THEOREM. 0.1 *(Taylor's) Let $f, f', \cdots, f^{(n)}$ be continuous on $[a,b]$ and $f^{(n+1)}$ is continuous on (a,b) then for all $x \in [a,b]$*

$$f(x) - \left(f(\alpha) + f'(\alpha)(x-\alpha) + \cdots + f^{(n)}(\alpha)\tfrac{(x-\alpha)^n}{n!}\right) = \tfrac{(x-\alpha)^{n+1} f^{(n+1)}(y)}{(n+1)!}$$

where y is between α and x.

THEOREM. 0.2 *Weierstrass approximation. Given $f \in C[a,b]$ and $\varepsilon > 0$ there exists $n = n(\varepsilon) \in \mathbb{N}$ and $p_n \in \mathcal{P}_n :=$ {polynomials of degree less than or equal to n} such that*

$$|f(x) - p_n(x)| < \varepsilon \quad \forall\ x \in [a,b].$$

1 Chebyshev Polynomials

Chebyshev polynomials of the first kind

The *Chebyshev polynomials of the first kind on* $[-1,1]$ satisfy

$$T_n(x) := \cos n\theta \qquad \text{where } \theta = \cos^{-1} x \tag{1.1}$$

satisfies $T_0(x) = 1$, $T_1(x) = x$ and the following three term recurrence relation

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x) \quad n = 1, 2, \cdots$$

from which it follows that $T_n(x) = 2^{n-1}x^n + \cdots$ for $n = 1, 2, \cdots$ and $|T_n(x)| \leqslant 1$.

Note that at the points $x_i = \cos\left(\frac{(2i+1)\pi}{2n}\right)$ we have $T_n(x_i) = 0$ and at $y_i = \cos(i\pi/n)$, between consecutive x_i's, $T_n(y_i) = (-1)^i$.

THEOREM. 1.1 *Let $w_n(x) = \prod_{i=0}^{n-1}(x - x_i) \in \mathcal{P}_n$. Among all possible choices for distinct x_i, $\max|w_n(x)|$ is minimised if $w_n(x) = 2^{1-n}T_n(x)$.*

PROOF. Firstly note that $w_n(x) = 2^{1-n}T_n(x) \in \mathcal{P}_n$ is a monic polynomial with distinct roots. Also $w_n(y_i) = 2^{1-n}(-1)^i, 0 < i < n$, where $y_i = \cos(i\pi/(n+1))$.

Now assume that there is another polynomial $v_n(x) \in \mathcal{P}_n$, with leading coefficient 1 such that $\max|v_n(x)| < \max|w_n(x)|$. Then, in particular, if i is even $v_n(y_i) < w_n(y_i)$ and if i is odd $v_n(y_i) > w_n(y_i)$. This implies that $p_{n-1}(x) = v_n(x) - w_n(x) \in \mathcal{P}_{n-1}$ changes sign n times and therefore has n roots. But $p_{n-1}(x) \in \mathcal{P}_{n-1}$ and therefore $p_{n-1}(x) \equiv 0$. □

We can replace the interval $[-1,1]$ by $[a,b]$ and Chebyshev polynomial of degree n becomes $T_n(\frac{2x-(a+b)}{b-a})$.

Chebyshev Economization of power series

The Taylor series of f about $\alpha = 0$ is

$$f(x) \sim \sum_{j=0}^{\infty} d_j x^j$$

where $d_j = f^{(j)}(0)$. Similar to a Fourier expansion, for $x \in [-1,1]$ consider writing a continuous function f as a Chebyshev series

$$f(x) = \tfrac{1}{2}c_0 + \sum_{j=1}^{\infty} c_j T_j(x) \quad \text{where} \quad c_j = \frac{2}{\pi}\int_{-1}^{1} \frac{f(x)T_j(x)}{\sqrt{1-x^2}}\mathrm{d}x.$$

Unfortunately in all but the simplest of cases it is difficult to calculate this integral. One way to approximate $f(x)$ by a polynomial of degree n is to "chop" the Chebyshev series

$$f(x) - \left(\tfrac{1}{2}c_0 + \sum_{j=1}^{n} c_j T_j(x)\right) = \sum_{j=n+1}^{\infty} c_j T_j(x) \approx c_{n+1}T_{n+1}(x)$$

if the coefficients c_j decrease rapidly (noting $|T_j(x)| \leqslant 1$). Thus, as we have seen, the error is as small as possible and uniformly spread across $[-1,1]$, unlike the Taylor polynomial.

Chebyshev economization Given an interval $[a,b]$ and a function $f(x)$. Compute the Taylor polynomial of degree n, p_n, about $\alpha = 0$ and bound the remainder term in Taylor's theorem. Now compute $q_{j-1}(x) = q_j(x) - \alpha_j T_j(x)$ where $q_n(x) = p_n(x)$, T_j is the appropriate Chebyshev polynomial for the interval $[a,b]$ and α_j is chosen so that $q_{j-1} \in \mathcal{P}_{j-1}$.

The *Chebyshev polynomials of the second kind* satisfy

$$U_n(x) := \frac{\sin((n+1)\theta)}{\sin\theta} \qquad \text{where } \theta = \cos^{-1} x, \tag{1.2}$$

$U_0(x) = 1$, $U_1(x) = 2x$ and the following three term recurrence relation

$$U_{n+1}(x) = 2xU_n(x) - U_{n-1}(x) \quad n = 1, 2, \cdots$$

2 Polynomial Interpolation

When presented with $n+1$ data points $(x_i, f(x_i))$ $(i = 0, 1, \cdots, n)$ a scientist may want to draw a curve through these points so that information might be obtained at intermediate values. *Polynomial Interpolation* is the process of finding a polynomial passing through these points namely

$$p(x_i) = f(x_i) \qquad \text{for } i = 0, 1, \cdots, n.$$

Interpolation tells us something about intermediate values, *extrapolation* tells us about values beyond what we have.

EXAMPLE. Let $(x_i, f(x_i))$ $(i = 0, 1, 2)$ be three points $(n = 2)$ with distinct x_i's. Is there a unique interpolating polynomial of degree at most two

$$p_2(x) = a_0 + a_1 x + a_2 x^2?$$

(Three points to fit and three unknown coefficients.)

Solve $a_0 + a_1 x_i + a_2 x_i^2 = f(x_i)$ $(i = 0, 1, 2)$. Writing as a matrix equation

$$\underbrace{\begin{pmatrix} 1 & x_0 & x_0^2 \\ 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \end{pmatrix}}_{X} \underbrace{\begin{pmatrix} a_0 \\ a_1 \\ a_2 \end{pmatrix}}_{\boldsymbol{a}} = \underbrace{\begin{pmatrix} f(x_0) \\ f(x_1) \\ f(x_2) \end{pmatrix}}_{\boldsymbol{f}}$$

we know that $\boldsymbol{a}$ will exist and be unique if X is invertible, i.e. $\det X \neq 0$. However, $\det X = (x_0 - x_1)(x_0 - x_2)(x_2 - x_1) \neq 0$, as the nodes are distinct. □

THEOREM. 2.1 *Let f be a continuous function on $[a, b]$ and let $x_0, x_1, \cdots, x_n$ be distinct nodes lying in $[a, b]$. Then there exists a unique polynomial $p_n \in \mathcal{P}_n$ which interpolates f*

PROOF. Existence is proved by construction. Define the *Lagrange polynomials* of degree n by

$$l_j(x) := \frac{(x - x_0)\cdots(x - x_{j-1})(x - x_{j+1})\cdots(x - x_n)}{(x_j - x_0)\cdots(x_j - x_{j-1})(x_j - x_{j+1})\cdots(x_j - x_n)} = \prod_{\substack{k=0 \\ k\neq j}}^{n} \frac{x - x_k}{x_j - x_k}$$

and observe that $l_j(x_i) = \delta_{ij}$. Now the *interpolating Lagrange polynomial* of degree at most n, p_n, is defined to be

$$p_n(x) = \sum_{j=0}^{n} f(x_j) l_j(x) \quad \text{so that} \quad p_n(x_i) = \sum_{j=0}^{n} f(x_j) l_j(x_i) = f(x_i) \quad i = 0, 1, \cdots, n.$$

To prove uniqueness we use proof by contradiction. Suppose that $p_n \neq q_n$ are both interpolating polynomials of degree at most n, i.e. $p_n(x_i) = q_n(x_i) = f(x_i)$ $(i = 0, 1, \cdots n)$. Let $r_n(x) := p_n(x) - q_n(x) \in \mathcal{P}_n$. Notice that

$$r_n(x_i) = p_n(x_i) - q_n(x_i) = 0, \qquad i = 0, 1, \cdots, n,$$

i.e. r_n has at least $n + 1$ real zeros, but it can have at most n! □

Notice we can rewrite

$$l_i(x) = \frac{w_{n+1}(x)}{(x - x_i) w'_{n+1}(x_i)} \quad \text{where} \quad w_{n+1}(x) := \prod_{j=0}^{n} (x - x_j).$$

THEOREM. 2.2 *(The truncation error theorem) Let $f, f', \cdots, f^{(n+1)}$ be continuous on $[a, b]$ and let $p_n \in \mathcal{P}_n$ interpolate f at the distinct points $x_0, x_1, \cdots, x_n$ in $[a, b]$. Define $w_{n+1} = (x - x_0)(x - x_1)\cdots(x - x_n)$. For each $x \in [a, b]$ there is a point $\xi \in (a, b)$ such that*

$$f(x) - p_n(x) = \frac{w_{n+1}(x)}{(n + 1)!} f^{(n+1)}(\xi).$$

PROOF. If $x = x_i$ $(i = 0, \cdots, n)$ then

$$f(x) - p_n(x) = 0 \quad \text{and} \quad w_{n+1}(x) = 0,$$

and the theorem is trivial. So assume that $x \neq x_i$ is given (fixed). Define g to be

$$g(t) = f(t) - p_n(t) - \frac{w_{n+1}(t)}{w_{n+1}(x)}(f(x) - p_n(x)),$$

which is $n + 1$ times continuously differentiable on $[a, b]$. Notice that $w_{n+1}(x) \neq 0$ so g is well-defined. Then $g(x) = 0$ and $g(x_i) = 0$, $i = 0, 1, \cdots, n$. That is, g has $n + 2$ distinct zeros in $[a, b]$. So from Rolle's theorem g' has $n + 1$ distinct zeros in (a, b). Repeated application of Rolle's theorem gives $g^{(n+1)}(\xi) = 0$ for some $c \in (a, b)$. The result now follows from

$$0 = g^{(n+1)}(\xi) = f^{(n+1)}(\xi) - \frac{(n + 1)!}{w_{n+1}(x)}[f(x) - p_n(x)].\square$$

Interpolation at Chebyshev nodes

It should be noted that truncation error theorem doesn't guarantee convergence of the interpolant as $n \to \infty$. A simple example ($f(x) = 1/(1+25x^2)$ with equally spaced nodes) can be used to show that we don't necessarily get a better approximation by putting in more points. (The essence of the problems is that, even though $f(x)$ is infinitely continuous the maximum values of the derivatives grows rapidly as we take higher derivatives). If we examine the error estimate

$$f(x) - p(x) = \frac{f^{(n+1)}(\xi)}{(n + 1)!} w_{n+1}(x) \in (a, b).$$

we see that we have little control over the $f^{(n+1)}(\xi)/(n + 1)!$ term. However we can try to choose the interpolation points to minimise the maximum value of $w_{n+1}(x)$ which is done by choosing the x_i's to be the zero's of $T_{n+1}(x)$, i.e. $x_i = \cos\left(\frac{(2i+1)\pi}{2(n+1)}\right)$ so that from before

$$|f(x) - p(x)| \leqslant \frac{|f^{(n+1)}(\xi)|}{(n + 1)! 2^n}.$$

Hermite Interpolation

If we ask to produce a polynomial interpolant which at distinct nodes $\{x_i\}_{i=0}^n$ fits heights $\{y_i\}_{i=0}^n$ and slopes $\{y_i'\}_{i=0}^n$ we produce the Hermite interpolant.

THEOREM. 2.3 *The Hermite interpolation polynomial* $p_{2n+1}(x) := \sum_{i=0}^{n} \left[h_i(x)y_i + \overline{h}_i(x)y_i'\right] \in \mathcal{P}_{2n+1}$ *where*

$$\overline{h}_i(x) := (x - x_i)l_i^2(x), \quad h_i(x) := [1 - 2(x - x_i)l_i'(x_i)]\, l_i^2(x)$$

is the only polynomial with the properties $p_{2n+1}(x_i) = y_i$ *and* $p_{2n+1}'(x_i) = y_i'$ *for* $i = 0 \to n$.

PROOF. Existence is automatic since

$$h_i(x_j) = \delta_{ij},\ h_i'(x_j) = 0,\ \overline{h}_i(x_j) = 0 \text{ and } \overline{h}_i'(x_j) = \delta_{ij}.$$

Let $p(x), q(x) \in \mathcal{P}_{2n+1}$ satisfy the interpolation conditions, then $p(x) - q(x) \in \mathcal{P}_{2n+1}$ and $p(x_i) - q(x_i) = 0$, $p'(x_i) - q'(x_i) = 0$. Thus $p(x) - q(x)$ is an $2n + 1$ degree polynomial with $2n + 2$ roots. Therefore by the fundamental theorem of algebra $p(x) - q(x) \equiv 0$.

THEOREM. 2.4 *(Truncation Error) Let* $f, f', \cdots, f^{(2n+2)}$ *be continuous on* $[a, b]$ *and* p_{2n+1} *be the interpolating Hermite polynomial at the distinct nodes* x_i $(i = 0 \to n)$. *Then for all* $x \in [a, b]$

$$E(x) := f(x) - p_{2n+1}(x) = \frac{[w_{n+1}(x)]^2}{(2n+2)!} f^{(2n+2)}(\xi) \qquad \xi \in (a, b) \qquad (2.3)$$

PROOF. The theorem is plainly true at the interpolation points. Fix $x \neq x_i$ and define

$$g(t) = f(t) - p_{2n+1}(t) - \frac{f(x) - p_{2n+1}(x)}{[w_{n+1}(x)]^2}[w_{n+1}(t)]^2,$$

then $g(t)$ has at least $n + 1$ double roots in $[a, b]$ and $g(x) = 0$. Hence $g(t)$ has at least $n + 2$ roots ($(n + 1)$ of which are double) in $[a, b]$. One application of Rollé's theorem gives that $g'(t)$ has $n+1$ roots in the open intervals defined by the roots of $g(t)$, therefore (from the double roots) $g'(t)$ has at least $2n + 2$ distinct roots in $[a, b]$. Now repeated application of Rollé's theorem gives that $g^{(2n+2)}$ has at least one root in $\xi \in (a, b)$ where

$$0 = g^{(2n+2)}(\xi) = f^{(2n+2)}(\xi) - \frac{f(x) - p_{2n+1}(x)}{[w_{n+1}(x)]^2}(2n + 2)!$$

□

Piecewise linear interpolation

The continuous, piecewise linear function, p_1, interpolating f at $x_0 < x_1 < \cdots < x_n$ is defined by

$$p_1(x) = \frac{x_{j+1} - x}{x_{j+1} - x_j} f(x_j) + \frac{x - x_j}{x_{j+1} - x_j} f(x_{j+1}) \quad x \in [x_i, x_{i+1}]\ (i = 0 \to n - 1).$$

Notice that if f, f', f'' are all continuous on $[a, b]$, then from linear interpolation for $x \in [x_i, x_{i+1}]$,

$$|f(x) - p_1(x)| \leqslant \frac{(x_{i+1} - x_i)^2}{8} M$$

where $|f''(x)| \leqslant M$ for all $x \in [a, b]$. Hence for all $x \in [a, b]$

$$|f(x) - p_1(x)| \leqslant \frac{h^2}{8} M \qquad \text{where } h = \max_i x_{i+1} - x_i.$$

3 Continuous least-squares approximation

In this section we try and make the error in approximation as small as possible, for instance for a given n minimize

$$E(d_0, \cdots, d_n) = \int_a^b \left(f(x) - \sum_{j=0}^{n} d_j x^j\right)^2 \mathrm{d}x$$

(note we could use another measure for the error, see §1, we have just decided to use the integral), we need to solve for $k = 0 \to n$

$$0 = \frac{\partial E}{\partial d_k} = -2 \int_a^b \left(f(x) - \sum_{j=0}^{n} d_j x^j\right) x^k \mathrm{d}x$$

$$\begin{array}{llllll} k = 0: & s_0 d_0 & +s_1 d_1 & + \cdots & +s_n d_n & = \rho_0 \\ k = 1: & s_1 d_0 & +s_2 d_1 & + \cdots & +s_{n+1} d_n & = \rho_1 \\ \vdots & & & \vdots & \vdots & \\ k = n: & s_n d_0 & +s_{n+1} d_1 & + \cdots & +s_{2n} d_n & = \rho_n \end{array}$$

where $s_k = \int_a^b x^k \mathrm{d}x$ and $\rho_k = \int_a^b x^k f(x) \mathrm{d}x$, a tricky set of $n+1$ simultaneous ill-conditioned equations. If it were the case that for $j \neq k$ that

$$\int_a^b \left(f(x) - \sum_{j=0}^{n} d_j x^j\right) x^k \mathrm{d}x$$

then we would be left with an explicit expression for d_k. We spend some time developing the idea of orthogonal polynomials to make the algebra easy.

Orthogonal polynomials

Given $\omega(x) \geqslant 0$ for all $x \in (a,b)$, continuous and $\int_a^b w(x)\mathrm{d}x > 0$, i.e. $\omega(x) \not\equiv 0$. We can define an inner-product

$$(f,g) := \int_a^b \omega(x) f(x) g(x) \mathrm{d}x \quad \text{and} \quad \|f\| := [(f,f)]^{1/2}.$$

Obviously the inner-product satisfies the following three key relations

1. $\|f\| \geqslant 0$ and $\|f\| = 0$ iff $f \equiv 0$;
2. $(\alpha f + \beta g, h) = \alpha(f,h) + \beta(g,h)$;
3. $(f,g) = (g,f)$.

This is actually the definition of an inner-product.

The sequence $\{\phi_n\}$ is an *orthogonal polynomial sequence* if $\phi_n(x)$ is a polynomial of degree n and $(\phi_n, \phi_m) = 0$ for $n \neq m$.

THEOREM. 3.1 *(Gram-Schmidt) Every inner-product, as defined above, has a monic orthogonal polynomial sequence. Moreover, $\{\phi_n\}$ satisfies the three term recurrence relation*

$$\phi_n(x) = (x + \alpha_{n-1})\phi_{n-1}(x) + \beta_{n-1}\phi_{n-2}(x) \quad n \geqslant 2$$

where $\alpha_{n-1}, b_{n-1} \in \mathbb{R}$.

PROOF. Let $\phi_0(x) \equiv 1$. Let $\phi_1(x) = x + a_{1,0}\phi_0(x) \in \mathcal{P}_1$ where $a_{1,0} = -(x, \phi_0)$ so that

$$(\phi_1, \phi_0) = (x, \phi_0) + a_{1,0}(\phi_0, \phi_0) = 0.$$

We now use mathematical induction. Let $n \geqslant 2$ Suppose that $\phi_0(x), \cdots, \phi_{n-1}(x)$ satisfy $\phi_j \in \mathcal{P}_j$ and $(\phi_i, \phi_j) = 0$ if $i \neq j$. Let

$$\phi_n(x) = x\phi_{n-1}(x) + a_{n,n-1}\phi_{n-1}(x) + \cdots + a_{n,0}\phi_0(x) \in \mathcal{P}_n$$

where we choose $a_{n,j}$ $j = 0 \to n-1$ so that $(\phi_n, \phi_j) = 0$, that is

$$a_{n,j} = \begin{cases} 0 & j = 0 \to n-3 \\ -\frac{(x\phi_{n-1}, \phi_{n-2})}{(\phi_{n-2}, \phi_{n-2})} & j = n-2 \\ -\frac{(x\phi_{n-1}, \phi_{n-1})}{(\phi_{n-1}, \phi_{n-1})} & j = n-1 \end{cases}$$

EXAMPLES.

nial name	$\omega(x)$	Interval	Recurrence relation	$n = 0,\ 1$
hev	$(1-x^2)^{-1/2}$	$[-1,1]$	$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x)$	$T_0(x) = 1,\ T_1(x) = x$
re	1	$[-1,1]$	$P_{n+1}(x) = \frac{(2n+1)}{n+1} x P_n(x) - \frac{n}{n+1} P_{n-1}(x)$	$P_0(x) = 1,\ P_1(x) = x$
e	e^{-x}	$[0,\infty)$	$L_{n+1}(x) = \frac{(2n+1)-x}{n+1} L_n(x) - \frac{n}{n+1} L_{n-1}(x)$	$L_0(x) = 1,\ L_1(x) = 1-x$
e	e^{-x^2}	$(-\infty,\infty)$	$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x)$	$H_0(x) = 1,\ H_1(x) = 2x$

Continuous least-squares

Taking the usual inner-product, let $\{\phi_n\}$ be the orthogonal monic polynomial sequence. For a given n we minimize

$$E(c_0, \cdots, c_n) = \int_a^b \omega(x) \left(f(x) - \sum_{j=0}^n c_j \phi_j(x) \right)^2 \mathrm{d}x$$

That is we want to solve

$$\begin{aligned} 0 &= \frac{\partial E}{\partial c_k} = -2\int_a^b \omega(x) \left(f(x) - \sum_{j=0}^n c_j\phi_j(x) \right) \phi_k(x)\mathrm{d}x \\ &= -2(f - \sum_{j=0}^n c_j\phi_j, \phi_k) = -2(f - c_k\phi_k, \phi_k) \Longrightarrow c_k = \frac{(f,\phi_k)}{(\phi_k,\phi_k)} \end{aligned}$$

Analogous theory holds where one works with a discrete inner-product, e.g. given distinct x_i and $\omega_i > 0$ define

$$(f,g) := \sum_{i=0}^n \omega_i f(x_i) g(x_i).$$

where f and g are polynomials of degree n.

4 Numerical Integration

Introduction

It is easy to write down an integral where we cannot write down the answer in a closed form, for example

$$\int_0^x e^{-t^2}\mathrm{d}t \text{ or } \int_0^1 \frac{\sin x}{x}\mathrm{d}x,$$

or the integrand may be complicated to write down. To find the value of the integral we may have to resort to *Numerical Integration*.

Let f be a continuous function and x_i $(i = 0 \to n)$ be interpolation points. Then integrating the Lagrange interpolation polynomial over the interval $[a,b]$ yields the $(n+1)$ point interpolation formula which is exact for polynomials of degree $\leqslant$ n

$$\int_a^b f(x)\mathrm{d}x \approx \sum_{i=0}^n H_i f(x_i) \quad \text{where} \quad H_i = \int_a^b l_i(x)\mathrm{d}x = \int_a^b \prod_{\substack{j=0 \\ j\neq i}}^n \frac{x - x_j}{x_i - x_j}\mathrm{d}x.$$

If $f, f', \cdots, f^{(n+1)}$ are continuous on $[a,b]$ then using the Lagrange interpolation error formula

$$\int_a^b f(x)\mathrm{d}x - \sum_{i=0}^n H_i f(x_i) = \int_a^b \frac{w_{n+1}(x)}{(n+1)!} f^{(n+1)}(\zeta)\mathrm{d}x.$$