Mathematical Tripos Part IB: Lent 2020

Numerical Analysis – Lecture 5[1]

We commence our construction of *Gaussian quadrature* by choosing pairwise-distinct nodes $c_1, c_2, \ldots, c_\nu \in [a,b]$ and define the *interpolatory weights*

$$b_k := \int_a^b w(x) \prod_{\substack{j=1 \\ j\neq k}}^{\nu} \frac{x-c_j}{c_k-c_j}\,\mathrm{d}x, \qquad k=1,2,\ldots,\nu.$$

Theorem The quadrature formula with the above choice is exact for all $f \in \mathbb{P}_{\nu-1}[x]$. Moreover, if $c_1, c_2, \ldots, c_\nu$ are the zeros of p_ν then it is exact for all $f \in \mathbb{P}_{2\nu-1}[x]$.

Proof. Every $f \in \mathbb{P}_{\nu-1}[x]$ is its own interpolating polynomial, hence by Lagrange's formula

$$f(x) = \sum_{k=1}^{\nu} f(c_k) \prod_{\substack{j=1 \\ j\neq k}}^{\nu} \frac{x-c_j}{c_k-c_j}. \tag{2.7}$$

The quadrature is exact for all $f \in \mathbb{P}_{\nu-1}[x]$ if $\int_a^b w(x)f(x)\,\mathrm{d}x = \sum_{k=1}^{\nu} b_k f(c_k)$, and this, in tandem with the interpolating-polynomial representation, yields the stipulated form of $b_1, \ldots, b_\nu$.

Let $c_1, \ldots, c_\nu$ be the zeros of p_ν. Given any $f \in \mathbb{P}_{2\nu-1}[x]$, we can represent it uniquely as $f = qp_\nu + r$, where $q, r \in \mathbb{P}_{\nu-1}[x]$. Thus, by orthogonality,

$$\begin{aligned}\int_a^b w(x)f(x)\,\mathrm{d}x &= \int_a^b w(x)[q(x)p_\nu(x)+r(x)]\,\mathrm{d}x = \langle q, p_\nu\rangle + \int_a^b w(x)r(x)\,\mathrm{d}x \\ &= \int_a^b w(x)r(x)\,\mathrm{d}x.\end{aligned}$$

On the other hand, the choice of quadrature knots gives

$$\sum_{k=1}^{\nu} b_k f(c_k) = \sum_{k=1}^{\nu} b_k[q(c_k)p_\nu(c_k)+r(c_k)] = \sum_{k=1}^{\nu} b_k r(c_k).$$

Hence the integral and its approximation coincide, because $r \in \mathbb{P}_{\nu-1}[x]$ and the quadrature is exact for all polynomials in $\mathbb{P}_{\nu-1}[x]$. □

Example Let $[a,b]=[-1,1]$, $w(x)\equiv 1$. Then the underlying orthogonal polynomials are the *Legendre polynomials:* $P_0 \equiv 1$, $P_1(x)=x$, $P_2(x)=\frac{3}{2}x^2-\frac{1}{2}$, $P_3(x)=\frac{5}{2}x^3-\frac{3}{2}x$, $P_4(x)=\frac{35}{8}x^4-\frac{15}{4}x^2+\frac{3}{8}$ (it is customary to use this, non-monic, normalisation). The nodes of Gaussian quadrature are

$\nu=1$: $c_1=0$;

$\nu=2$: $c_1=-\frac{\sqrt{3}}{3}$, $c_2=\frac{\sqrt{3}}{3}$;

$\nu=3$: $c_1=-\frac{\sqrt{15}}{5}$, $c_2=0$, $c_3=\frac{\sqrt{15}}{5}$;

$\nu=4$: $c_1=-\sqrt{\frac{3}{7}+\frac{2}{35}\sqrt{30}}$, $c_2=-\sqrt{\frac{3}{7}-\frac{2}{35}\sqrt{30}}$, $c_3=\sqrt{\frac{3}{7}-\frac{2}{35}\sqrt{30}}$, $c_4=\sqrt{\frac{3}{7}+\frac{2}{35}\sqrt{30}}$.

3 The Peano kernel theorem

In the previous section we looked at quadrature formulae that are exact for polynomials up to certain degree n. The aim of this section is to present a tool that allows us to bound the error if we use the quadrature formula for functions f that are not in $\mathbb{P}_n[x]$. The result we will state is actually quite general, and is not

[1] Corrections and suggestions to these notes should be emailed to `h.fawzi@damtp.cam.ac.uk`.

restricted to quadrature formulae, however we will use quadrature formulae as a running example for the sake of motivation. The error function for a quadrature formula is

$$L(f) = \int_a^b w(x)f(x)dx - \sum_{k=1}^{\nu} b_k f(c_k).$$

Assume that $f \in \mathrm{C}^{n+1}[a,b]$ and consider Taylor's formula with integral remainder:

$$f(x) = \underbrace{f(a) + (x-a)f'(a) + \frac{(x-a)^2}{2!}f''(a) + \cdots + \frac{(x-a)^n}{n!}f^{(n)}(a)}_{g(x)} + \frac{1}{n!}\int_a^x (x-\theta)^n f^{(n+1)}(\theta)\,\mathrm{d}\theta. \quad (3.1)$$

Since g is a polynomial of degree n, and since our quadrature formula is exact for polynomials up to degree n we have $L(g) = 0$. It thus follows, since L is linear that

$$L(f) = L\left\{x \mapsto \frac{1}{n!}\int_a^x (x-\theta)^n f^{(n+1)}(\theta)\,\mathrm{d}\theta\right\}.$$

To make the range of integration independent of x, we introduce the notation

$$(x-\theta)_+^n := \begin{cases} (x-\theta)^n, & x \geq \theta, \\ 0, & x \leq \theta, \end{cases} \qquad \text{whence} \qquad L(f) = \frac{1}{n!}L\left\{x \mapsto \int_a^b (x-\theta)_+^n f^{(n+1)}(\theta)\,\mathrm{d}\theta\right\}.$$

Let $K(\theta) := L[x \mapsto (x-\theta)_+^n]$ for $x \in [a,b]$. *[Note: K is independent of f.]* The function K is called the *Peano kernel* of L. ***Suppose that it is allowed to exchange the order of action of $\int$ and L.*** Because of the linearity of L, we then have

$$L(f) = \frac{1}{n!}\int_a^b K(\theta) f^{(n+1)}(\theta)\,\mathrm{d}\theta. \quad (3.2)$$

The Peano kernel theorem Let L be a linear functional such that $L(f) = 0$ for all $f \in \mathbb{P}_n[x]$. Provided that $f \in \mathrm{C}^{n+1}[a,b]$ and the above exchange of L with the integration sign is valid, the formula (3.2) is true. □

Example Consider Simpson's rule $\int_{-1}^{1} f(x)\,\mathrm{d}x \approx \frac{1}{3}(f(-1)+4f(0)+f(1))$. One can verify that the Simpson rule is exact for polynomials up to degree 2 (in fact it is also true for polynomials up to degree 3). Let $L(f) = \int_{-1}^{1} f(x)dx - \frac{1}{3}(f(-1)+4f(0)+f(1))$. Peano kernel theorem tells us that for any $f \in \mathrm{C}^3[-1,1]$ we have

$$L(f) = \frac{1}{2}\int_{-1}^{1} K(\theta) f'''(\theta)\,\mathrm{d}\theta,$$

where $K(\theta) = L(x \mapsto (x-\theta)_+^2)$. Since $\int_{-1}^{1}(x-\theta)_+^2\,\mathrm{d}x = \frac{(1-\theta)^3}{3}$ we can verify that

$$\begin{aligned} K(\theta) &= \begin{cases} \frac{(1-\theta)^3}{3} - \frac{1}{3}(0 + 4\theta^2 + (1-\theta)^2) & -1 \leq \theta \leq 0 \\ \frac{(1-\theta)^3}{3} - \frac{1}{3}(0 + 4\cdot 0 + (1-\theta)^2) & 0 \leq \theta \leq 1 \end{cases} \\ &= \begin{cases} -\frac{1}{3}\theta(1+\theta)^2 & -1 \leq \theta \leq 0 \\ -\frac{1}{3}\theta(1-\theta)^2 & 0 \leq \theta \leq 1. \end{cases} \end{aligned} \quad (3.3)$$

This allows us to bound the approximation error for Simpson's rule. Indeed for any $f \in \mathrm{C}^3[-1,1]$ we get

$$|L(f)| \leq \frac{1}{2}\int_{-1}^{1} |K(\theta)||f'''(\theta)|\,\mathrm{d}\theta \leq \frac{1}{36}\|f'''\|_\infty$$

where $\|f'''\|_\infty := \max_{x\in[-1,1]} |f'''(\theta)|$ and where we used the fact $\int_{-1}^{1} |K(\theta)|\,\mathrm{d}\theta = \frac{1}{18}$ which can be easily verified from (3.3).