Mathematical Tripos Part IB: Easter Term 2003

Numerical Analysis – Lecture 11

11 Approximation of linear functionals

Given a vector space $\mathbb{X}$ (e.g., $\mathbb{R}^n$, or $C^m[a,b]$), a *linear functional* is any linear mapping

$$\lambda : \mathbb{X} \to \mathbb{R} \qquad \Big(\text{so } \lambda(\alpha f + \beta g) = \alpha\lambda(f) + \beta\lambda(g), \quad \forall f, g \in \mathbb{X} \text{ and } \forall \alpha, \beta \in \mathbb{R}\Big).$$

We will treat the space $\mathbb{X} = C^{n+1}[a,b]$, and the functionals

$$1)\ \ \lambda(f) = f^{(k)}(\bar{x}), \quad (\bar{x}, k \text{ being fixed}), \qquad 2)\ \ \lambda(f) = \textstyle\int_a^b f(x)\, w(x) dx.$$

Our goal is to find an approximation of the form

$$\lambda(f) \approx \textstyle\sum_{i=0}^N a_i f(x_i), \qquad f \in C^{n+1}[a,b] \tag{11.1}$$

For the functionals 1)–2), this is called *numerical differentiation* and *numerical integration*, respectively.

Method 11.1 A suggestive approximation method is to interpolate f by $p \in \mathcal{P}_n$ and take $\lambda(f) \approx \lambda(p)$. This is called the *interpolating formula* (of degree n), in this case $N = n$. We have already seen an interpolating formula, namely that of Lagrange for the functional $\lambda(f) = f(\bar{x})$:

$$f(\bar{x}) \approx p(\bar{x}) = \textstyle\sum_{i=0}^n \ell_i(\bar{x}) f(x_i)$$

By linearity of λ, we have $\lambda(p) = \sum_{i=0}^n \lambda(\ell_i) p(x_i)$, thus the interpolating formula has the form

$$\lambda(f) \approx \textstyle\sum_{i=0}^n \lambda(\ell_i) f(x_i). \tag{11.2}$$

Method 11.2 Another method is to require from the formula (11.1) to be *exact on $\mathcal{P}_n$*, that is to become equality for any $f \in \mathcal{P}_n$. In this case the number N of terms (almost) need not to be restricted, and if $N > n$, then it is certainly not a polynomial of degree n that substitutes the function. If $N < n$, then the formula is of *high accuracy*. However, if $N = n$, then both methods are the same.

Lemma 11.3 *The formula $\lambda(f) \approx \sum_{i=0}^n a_i f(x_i)$ is interpolating $\quad\Leftrightarrow\quad$ it is exact on $\mathcal{P}_n$.*

Proof. The interpolating formula (11.2) is exact on $\mathcal{P}_n$ by definition. Conversely, if the formula in the lemma is exact on $\mathcal{P}_n$, take $f(x) = \ell_j(x)$ to obtain $\lambda(\ell_j) = \sum_{i=0}^n a_i \ell_j(x_i) = a_j$, i.e., (11.2). ∎

11.1 Numerical integration

A formula of numerical integration

$$\lambda(f) := I(f) := \int_a^b f(x)\, w(x)\, dx \approx \sum_{i=0}^n a_i f(x_i), \qquad f \in C[a,b].$$

is called a *quadrature formula* with *nodes* (x_i) and *weights* (a_i). By Lemma 11.3, for any $n+1$ *fixed* (x_i), the interpolating formula $a_i = I(\ell_i)$ is exact on $\mathcal{P}_n$. Can one find a *quadrature of higher accuracy* which is exact on $\mathcal{P}_m$ with some $m > n$? Since we are free in choosing $n+1$ nodes (x_i), we may hope to increase the degree of accuracy n up to $2n+1$. More is impossible.

Claim 11.4 *No quadrature formula with $n+1$ nodes is exact for all $p \in \mathcal{P}_m$ if $m \geq 2n+2$.*

Proof. Take $p(x) = \prod_{i=0}^n (x - x_i)^2 \geq 0$. Then $p \in \mathcal{P}_{2n+2}$, and $I(p) > 0$, but $\sum_{i=0}^n a_i p(x_i) = 0$ for any a_is. Hence the integral and the quadrature do not match. ∎

Our next goal is to show that $m = 2n+1$ can be attained. For this we need

Lemma 11.5 *Let Q_{n+1} be orthogonal to all $p_n \in \mathcal{P}_n$ on $[a,b]$. Then all the zeros of Q_{n+1} are real, distinct and lie in the interval (a,b).*

Proof. Denote by k the number of the sign changes of Q_{n+1} in (a,b) and assume that $k \le n$. If $k = 0$ set $p_k \equiv 1$, and if $1 \le k \le n$ set $p_k(x) := \prod_{i=1}^k (x - t_i)$ where t_is are the points where a sign change of Q_{n+1} occurs. Then $p_k \in \mathcal{P}_k$, $k \le n$, hence $(Q_{n+1}, p_k) = 0$. On the other hand, by construction, $Q_{n+1}(x)p_k(x)$ does not change sign throughout $[a,b]$ and vanishes at a finite number of points, hence $|(Q_{n+1}, p_k)| := \left|\int_a^b Q_{n+1}(x)p_k(x)w(x)dx\right| = \int_a^b |Q_{n+1}(x)p_k(x)|\, w(x)dx > 0$, a contradiction. Thus, $k \ge n+1$ (hence $k = n+1$) and the statement follows. ∎

Theorem 11.6 *Let a quadrature with $n+1$ nodes $(x_i)_{i=0}^n$ be exact on $\mathcal{P}_n$ (i.e. interpolating). Then it is exact on $\mathcal{P}_{2n+1}$ if and only if its nodes $(x_i)_{i=0}^n$ are the zeros of the $(n+1)$-st orthogonal polynomial Q_{n+1}.*

Proof. 1) Let $(x_i)_{i=0}^n$ be the zeros of Q_{n+1}. Given any $p_{2n+1} \in \mathcal{P}_{2n+1}$, we can represent it uniquely as

$$p_{2n+1}(x) = Q_{n+1}(x)r_n(x) + s_n(x), \quad \text{with some} \quad r_n, s_n \in \mathcal{P}_n.$$

Since Q_{n+1} is orthogonal to r_n, we have

$$I(p_{2n+1}) = \int_a^b p_{2n+1}(x)\, w(x)dx = \int_a^b s_n(x)\, w(x)dx = I(s_n).$$

On the other hand, because $Q_{n+1}(x_i) = 0$,

$$\sum_{i=0}^n a_i p_{2n+1}(x_i) = \sum_{i=1}^n a_i s_n(x_i).$$

But $s_n \in \mathcal{P}_n$ while the quadrature is exact on $\mathcal{P}_n$, hence $I(s_n) = \sum a_i s_n(x_i)$, i.e., the right-hand sides of two previous equalities coincide, therefore the left-hand sides coincide too, i.e., $I(p_{2n+1}) = \sum a_i p_{2n+1}(x_i)$.

2) Conversely, if a quadrature with $n+1$ nodes (x_i) is exact for all $p \in \mathcal{P}_{2n+1}$, then letting $Q_{n+1}(x) := \prod_{i=0}^n (x - x_i) \in \mathcal{P}_{n+1}$ and taking any $q_n \in \mathcal{P}_n$ we find

$$\int_a^b Q_{n+1}(x)q_n(x)w(x)dx = \sum_{i=0}^n a_i[Q_{n+1}(x_i)q_n(x_i)] = 0$$

i.e., Q_{n+1} is orthogonal to all $q_n \in \mathcal{P}_n$. ∎

Definition 11.7 A quadrature with $n+1$ nodes that is exact on $\mathcal{P}_{2n+1}$ is called *Gaussian quadrature.*

Example 11.8 For $[a,b] = [-1,1]$ and $w(x) \equiv 1$, the underlying orthogonal polynomials are the *Legendre polynomials*. The corresponding weights and nodes of the Gaussian quadratures are as follows.

$P_1(x) = x$	$x_0 = 0$	$a_0 = 2;$
$P_2(x) = \frac{3}{2}(x^2 - \frac{1}{3})$	$x_0 = -\frac{1}{\sqrt{3}}, x_1 = \frac{1}{\sqrt{3}}$	$a_0 = 1, a_1 = 1$
$P_3(x) = \frac{5}{2}(x^3 - \frac{3}{5}x)$	$x_0 = -\sqrt{\frac{3}{5}}, x_1 = 0, x_2 = \sqrt{\frac{3}{5}}$	$a_0 = \frac{5}{9}, a_1 = \frac{8}{9}, a_2 = \frac{5}{9}$

Example 11.9 For $[a,b] = [-1,1]$ and $w(x) = (1-x^2)^{-1/2}$, the orthogonal polynomials are the *Chebyshev polynomials* and the qudrature rule is particularly attractive:

$$T_{n+1}(x) = \cos(n+1)\arccos x, \qquad x_i = \cos\tfrac{2i+1}{2n+2}\pi, \qquad a_i = \tfrac{\pi}{n+1}, \qquad i = 0, \dots, n.$$

Example 11.10 (Simplest quadrature formulae $(w \equiv 1)$).

the rectangle rule:	$\boxed{I(f) \approx (b-a)f(a)}$	1-point, non-Gaussian exact on constants
the midpoint rule:	$\boxed{I(f) \approx (b-a)f(\frac{a+b}{2})}$	1-point, Gaussian, exact on linear fns
the trapezoidal rule:	$\boxed{I(f) \approx (b-a)[\frac{1}{2}f(a) + \frac{1}{2}f(b)]}$	2-point, non-Gaussian, exact on linear fns
the Simpson rule:	$\boxed{I(f) \approx (b-a)[\frac{1}{6}f(a) + \frac{2}{3}f(\frac{a+b}{2}) + \frac{1}{6}f(b)]}$	3-point, non-Gaussian, but of higher accuracy (exact on cubics)

11.2 Numerical differentiation

Consider the interpolating formulae for numerical differentiation

$$\lambda(f) = f^{(k)}(\bar{x}) \approx \textstyle\sum_{i=0}^{n} a_i f(x_i), \qquad a_i = \lambda(\ell_i) = \ell_i^{(k)}(\bar{x}),$$

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

Example 11.11

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

Example 11.12 $2 = n > k = 1$, $[a, b] = [0, 2]$. (Of course, one can transform any formula to any interval.)

$$f'(0) \approx p_2'(0) = -\tfrac{3}{2} f(0) + 2f(1) - \tfrac{1}{2} f(2)\,. \tag{11.3}$$

11.3 Exercises

11.1. Suppose that the function values $f(0), f(1), f(2)$ and $f(3)$ are given and that we wish to estimate

$$f(6), \quad f'(0) \quad \text{and} \quad \int_0^3 f(x)\,dx.$$

One method is to let p be the cubic polynomial that interpolates these function values, and then to employ the approximants

$$p(6), \quad p'(0) \quad \text{and} \quad \int_0^3 p(x)\,dx$$

respectively. Deduce from the Lagrange formula for p that each approximant is a linear combination of the four data with constant coefficients. Calculate the numerical values of these constants. Verify your work by showing that the approximants are exact when f is an arbitrary cubic polynomial.

11.2. Calculate the weights a_1, a_2 and nodes x_1, x_2 so that the approximant

$$\int_0^1 f(x)\,dx \approx a_1 f(x_1) + a_2 f(x_2)$$

is exact when f is a cubic polynomial. You may exploit the fact that x_1 and x_2 are the zeros of a quadratic polynomial that is orthogonal to all linear polynomials. Verify your calculation by testing the formula when $f(x) = 1, x, x^2$ and x^3.