The math behind the methods

and some madness...
part 2

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PH3105, Autumn Semester 2017

Orthogonal Polynomials

Weight functions

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Inner product

Given a weight function on (a, b) we can define the **inner product** of $f, g \in C[a, b]$ by

$$(f, g) \equiv \int_a^b w(x) f(x) g(x) \, dx$$

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The **Cauchy-Scwarz inequality**

$$\forall f, g \in C[a,b], \qquad |(f,g)| \leq ||f||_2\,||g||_2$$

allows us to show that the Euclidean norm obeys the **triangle inequality**

$$||f+g||_2 \leq ||f||_2 + ||g||_2$$

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(Gram-Schmidt) There exists a sequence of polynomials $\{\phi_n(x) \,|\, n \geq 0\}$ *with* $degree(\phi_n) = n$*, for all* n *and*

$$(\phi_n, \phi_m) = 0 \qquad \forall n \neq m, \quad n, m \geq 0$$

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In addition, we can impose the following properties:
(i) $(\phi_n, \phi_n) = 1$, for all n;
(ii) the coefficient of x^n in $\phi_n(x)$ is positive
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For $w(x) = 1$ on $(-1, 1)$ we can find

$$\phi_0(x) = \sqrt{\frac{1}{2}}, \qquad \phi_1(x) = \sqrt{\frac{3}{2}}x, \qquad \phi_2(x) = \sqrt{\frac{5}{2}}\frac{1}{2}\left(3x^2 - 1\right), \qquad \ldots$$

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Legendre polynomials

For $w(x) = 1$ on $(-1, 1)$ define

$$P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} \left[\left(x^2 - 1 \right)^n \right]$$

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$$\phi_n(x) = \sqrt{\frac{2n+1}{2}} P_n(x)$$

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From $\cos(A \pm B) = \cos A \cos B \mp \sin A \sin B$ we can show that

$$T_{n+1}(x) = 2x T_n(x) - T_{n-1}(x), \qquad n \ge 1$$

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$$(T_n, T_m) = \begin{cases} 0 & n \ne m \\ \pi & m = n = 0 \\ \dfrac{\pi}{2} & m = n > 0 \end{cases}$$

Theorem

Let $\{\phi_n(x) \,|\, n \geq 0\}$ *be an orthogonal family of polynomials on* (a,b)*with weight function* $w(x)$*. If* $f(x)$ *is a polynomial of degree* m *we have*

$$f(x) = \sum_{n-0}^{m} \frac{(f.\phi_n)}{(\phi_n, \phi_n)} \phi_n(x)$$

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Corollary

Let $f(x)$ *be a polynomial of degree* $\leq m-1$*. Then*

$$(f,\phi_m) = 0$$

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Let $x_1, x_2 \ldots, x_m$ be all the roots of $\phi_n(x)$ in (a, b) at which $\phi_n(x)$ changes sign.

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However, degree$(B(x)) = m < n$ - and so $(B, \phi_n) = 0$ - a contradiction!

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$$\phi_n(x) = A_n\left(x - x_1^{(n)}\right)\left(x - x_2^{(n)}\right)\ldots\left(x - x_n^{(n)}\right)$$

$$= A_n x^n + B_n x^{n-1} + \ldots$$

Theorem

Triple Recursion Relation

For $n \geq 1$

$$\phi_{n+1}(x) = (a_n x + b_n)\,\phi_n(x) - c_n \phi_{n-1}(x)$$

where $a_n = \dfrac{A_{n+1}}{A_n}, \qquad b_n = a_n\left[\dfrac{B_{n+1}}{A_{n+1}} - \dfrac{B_n}{A_n}\right]$ *and*

$$c_n = \frac{A_{n+1}A_{n-1}}{A_n^2}\,\frac{(\phi_n, \phi_n)}{(\phi_{n-1}, \phi_{n-1})}$$

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We need to find $2n$ polynomials $h_1,\ldots h_n,\tilde{h}_1,\ldots\tilde{h}_n$, each of degree $2n-1$ satisfying

$$h_i\left(x_j\right)=\delta_{ij}, \qquad h_i'\left(x_j\right)=0$$

and

$$\tilde{h}_i\left(x_j\right)=0, \qquad \tilde{h}_i'\left(x_j\right)=\delta_{ij}$$

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$$h_i\left(x_j\right)=\delta_{ij}, \qquad h_i'\left(x_j\right)=0$$

and

$$\tilde{h}_i\left(x_j\right)=0, \qquad \tilde{h}_i'\left(x_j\right)=\delta_{ij}$$

Then

$$H_n\left(x\right)=\sum_{i=1}^{n}\left[y_i h_i\left(x\right)+y_i'\tilde{h}_i\left(x\right)\right]$$

is the Hermite interpolating polynomial.

Hermite interpolation

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Similarly

$$h_i(x) = \left(1 - 2L'_i(x_i)(x - x_i)\right)\left[L_i(x)\right]^2$$

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Thus $R(x)$must be identically zero!

The error can be shown to be

$$f(x) - H_n(x) = [\Psi_n(x)]^2 \frac{f^{(2n)}(x)}{(2n)!}$$

Gauss quadrature

Recall that the Gauss quadrature formula is

$$\int_{-1}^{1} f(x)\, dx \approx \sum_{i=1}^{n} w_i f(x_i)$$

where the freedom of choice of the n weights w_i and the n nodes x_i is expolited to get an expression that is correct for all polynomials up to degree $2n-1$.

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As we have already seen, in principle we can find the w_i and x_i from the $2n$ equations

$$\sum_{i=1}^{n} w_i x_i^j = \begin{cases} 0 & \text{for } j = 1, 3, \ldots, 2n-1 \\ \frac{2}{j+1} & \text{for } j = 2, 4, \ldots, 2n-2 \end{cases}$$

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This is a set of non-linear equations - not only are they difficult to solve, the existence of solutions for general n is not even clear *a priori.*

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for some $\eta \in (a, b)$.

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$$w_j = -\frac{a_n (\phi_n, \phi_n)}{\phi_n'(x_j)\, \phi_{n+1}(x_j)}$$

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Proof - an outline

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since degree $L_i(x) = n - 1$.

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Consider the composite trapezoidal estimate of an integral

$$I_0 \equiv \int_a^b f(x)\,dx = I(h) + E(h)$$

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$$\frac{E(h_1)}{E(h_2)} \approx \frac{h_1^2}{h_2^2} \implies \frac{E(h_1)}{h_1^2} = \frac{E(h_2)}{h_2^2} = \frac{E(h_2) - E(h_1)}{h_2^2 - h_1^2} = \frac{I(h_1) - I(h_2)}{h_2^2 - h_1^2}$$

Richardson extrapolation

A better estimate for I_0 would be

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In particular, we often use

$$I_0 \approx \frac{4}{3} I\left(\frac{h}{2}\right) - \frac{1}{3} I\left(h\right)$$

Richardson extrapolation

The next step

Using three step sizes h, $\frac{h}{2}$ and $\frac{h}{4}$, we can get two Richardson estimates

$$I_l \approx \frac{4}{3} I\left(\frac{h}{2}\right) - \frac{1}{3} I\left(h\right)$$

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and

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These can be similarly combined to give a better estimate

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We can repeat this with two $\mathcal{O}\left(h^6\right)$ estimates to get an even better estimate

$$I \approx \frac{64}{63} I_m - \frac{1}{63} I_l \qquad + \mathcal{O}\left(h^8\right)$$

Richardson extrapolation

The next step

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Extending this idea leads to the **Romberg integration** algorithm!