Dr A. Iserles
Easter 1997

Numerical Analysis – Lecture 11

7.5 Least squares fitting to discrete function values

Suppose that $m \geq n+1$. We are given m function values $f(x_1), f(x_2), \ldots, f(x_m)$, where the x_ks are pairwise distinct, and seek $p \in \mathbb{P}_n[x]$ that minimizes $\langle f-p, f-p\rangle$, where

$$\langle g, h\rangle := \sum_{k=1}^{m} g(x_k)h(x_k). \tag{7.1}$$

One alternative is to express p as $\sum_{\ell=0}^{n} c_\ell x^\ell$ and find optimal $c_0, \ldots, c_n$ as a solution of a linear least squares problem *à la* Section 5. An alternative is to construct orthogonal polynomials w.r.t. the scalar product (7.1). The theory is identical to that of subsections 7.1–4, except that we can evaluate only $p_0, p_1, \ldots, p_{m-1}$ – but we need just $p, p_1, \ldots, p_n$ and $n \leq m-1$, so it doesn't matter! Thus
1. Employ the three-term recurrence (7.2) to calculate $p_0, p_1, \ldots, p_n$ (of course, using the scalar product (7.1));
2. Form $p = \sum_{k=0}^{n}(\langle p_k, f\rangle / \langle p_k, p_k\rangle)p_k$.

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.

7.6 Gaussian quadrature

We are again in $C[a,b]$ and a scalar product is defined as in subsection 7.1, namely $\langle f, g\rangle = \int_a^b w(x)f(x)g(x)\,\mathrm{d}x$, where $w > 0$ in (a,b). Our goal is to approximate integrals by finite sums,

$$\int_a^b w(x)f(x)\,\mathrm{d}x \approx \sum_{k=1}^{\nu} b_k f(c_k), \qquad f \in C[a,b].$$

Here ν is given, whereas the points $b_1, \ldots, b_\nu$ (the *weights*) and $c_1, \ldots, c_\nu$ (the *nodes*) are independent of the choice of f.

A reasonable approach to achieving high accuracy is to require that the approximant is exact for all $f \in \mathbb{P}_m[x]$, where m is as large as possible – this results in *Gaussian quadrature* and we will demonstrate that $m = 2\nu - 1$ can be attained.

Firstly, we claim that $m = 2\nu$ is impossible. To prove this, note that $p(x) := \prod_{k=1}^{\nu}(x-c_k)^2$ lives in $\mathbb{P}_{2\nu}[x]$, $\int_a^b w(x)p(x)\,\mathrm{d}x > 0$ and $\sum_{k=1}^{\nu} b_k p(c_k) = 0$.

Let $p_0, p_1, p_2, \ldots$ denote, again, the monic polynomials which are orthogonal w.r.t. the underlying scalar product.

Theorem All the zeros of p_n are real, distinct and lie in the interval (a,b) for all $n \geq 1$.

Proof. Since $\int_a^b w(x)p_k(x)\,\mathrm{d}x = \int_a^b w(x)p_0(x)p_n(x)\,\mathrm{d}x = 0$, p_n changes sign at least once in (a,b). Let us denote by $m \geq 1$ the number of its sign changes in (a,b) and assume that $m \leq n-1$. Denoting the points where the sign change occurs by $\xi_1, \xi_2, \ldots, \xi_m$, we let $q(x) := \prod_{j=1}^{m}(x-\xi_j)$. Since $q \in \mathbb{P}_m[x]$, $m \leq n-1$, it follows that $\langle q, p_n\rangle = 0$. On the other hand, qp_n is of the same sign throughout $[a,b]$ and vanishes at a finite number of points, hence $|\langle q, p_n\rangle| = \left|\int_a^b w(x)q(x)p_n(x)\,\mathrm{d}x\right| =$

$\int_a^b w(x)|q(x)p_n(x)|\,\mathrm{d}x > 0$ – a contradiction. It follows that $m = n$ and the proof is complete. □

We commence by choosing pairwise-distinct $c_1, c_2, \ldots, c_\nu \in (a, b)$ 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 $f \in \mathbb{P}_{\nu-1}[x]$. However, 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

$$f(x) = \sum_{k=0}^{\nu} f(c_k) \prod_{\substack{j=1\\ j\neq k}}^{\nu} \frac{x - c_j}{c_k - c_j}. \tag{7.2}$$

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 $f \in \mathbb{P}_{2\nu-1}[x]$, 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 approximant coincide, because $r \in \mathbb{P}_{\nu-1}[x]$. □

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, normalization). Hence Gaussian quadrature nodes are

$n = 1$: $c_1 = 0$;

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

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

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