Mathematical Tripos Part IB: Lent 2020

Numerical Analysis – Lecture 4[1]

2.4 Least-squares polynomial fitting

Consider a scalar product

$$\langle g, h\rangle = \int_a^b w(x)g(x)h(x)\,\mathrm{d}x \tag{2.3}$$

on $C[a,b]$ where $w(x) > 0$ for $x \in (a,b)$. Given $f \in C[a,b]$ we want to find $p \in \mathbb{P}_n[x]$ so as to minimise $\langle f-p, f-p\rangle = \|f-p\|^2$. Call the optimal polynomial $\hat{p}_n$. The following theorem shows that $\hat{p}_n$ can be easily expressed in terms of the orthogonal polynomials associated to (2.3).

Theorem Let $p_0, p_1, p_2, \ldots$ be orthogonal polynomials associated to the inner product (2.3). Let $f \in C[a,b]$. Then the polynomial $\hat{p}_n \in \mathbb{P}_n[x]$ that minimises $\|f-p\|^2 = \langle f-p, f-p\rangle$ is given by

$$\hat{p}_n(x) = \sum_{k=0}^{n} \frac{\langle f, p_k\rangle}{\langle p_k, p_k\rangle} p_k(x). \tag{2.4}$$

Proof. Because $p_0, \ldots, p_n$ form a basis of $\mathbb{P}_n[x]$, any $p \in \mathbb{P}_n$ can be written as $p = \sum_{k=0}^n c_k p_k$ for some coefficients c_k. Thus we have, using orthogonality of the p_ks

$$\langle f-p, f-p\rangle = \left\langle f - \sum_{k=0}^n c_k p_k, f - \sum_{k=0}^n c_k p_k \right\rangle = \langle f, f\rangle - 2\sum_{k=0}^n c_k\langle p_k, f\rangle + \sum_{k=0}^n c_k^2 \langle p_k, p_k\rangle.$$

To minimise this expression we find values of the c_ks that make the gradient equal to 0. We have:

$$\frac{\partial}{\partial c_k}\langle f-p, f-p\rangle = -2\langle p_k, f\rangle + 2c_k\langle p_k, p_k\rangle, \qquad k = 0, 1, \ldots, n,$$

hence setting these to zero we get $c_k = \frac{\langle f, p_k\rangle}{\langle p_k, p_k\rangle}$ which gives the expression (2.4). □

The approximation error we get with $\hat{p}_n$ is

$$\langle f-\hat{p}_n, f-\hat{p}_n\rangle = \langle f, f\rangle - \sum_{k=0}^n \{2c_k\langle p_k, f\rangle - c_k^2\langle p_k, p_k\rangle\} = \langle f, f\rangle - \sum_{k=0}^n \frac{\langle p_k, f\rangle^2}{\langle p_k, p_k\rangle}. \tag{2.5}$$

This identity can be rewritten as $\langle f-\hat{p}_n, f-\hat{p}_n\rangle + \langle \hat{p}_n, \hat{p}_n\rangle = \langle f, f\rangle$, reminiscent of the Pythagoras theorem. It is clear that increasing n brings the approximation error down. A natural question is: if we keep increasing n does the approximation error eventually reach 0? The answer is yes and this is a consequence of Weierstrass's theorem (which we are going to admit without proof):

Theorem *(Weierstrass theorem)* Let $[a,b]$ be finite and let $f \in C[a,b]$. For any $\epsilon > 0$ there is a polynomial p of high enough degree such that $|f(x) - p(x)| \le \epsilon$ for all $x \in [a,b]$.

To prove that $\|f - \hat{p}_n\|^2 \to 0$ as $n \to \infty$, note that by our definition of inner product (2.3) we have, for any p

$$\|f-p\|^2 = \int_a^b w(x)(f(x)-p(x))^2 dx \le \left(\max_{x\in[a,b]} |f(x)-p(x)|\right)^2 \int_a^b w(x)dx.$$

For any $\delta > 0$ we know by Weierstrass theorem that there is a polynomial p of degree n (with n large enough) such that $\max_{x\in[a,b]} |f(x)-p(x)| \le \sqrt{\delta / \int_a^b w(x)dx}$. So for any $N \ge n$ we have

$$\|f - \hat{p}_N\|^2 \le \|f-p\|^2 \le \left(\sqrt{\frac{\delta}{\int_a^b w(x)dx}}\right)^2 \int_a^b w(x)dx \le \delta.$$

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

This is true for any $\delta > 0$ and so shows that $\|f - \hat{p}_n\|^2 \to 0$ as $n \to \infty$. Using the identity (2.5) we get the following consequence:

Theorem *(The Parseval identity)* Let $[a, b]$ be finite, and let $p_0, p_1, p_2, \ldots$ be orthogonal polynomials for (2.3). Then for any $f \in C[a, b]$,

$$\sum_{k=0}^{\infty} \frac{\langle p_k, f\rangle^2}{\langle p_k, p_k\rangle} = \langle f, f\rangle. \tag{2.6}$$

2.5 Least-squares fitting to discrete function values

Consider now the following problem: 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 minimises $\sum_{k=1}^{m}(f(x_k) - p(x_k))^2$. This corresponds to minimising $\langle f - p, f - p\rangle$ with the following inner product:

$$\langle g, h\rangle := \sum_{k=1}^{m} g(x_k)h(x_k). \tag{2.7}$$

The result from the previous subsection extends directly to this situation as long as $n \le m-1$ (note that (2.7) does not define a valid inner product on polynomials of degree greater than or equal m). So for $n \le m - 1$ we can solve the problem as follows:

1. Employ the three-term recurrence (2.3) to calculate $p_0, p_1, \ldots, p_n$ (of course, using the scalar product (2.7));
2. Form $p(x) = \sum_{k=0}^{n} \frac{\langle p_k, f\rangle}{\langle p_k, p_k\rangle} p_k(x)$.

2.6 Gaussian quadrature

We are again in $C[a, b]$ and a scalar product is defined as in subsection 2.1, namely $\langle f, g\rangle = \int_a^b w(x)f(x)g(x)\,\mathrm{d}x$, where $w(x) > 0$ for $x \in (a, b)$. Our goal is to approximate integrals by finite sums,

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

The above is known as a *quadrature formula.* 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 approximation 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, choose arbitrary nodes $c_1, \ldots, c_\nu$ and note that $p(x) := \prod_{k=1}^{\nu}(x - c_k)^2$ lives in $\mathbb{P}_{2\nu}[x]$. But $\int_a^b w(x)p(x)\,\mathrm{d}x > 0$, while $\sum_{k=1}^{\nu} b_k p(c_k) = 0$ for any choice of weights $b_1, \ldots, b_\nu$. Hence the integral and the quadrature do not match.
Let $p_0, p_1, p_2, \ldots$ denote, as before, the monic polynomials which are orthogonal w.r.t. the underlying scalar product.

Theorem Given $n \ge 1$, p_n has n real distinct zeros in the interval (a, b).

Proof. Let $\xi_1, \ldots, \xi_m$ be the points in (a, b) where p_n changes signs (equivalently these are the zeros of p of odd multiplicity) and let $q(x) = \prod_{i=1}^{m}(x - \xi_i)$. Observe that the polynomial $p_n(x)q(x)$ does not change signs in (a, b): this is because all the roots of $p_n(x)q(x)$ in (a, b) have even multiplicity. It thus follows that

$$|\langle q, p_n\rangle| = \left|\int_a^b w(x)q(x)p_n(x)\,\mathrm{d}x\right| = \int_a^b w(x)|q(x)p_n(x)|\,\mathrm{d}x > 0.$$

Since p_n is orthogonal to all polynomials of degree $\le n - 1$ it follows that q must be of degree *at least* n, i.e., $m \ge n$. On the other hand, since p_n is of degree n it can have at most n roots. Finally this means that p_n has n distinct real roots in (a, b). □