)}$ that provides equality in (5.6) is not continuous, whereas we consider $f \in C^{n+1}$.

Informally, we just *allow* the functions with piecewise continuous $(n+1)$ -st derivative, like $|x|^{n+1}$, to be considered together with $f \in C^{n+1}$.

Formally, we can approximate a discontinuous sign-function $f_0^{(n+1)}$ by a continuous function $f_\epsilon^{(n+1)}$ changing $f_0^{(n+1)}$ by a linear function on arbitrarily small intervals, say of length ϵ' , around the jumps. This will change the integral value in (5.5) by ϵ'' , hence for such f_ϵ we get the estimate $e_\lambda(f_\epsilon) > (c_\lambda - \epsilon) \|f_\epsilon^{(n+1)}\|_\infty$. Thus, c_λ in (5.6) is the least possible constant on C^{n+1} as well.

Finally, here are two general results on the sharp constants in numerical integration and numerical differentiation.

Theorem 5.6 (Error of Gaussian quadrature) Given $n \in \mathbb{N}$ and $w(x) \geq 0$, let $(a_i)_{i=0}^n$ and $(x_i)_{i=0}^n$ be the weights and nodes of the Gaussian quadrature, respectively, i.e., (x_i) are zeros of the monic orthogonal polynomial Q_{n+1} . Then we have the sharp inequality

$$\left| \int_a^b f(x) w(x) dx - \sum_{i=0}^n a_i f(x_i) \right| \leq \frac{1}{(2n+2)!} \|Q_{n+1}\|_2^2 \|f^{(2n+2)}\|_\infty.$$

Theorem 5.7 (Shadrin) For any $n \in \mathbb{N}$ and any $\Delta = (x_i)_{i=0}^n$, let $\ell_\Delta \in \mathcal{P}_n$ be the polynomial that interpolates f on Δ . Then, for any $1 \leq k \leq n$, we have the sharp inequality

$$\|f^{(k)} - \ell_\Delta^{(k)}\|_\infty \leq \frac{1}{(n+1)!} \|\omega_\Delta^{(k)}\|_\infty \|f^{(n+1)}\|_\infty.$$

5.3 Examples

Example 5.8 Take formula (4.4):

$$f'(0) \approx -\frac{3}{2}f(0) + 2f(1) - \frac{1}{2}f(2).$$

It is exact on $\mathcal{P}_2$, hence the error on $C^3[0, 2]$ can be expressed as

$$e(f) := f'(0) - \left[-\frac{3}{2}f(0) + 2f(1) - \frac{1}{2}f(2) \right] = \frac{1}{2!} \int_0^2 K(t) f'''(t) dt.$$

Here, with $g_t(x) := (x - t)_+^2$, the Peano kernel K has the form

$$\begin{aligned} K(t) = e(g_t) &= 2(0 - t)_+^1 + \frac{3}{2}(0 - t)_+^2 - 2(1 - t)_+^2 + \frac{1}{2}(2 - t)_+^2 \\ &= \begin{cases} -2(1 - t)^2 + \frac{1}{2}(2 - t)^2 & t \in [0, 1], \\ \frac{1}{2}(2 - t)^2 & t \in [1, 2]. \end{cases} \end{aligned}$$

So, $K(t) \geq 0$, and integration gives the value

$$\|K\|_1 := \int_0^2 |K(t)| dt = \left(\int_0^1 + \int_1^2 \right) K(t) dt = \frac{1}{2} + \frac{1}{6} = \frac{2}{3}.$$

Therefore, we have the estimate

$$|e(f)| \leq \frac{1}{2!} \frac{2}{3} \|f'''\|_\infty = \frac{1}{3} \|f'''\|_\infty.$$

The constant $c = \frac{1}{3}$ is sharp: since $K(t) \geq 0$, we will get equality for $f''' \equiv \text{const}$, e.g. for $f(x) = x^3$.

Example 5.9 The Simpson's rule,

$$\int_{-1}^1 f(t) dt \approx \int_{-1}^1 p_2(t) dt = \frac{1}{3}f(-1) + \frac{4}{3}f(0) + \frac{1}{3}f(1),$$

is exact on $\mathcal{P}_2$, hence the error on $C^3[-1, 1]$ is

$$e(f) = \int_{-1}^1 f(t) dt - \frac{1}{3}f(-1) - \frac{4}{3}f(0) - \frac{1}{3}f(1) = \frac{1}{2!} \int_{-1}^1 K(t) f'''(t) dt,$$

where with $g_t(x) := (x - t)_+^2$

$$\begin{aligned} K(t) = e(g_t) &= \int_{-1}^1 (x - t)_+^2 dx - \frac{1}{3}(-1 - t)_+^2 - \frac{4}{3}(0 - t)_+^2 - \frac{1}{3}(1 - t)_+^2 \\ &= \begin{cases} \frac{1}{3}(1 - t)^3 - \frac{4}{3}t^2 - \frac{1}{3}(1 - t)^2 & t \in [-1, 0] \\ \frac{1}{3}(1 - t)^3 - \frac{1}{3}(1 - t)^2 & t \in [0, 1] \end{cases} \end{aligned}$$

Now, $K(t)$ changes its sign at $t = 0$, so its L_1 -norm has the value

$$\|K\|_1 := \int_{-1}^1 |K(t)| dt = \left(\int_{-1}^0 - \int_0^1 \right) K(t) dt = 2 \cdot \frac{1}{3} \left(\frac{1}{2} - \frac{2}{3} + \frac{1}{4} \right) = \frac{1}{18},$$

so that

$$e(f) \leq \frac{1}{2!} \frac{1}{18} \|f'''\|_\infty = \frac{1}{36} \|f'''\|_\infty.$$

The constant $c = \frac{1}{36}$ is sharp again: since $K(t)$ changes its sign at one point $t = 0$, we get equality for $f'''(t) = C \operatorname{sgn} t$, e.g. for $f(x) = |x|^3$. For this f its third derivative has a jump, but for any $\epsilon > 0$ it can be approximated by $f_\epsilon \in C^3$ for which the constant would be $c > \frac{1}{36} - \epsilon$, i.e.

$$e(f_\epsilon) > \left(\frac{1}{36} - \epsilon \right) \|f_\epsilon'''\|_\infty.$$