Mathematical Tripos Part IB: Easter 2001

Numerical Analysis – Lecture 11[1]

7.5 Least-squares fitting to discrete function values

Suppose we are given $m+1$ function values $f(x_0),\dots,f(x_m)$ (e.g., the results of observations), where the x_ks are pairwise distinct, and we expect that f should coin with a polynomial of degree n. If $m \le n$, then one can use interpolation. If $m > n$, then the least squares problem can be solved.

Least squares problem. Given $(f(x_i))_{i=0}^m$, find $p^* = \arg\min_{p\in P_n} \sum_{i=0}^m |f(x_i) - p(x_i)|^2 w(x_i)$.

For the weight function w one usually chooses $w \equiv 1$, the different values $w(x_i)$ are being used when accuracy of data depends on x_i (e.g., to supress inaccurate data). With $\|f\| := \langle f, f\rangle^{1/2}$ and $\langle f, g\rangle_w := \sum_{i=0}^m f(x_i)g(x_i)w(x_i)$, it is simply the minimization problem $p^* = \arg\min_{p\in P_n} \|f-p\|$.

Solution. One possibility is to express p as $\sum_{j=0}^n c_j x^j$ and find optimal c_js as a solution of a linear least squares problem (see §5), using QR factorization. An alternative is to construct orthogonal polynomials w.r.t. the scalar product $\langle f, g\rangle_w$. The theory is identical to that of §§7.1–4, except that we have enough data to evaluate p_k only for $k \le m$. However, we need just p_k for $k \le n$ and $n < m$. Thus

1. Employ the recurrence (7.3) to calculate monic $(\tilde p_k)_{k=0}^n$
2. Normalize $p_k = \tilde p_k / \langle \tilde p_k, \tilde p_k\rangle_w^{1/2}$ and form $p(x) = \sum_{k=0}^n \langle p_k, f\rangle p_k(x)$.

Since the work for each k is bounded by a constant multiple of m, the complete cost is $\mathcal{O}(mn)$, as compared with $\mathcal{O}(n^2 m)$ if QR is used.

8 Approximation of linear functionals

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

$$\ell : \mathbb{X} \to \mathbb{R} \qquad (\text{s.t. } \ell(\alpha f + \beta g) = \alpha\ell(f) + \beta\ell(g), \quad \forall f, g \in \mathbb{X}).$$

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

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

Suppose we are given n values $(f(x_i))_{i=0}^n$ only. Our goal is to find an approximation

$$\ell(f) \approx \sum_{i=0}^n a_i f(x_i). \tag{8.1}$$

For the functionals 1)–2), this is called *numerical differentiation* and *numerical integration*, respectively. A natural solution is to interpolate f by $p \in \mathbb{P}_n$ and take $\ell(f) \approx \ell(p)$. This is called the *interpolating formula* (of degree n). We have already seen an interpolating formula, namely that of Lagrange for the functional $\ell(f) = f(x)$:

$$f(x) \approx p(x) = \sum_{i=0}^n L_i(x) f(x_i), \qquad L_i(x) = \prod_{j=0, j\ne i}^n \frac{(x-x_j)}{(x_i - x_j)}$$

By linearity, $\ell(p) = \sum_{i=0}^n \ell(L_i) p(x_i)$, thus the interpolating formula has the form

$$\ell(f) \approx \sum_{i=0}^n \ell(L_i) f(x_i).$$

It is exact on $\mathbb{P}_n$, by definition. The converse is true as well. For if (8.1) is exact on $\mathbb{P}_n$, take $f(x) = L_j(x)$ to obtain $\ell(L_j) = \sum_{i=0}^n a_i L_j(x_i) = a_j$. Hence, we have just proved

Lemma. The formula $\ell(f) \approx \sum_{i=0}^n a_i f(x_i)$ is interpolating $\Leftrightarrow$ it is exact for all $p \in \mathbb{P}_n$.

[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`.

8.1 Numerical integration

A formula of numerical integration

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

is called a *quadrature formula* with the *nodes* (x_i) and the *weights* (a_i). For any $n+1$ fixed x_is, the interpolating formula $a_i = I(L_i)$ is exact on $\mathbb{P}_n$. Can one find a *quadrature of higher accuracy* which is exact for all $p \in \mathbb{P}_m$ with some $m > n$?

Claim. No quadrature formula with $n+1$ nodes is exact for all $q \in \mathbb{P}_m$ if $m > 2n+1$.

Proof. Take $q(x) = \prod_{i=0}^n (x-x_i)^2 \ge 0$. Then $q \in \mathbb{P}_{2n+2}$, and $I(q) > 0$, but $\sum_{i=0}^n a_i q(x_i) = 0$ 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. Let p_{n+1} be the $(n+1)$-st orthogonal polynomial. Then all the zeros of p_{n+1} are real, distinct and lie in the interval (a,b).

Proof. Denote by k the number of the sign changes of p_{n+1} in (a,b) and assume that $k \le n$. If $k=0$, set $q \equiv 1$. For $1 \le k \le n$, we let $q(x) := \prod_{j=1}^k (x-\xi_j)$ where ξ_js are the points where a sign change of p_n occurs. Then $q \in \mathbb{P}_k$, $k \le n$, thus $\langle p_{n+1}, q\rangle = 0$. On the other hand, by construction, $q(x)p_{n+1}(x)$ does not change sign throughout $[a,b]$ and vanishes at a finite number of points, hence $|\langle q, p_{n+1}\rangle| = \left|\int_a^b q(x)p_{n+1}(x)w(x)\,\mathrm{d}x\right| = \int_a^b |q(x)p_{n+1}(x)|w(x)\,\mathrm{d}x > 0$, a contradiction. Thus, $k = n+1$. □

Theorem. The interpolating quadrature with $n+1$ nodes $(x_i)_{i=0}^n$ is exact for all $q \in \mathbb{P}_{2n+1}$ iff $(x_i)_{i=0}^n$ are the zeros of $(n+1)$-st orthogonal polynomial p_{n+1}.

Proof. Let $(x_i)_{i=0}^n$ be the zeros of p_{n+1}. Given any $q \in \mathbb{P}_{2n+1}$, we can represent it uniquely as $q(x) = r(x)p_{n+1}(x) + s(x)$, where $r, s \in \mathbb{P}_n$. Since p_{n+1} is orthogonal to r,

$$I(q) = \int_a^b q(x)w(x)\,\mathrm{d}x = \int_a^b s(x)w(x)\,\mathrm{d}x = I(s).$$

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

$$\sum_{i=0}^n a_i q(x_i) = \sum_{i=1}^n a_i s(x_i).$$

But $s \in \mathbb{P}_n$ and the interpolating quadrature is exact on $\mathbb{P}_n$, hence $I(s) = \sum a_i s(x_i)$, and therefore $I(q) = \sum a_i q(x_i)$ for all $q \in \mathbb{P}_{2n+1}$.

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

$$\int_a^b q(x)p_n(x)w(x)\,\mathrm{d}x = \sum_{i=0}^n a_i[q(x_i)p_n(x_i)] = 0$$

i.e., p_{n+1} is orthogonal to all $q \in \mathbb{P}_n$. □

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

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

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

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

Example (*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 f-ns
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 f-ns
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)