Differentiation via Polynomial interpolation

The previous formulas and many others can be obtained by differentiating the interpolating polynomial.

Let $x_0, x_1, \dots x_n$ be $n+1$ distinct nodes

$$f(x) = \underbrace{\sum_{i=0}^{n} f(x_i)\, l_i(x)}_{\text{interp poly of } f \text{ at nodes } x_i.} + \underbrace{\frac{1}{(n+1)!} f^{(n+1)}(\xi_x)\, w(x)}_{\text{error term where}}$$

$$w(x) = \prod_{i=0}^{n} (x - x_i).$$

Differentiate:

$$f'(x) = \sum_{i=0}^{n} f(x_i)\, l_i'(x) + \frac{1}{(n+1)!} \frac{d}{dx}\left[f^{(n+1)}(\xi_x) \right] w(x)$$

$$+ \frac{1}{(n+1)!} f^{(n+1)}(\xi_x)\, w'(x)$$

Take $x = x_\alpha$ = one of the nodes:

$$f'(x_\alpha) = \sum_{i=0}^{n} f(x_i)\, l_i'(x_\alpha) + \frac{1}{(n+1)!} f^{(n+1)}(\xi_{x_\alpha})\, w'(x_\alpha)$$

Moreover:

$$w'(x) = \sum_{i=0}^{n} \prod_{\substack{j=0 \\ j \neq i}}^{n} (x - x_j)$$

$$\Rightarrow \quad w'(x_\alpha) = \prod_{\substack{j=0 \\ j \neq \alpha}}^{n} (x_\alpha - x_j)$$

(There is only one term in sum above that does not contain x_α as a root)

We get the differentiation formula:

$$\boxed{f'(x_\alpha) = \sum_{i=0}^{n} f(x_i)\, l_i'(x_\alpha) + \frac{1}{(n+1)!} f^{(n+1)}(\xi_\alpha) \prod_{\substack{j=0 \\ j\neq\alpha}}^{n} (x_\alpha - x_j)}$$

$\rightsquigarrow$ $n+1$ point formula to approx $f'(x_\alpha)$.

Most common formulas are for $n=2$ and 4.

$\underline{n=2}$: $$l_0(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} \rightarrow l_0'(x) = \frac{2x - x_1 - x_2}{(x_0-x_1)(x_0-x_2)}$$

$$l_1(x) = \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} \rightsquigarrow l_1'(x) = \frac{2x - x_0 - x_2}{(x_1-x_0)(x_1-x_2)}$$

$$l_2(x) = \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} \rightsquigarrow l_2'(x) = \frac{2x - x_0 - x_1}{(x_2-x_0)(x_2-x_1)}$$

So we get formulas of the form:

$$f'(x_j) = f(x_0)\frac{2x_j - x_1 - x_2}{(x_0-x_1)(x_0-x_2)} + f(x_1)\frac{2x_j - x_0 - x_2}{(x_1-x_0)(x_1-x_2)}$$

$$+ f(x_2)\frac{2x_j - x_1 - x_2}{(x_2-x_1)(x_2-x_0)} + \frac{1}{6} f^{(3)}(\xi_j) \prod_{\substack{k=0 \\ k\neq j}}^{2} (x - x_k)$$

dep. on x_j

Most commonly the points are evenly spaced:

$$x_0, \quad x_1 = x_0 + h, \quad x_2 = x_0 + 2h$$

which leads to the following differentiation formulas.

① $\underline{x_j = x_0}$ $$f'(x_0) = \frac{1}{h}\left[-\frac{3}{2}f(x_0) + 2f(x_0+h) - \frac{1}{2}f(x_0+2h)\right] + \frac{h^2}{3}f^{(3)}(\xi_0)$$

② $\underline{x_j = x_1}$ $$f'(x_0+h) = \frac{1}{h}\left[-\frac{1}{2}f(x_0) + \frac{1}{2}f(x_0+2h)\right] - \frac{h^2}{6}f^{(3)}(\xi_1)$$

③ $\underline{x_j = x_2}$ $$f'(x_0+2h) = \frac{1}{h}\left[\frac{1}{2}f(x_0+2h) - 2f(x_0+h) + \frac{3}{2}f(x_0+2h)\right] + \frac{h^2}{3}f^{(3)}(\xi_2)$$

Note: ② can be actually rewritten in the form:

$$f'(x_0) = \frac{1}{2h}\left[f(x_0+h) - f(x_0-h)\right] - \frac{h^2}{6}f^{(3)}(\xi_1)$$

which we already derived using Taylor's theorem

① and ③ are essentially same formula: simply change variables $x_0+2h \to x_0$ in ③ and $h = -h$ to get ①

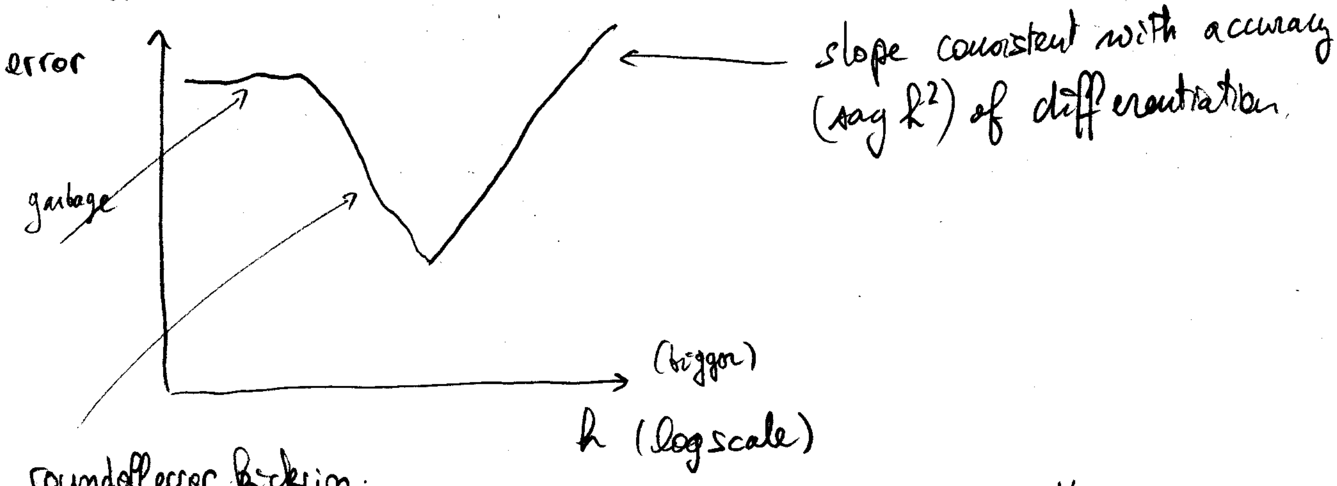
② is preferable over ① and ③ because error is half!

$\underline{n=4}$: five point formulas: (same technique)

one example is:

$$f'(x_0) = \frac{1}{12h}\left[f(x_0-2h) - 8f(x_0-h) + 8f(x_0+h) - f(x_0+2h)\right] + \frac{h^4}{30}f^{(5)}(\xi), \quad \xi \in (x_0-2h, x_0+2h).$$

Big problem with numerical differentiation is roundoff error.
A typical error plot for such methods is:



$\rightsquigarrow$ step must not be too small (e.g. taking $h = 10^{-16}$ is a very bad idea!)
not be too big (otherwise method is not accurate)

see HW problem. for numerical study of accuracy.

§4.2 Richardson's Extrapolation

This is a nice trick to get more accuracy out of numerical differentiation methods. Actually the idea is more general and can be used when the truncation error associated with method has the form:

$$M = \underbrace{N(h)}_{\text{approx}} + k_1 h + k_2 h^2 + k_3 h^3 + \cdots$$

(we shall see how to apply extrapolation methods to numerical integration and to solving ODEs.)

Idea: combine approx with different h in a certain way that cancels the leading order term

Here is an example with centered differences formula:

$$f(x+h) = \sum_{k=0}^{\infty} \frac{1}{k!} h^k f^{(k)}(x)$$

$$f(x-h) = \sum_{k=0}^{\infty} \frac{1}{k!} (-1)^k h^k f^{(k)}(x)$$

$$f(x+h) - f(x-h) = 2h f'(x) + \frac{2h^3}{3!} f^{(3)}(x) + \frac{2h^5}{5!} f^{(5)}(x) + \cdots$$

$$f'(x) = \underbrace{\frac{f(x+h) - f(x-h)}{2h}}_{\text{approx Centered differences}} - \underbrace{\left[\frac{h^2}{3!} f^{(3)}(x) + \frac{h^4}{5!} f^{(5)}(x) + \cdots \right]}_{\text{truncation error of method}}$$

$$M = N(h) + K_2 h^2 + K_4 h^4 + K_6 h^6 + \cdots$$

$$4\times \left[M = N(h/2) + \frac{K_2 h^2}{4} + \frac{K_4 h^4}{16} + \frac{K_6 h^6}{64} + \cdots \right]$$

$$3M = 4N(h/2) - N(h) - \frac{3K_4 h^4}{4} - \frac{15 K_6 h^6}{16} - \cdots$$

$$\boxed{M = \frac{4}{3} N\left(\frac{h}{2}\right) - \frac{1}{3} N(h) - \underbrace{\frac{K_4 h^4}{4} - \frac{5 K_6 h^6}{16}}_{} - \cdots}$$

By applying centered differences w/ h, $h/2$ we can get $O(h^4)$ error instead of $O(h^2)$!!

Can we do the same thing again? Yes!

Let $N_2(h) = \frac{4}{3} N\left(\frac{h}{2}\right) - \frac{1}{3} N(h)$ $\quad (O(h^4)$ accurate$)$

$$M = N_2(h) + L_4 h^4 + L_6 h^6 + \dots$$

$$16\times\left[M = N_2(h/2) + \frac{L_4 h^4}{16} + \frac{L_6 h^6}{64} + \dots \right]$$

$$15M = 16N_2(h/2) - N_2(h) - \frac{3L_6 h^6}{4} - \dots$$

Thus we get: $M = N_3(h) + O(h^6)$

where $N_3(h) = \frac{16}{15} N_2(h/2) - \frac{1}{15} N_2(h)$

in general:

$$\boxed{N_j(h) = \frac{4^j}{4^{j-1}-1} N_{j-1}(h/2) - \frac{1}{4^{j-1}-1} N_{j-1}(h) \quad \text{is accurate } O(h^{2j}).}$$

Richardson's extrapolation is simply using this recursive formula:

$$\begin{array}{cccc}
O(h^2) & O(h^4) & O(h^6) & O(h^8) \\
N_1(h) \equiv N(h) & \to N_2(h) & \to N_3(h) & \to N_4(h) \\
N_1(h/2) \equiv N(h/2) & \to N_2(h/2) & \to N_3(h/2) & \\
N_1(h/4) \equiv N(h/4) & \to N_2(h/4) & & \\
N_1(h/8) \equiv N(h/8) & & &
\end{array}$$

Of course we can't keep doing this forever... Why?

As we increase accuracy we need smaller $h/2^k$ which can become close to machine precision and give trouble.

§ 4.3 Numerical Integration

Numerical integration is sometimes called numerical quadrature (or cubature). Our goal is to design quadrature formulas of the kind

$$\int_a^b f(x)\,dx \approx \sum_{i=0}^{n} a_i f(x_i)$$

from polynomial interpolation, via a process similar to the one used for numerical differentiation.

Let $x_0, x_1, \ldots x_n$ be n distinct nodes on $[a,b]$ and let $p(x)$ be the interp poly of f at the nodes $x_0, x_1, \ldots x_n$, then:

$$p(x) = \sum_{i=0}^{n} f(x_i)\, l_i(x) \quad \text{(in Lagrange form)}$$

where $$l_i(x) = \prod_{\substack{j=0\\ j\neq i}}^{n} \frac{(x-x_j)}{(x_i-x_j)}, \quad i=0,\ldots,n.$$

Then $$\boxed{\int_a^b f(x)\,dx} \approx \int_a^b p(x)\,dx = \sum_{i=0}^{n} f(x_i) \underbrace{\int_a^b l_i(x)\,dx}$$

$$= \boxed{\sum_{i=0}^{n} f(x_i)\, A_i}$$

The A_i are integration weights that can be computed ahead of time. An integration formula of this kind is called Newton-Cotes formula if the nodes are equally spaced.

Trapezoidal rule

$\underline{n=1}$: $x_0 = a$, $x_1 = b$ then:

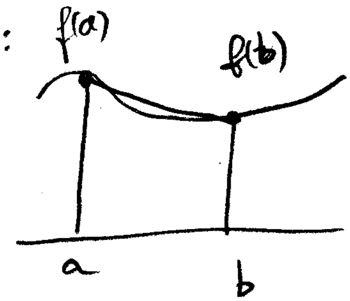
$$l_0(x) = \frac{b-x}{b-a}, \quad l_1(x) = \frac{x-a}{b-a}$$

$$A_0 = \int_a^b l_0(x)\,dx = \frac{1}{2}(b-a) = \int_a^b l_1(x)\,dx = A_1$$

We get formula:

$$\boxed{\int_a^b f(x)\,dx \approx \frac{b-a}{2}\left[f(a)+f(b)\right]}$$

Called Trapezoid rule because we approx integral by area of a trapezoid:



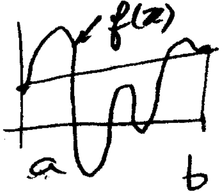
The error of trapezoidal rule can be shown to be in the form:

$$-\frac{1}{12}(b-a)^3 f''(\xi), \quad \text{for some } \xi \in (a,b)$$

method to get error is outlined in textbook and its main steps are:

- writing $f(x) - p_1(x) = f''(\xi_x)\dfrac{(x-a)(x-b)}{2}$
- using MVT for integrals (polynomial does not change signs)

Using trapezoidal rule on one single interval does not give good approx. to integral.



↝ subdivide or partition $[a,b]$ with nodes:

$$a = x_0 < x_1 < \dots < x_n = b$$

↝ apply trapz. rule on each subinterval and sum result:

$$\boxed{\int_a^b f(x)\,dx = \sum_{i=1}^{n} \int_{x_{i-1}}^{x_i} f(x)\,dx}$$

$$\boxed{\approx \frac{1}{2}\sum_{i=1}^{n} (x_i - x_{i-1})\,(f(x_i) + f(x_{i-1}))}$$

We obtain by this process a composite rule (i.e. applying same integration formula to many subintervals).

If the nodes x_i are equally space: $x_i = a + ih$, $i=0,\dots n$ where $h = \frac{b-a}{n}$, the composite trapz rule is:

$$\int_a^b f(x)\,dx \approx \frac{h}{2}\left[f(a) + 2\sum_{i=1}^{n-1} f(a+ih) + f(b)\right]$$

how do we get error?

$$\text{error of composite trapz} = \sum_{i=1}^{n} -\frac{1}{12} h^3 f''(\xi_i)$$

$$= -\frac{1}{12} h^3\, n\, f''(\xi), \quad \xi \in [a,b]$$

$$= -\frac{(b-a)}{12} h^2 f''(\xi)$$

Since there is a $\xi \in [a,b]$ s.t.

$$f''(\xi) = \frac{1}{n} \sum_{i=1}^{n} f''(\xi_i) \quad \text{and } \xi_i \in [a,b]$$

(think about this identity as a generalized intermediate value theorem)

Here is another way of deriving integration formulas:

<u>Method of undetermined coefficients:</u>

Since the interp poly at n+1 distinct nodes of a polynomial function is the polynomial itself, we see that with this procedure we can generate integration formulas that are exact for polynomials of degree $\leq n$.

So we can get same integration formulas by requiring that the formula be exact for all poly of degree $\leq n$.

<u>Example</u>: Derive formula of the form below and exact for poly of degree ≤ 2.

$$\int_0^1 f(x)\,dx \approx A_0 f(0) + A_2 f(1/2) + A_3 f(1).$$

If we use as basis for $\Pi_2 = \{1, x, x^2\}$ we get:

$$1 = \int_0^1 dx = A_0 + A_1 + A_2$$

$$\frac{1}{2} = \int_0^1 t\,dt = \frac{1}{2}A_1 + A_2$$

$$\frac{1}{3} = \int_0^1 t^2\,dt = \frac{1}{4}A_1 + A_2$$

We get 3×3 system that we can solve:

$$\begin{bmatrix} 1 & 1 & 1 \\ 0 & \frac{1}{2} & 1 \\ 0 & \frac{1}{4} & 1 \end{bmatrix} \begin{bmatrix} A_0 \\ A_1 \\ A_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1/2 \\ 1/3 \end{bmatrix}$$

get $A_0 = \frac{1}{6}$, $A_1 = \frac{2}{3}$, $A_2 = \frac{1}{6}$

$\rightsquigarrow$ we get an integration formula that is exact for any polynomial of degree 2:

Simpson's rule

$$\int_a^b f(x)\,dx \approx \frac{b-a}{6}\left[f(a) + 4 f\left(\frac{a+b}{2}\right) + f(b) \right]$$

Unexpectedly Simpson's rule is $\boxed{\text{exact for all polynomials of order 3,}}$ and error term is:

$$-\frac{1}{90}\left(\frac{b-a}{2}\right)^5 f^{(4)}(\xi)$$

<u>Note</u>: if you're given error term, how do you get degree for which formula is exact? Well the error term for Simpson's rule involves $f^{(4)}(\xi)$ which is identically zero for all poly of degree ≤ 3.

We can convince ourselves that error in Simpson's rule is $O(h^5)$ by using Taylor's theorem: let $h = \frac{b-a}{2}$

$$\int_a^{a+2h} f(x)\,dx \approx \frac{h}{3}\left[f(a) + 4 f(a+h) + f(a+2h) \right]$$

$$RHS = \frac{h}{3}\Big[f(a)$$
$$+4\left(f(a) + hf'(a) + \frac{h^2}{2}f''(a) + \frac{h^3}{3!}f'''(a) + \frac{h^4}{4!}f^{(4)}(a) + \cdots\right)$$
$$+ f(a) + 2hf'(a) + 2h^2 f''(a) + \frac{4}{3}h^3 f'''(a) + \frac{2}{3}h^4 f^{(4)}(a) + \cdots\Big]$$

$$= 2hf(a) + 2h^2 f'(a) + \frac{4}{3}h^3 f''(a) + \frac{2}{3}h^4 f^{(3)}(a) + \frac{100}{3.5!}h^5 f^{(4)}(a) + \cdots$$

Letting $F(x) = \int_a^x f(t)\,dt$:

$$LHS = F(a+2h) = \underbrace{F(a)}_{0} + 2h f(a) + 2h^2 f'(a) + \frac{4}{3}h^3 f''(a) + \frac{2}{3}h^4 f^{(3)}(a)$$
$$+ \frac{32}{5!}h^5 f^{(4)}(a)$$

Combining both equations we get:

$$\int_a^{a+2h} f(x)\,dx = \frac{h}{3}\left[f(a) + 4f(a+h) + f(a+2h)\right] - \frac{h^5}{90}f^{(4)}(a) - \cdots$$

<u>Composite Simpson's rule</u>: Let n be <u>even</u> and subdivide $[a,b]$ into n subintervals delimited by the node:

$$x_i = a + ih, \quad i = 0, \dots, n, \quad h = \frac{b-a}{n}$$

then:

$$\int_a^b f(x)\,dx = \int_{x_0}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx + \cdots + \int_{x_{n-2}}^{x_n} f(x)dx$$

$$= \sum_{i=1}^{n/2} \int_{x_{2i-2}}^{x_{2i}} f(x)\,dx$$

$$\approx \frac{h}{3}\sum_{i=1}^{n/2}\left[f(x_{2i-2}) + 4f(x_{2i-1}) + f(x_{2i})\right]$$

using Simpson's rule for each subinterval

To avoid repetition of terms the composite Simpson's rule can be written as:

$$\int_a^b f(x)\,dx \approx \frac{h}{3}\Big[f(x_0) + 2\sum_{i=2}^{n/2} f(x_{2i-2}) + 4\sum_{i=1}^{n/2} f(x_{2i-1}) + f(x_n) \Big]$$

Since error term for Simpson's rule is $-\dfrac{h^5}{90} f^{(4)}(\xi)$

the error for composite Simpson's rule should be:

$$\frac{n}{2}\left(-\frac{h^5}{90}\right) f^{(4)}(\xi)$$

$$\boxed{= -\frac{(b-a)}{180} h^4 f^{(4)}(\xi)}$$

Now the more general cases:

The degree of accuracy or precision of a quadrature formula is largest n s.t. formula is exact for

$$\Pi_n = \operatorname{span}\{1, x, x^2, \dots, x^n\}$$

– poly of degree $\le n$.

Recall the $(n+1)$-th Newton Cotes formula is obtained from interp poly of f at a set of equally spaced points

$$x_i = a + ih, \quad i = 0, \dots, n, \quad h = \frac{b-a}{n}.$$

and is of the form:

$$\int_a^b f(x)\,dx \approx \sum_{i=0}^{n} A_i f(x_i)$$

where $$A_i = \int_a^b l_i(x)\,dx = \int_a^b \left(\prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{x - x_j}{x_i - x_j} \right) dx$$

<u>Theorem on Newton Cotes formula:</u> Assuming f is smooth enough:

<u>n even:</u> $\exists\, \xi \in (a,b)$ for which

$$\int_a^b f(x)\,dx = \sum_{i=0}^{n} A_i f(x_i) + \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!} \int_0^n t \prod_{i=0}^{n} (t-i)\,dt$$

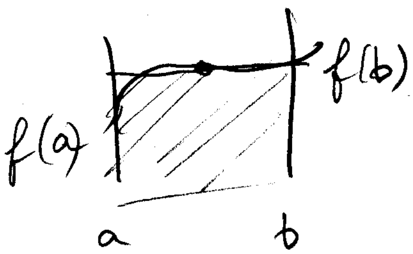
(exact for poly of degree $n+1$ $\rightsquigarrow$ like Simpson's we get one degree more of accuracy than we were expecting:

<u>n odd</u>: $\exists\, \xi \in (a,b)$ for which:

$$\int_a^b f(x)\,dx = \sum_{i=0}^{n} A_i f(x_i) + \frac{h^{n+2} f^{(n+1)}(\xi)}{(n+1)!} \int_0^n \prod_{i=0}^{n} (t-i)\,dt$$

→ just remember quantitatively order of error

One other useful integration formula is <u>midpoint rule</u>.

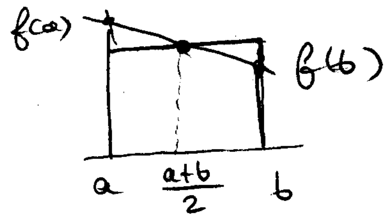


approximate integral by rectangle of height $f\left(\frac{a+b}{2}\right)$.

$$\int_a^b f(x)\,dx = (b-a)\,f\left(\frac{a+b}{2}\right) + \frac{(b-a)^3}{\quad} f''(\xi)$$

where $\xi \in [a,b]$.

(exact for linear since area of trapezium and rectangle below are same.



and <u>composite midpoint rule</u> $x_i = a + ih$, $i = 0, \dots, n$, $h = \frac{b-a}{n}$

and <u>n even</u>:

$$\int_a^b f(x)\,dx = \sum_{i=1}^{n/2} \int_{x_{2i-2}}^{x_{2i}} f(x)\,dx \approx 2h \sum_{i=1}^{n/2} f(x_{2i-1})$$

General integration formulas

Same ideas we used to obtain Newton Cotes integration formulas can be applied to approximating:

$$\int_a^b f(x)\, w(x)\,dx \approx \sum_{i=0}^{n} A_i f(x_i),$$

where $w(x) \equiv$ <u>weight function</u>

The only thing we need to do is set:

$$\boxed{A_i = \int_a^b l_i(x)\, w(x)\, dx.}$$

note: $w(x)$ doesn't need to be positive.

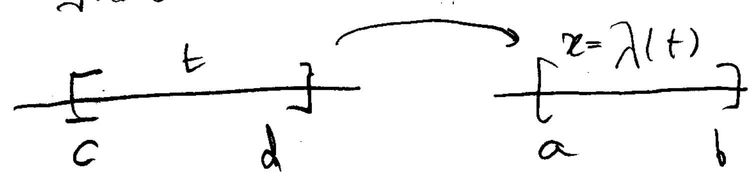
Change of intervals

How do we transform a quadrature formula given for:

$$\int_c^d f(t)\,dt \approx \sum_{i=0}^{n} A_i f(x_i)$$

with degree k accuracy into a formula for interval $[a,b]$ with same accuracy?

We use change of variables. Indeed:



$$\left.\begin{array}{l}\lambda(c) = a \\ \lambda(d) = b\end{array}\right\} \Rightarrow \lambda(t) = a\,\frac{t-d}{c-d} + b\,\frac{c-t}{c-d}$$

$x = \lambda(t)$

$$dx = \lambda'(t)\,dt = \frac{a-b}{c-d}\,dt$$

$$\int_a^b f(x)\,dx = \frac{a-b}{c-d}\int_c^d f(\lambda(t))\,dt$$

$$\approx \frac{a-b}{c-d}\sum_{i=0}^{n} A_i f(\lambda(t_i))$$

§ 4.7 Gaussian Quadrature

(§4.5 and 4.6 will be seen later)

Let $x_0, x_1, \dots, x_n$ be $n+1$ distinct nodes in $[a,b]$

We know we can design quadrature formulas of the kind:

$$\int_a^b f(x)\, w(x)\, dx \approx \sum_{i=0}^{n} A_i f(x_i) \qquad (*)$$

where $w(x) > 0$ is a weight function.

Assume $(*)$ is exact for poly of degree $\leq n$ then

$$A_i = \int_a^b w(x) \underbrace{\prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{x - x_j}{x_i - x_j}}_{l_i(x)} dx \qquad (**)$$

(since interp poly at the nodes $x_0, \dots x_n$ of a poly of degree $\leq n$ is the poly. itself)

How can we improve accuracy of $(*)$? How many degrees of freedom do we have?

$A_i \quad i = 0, \dots, n \quad \equiv n+1$ degrees of freedom

$x_i \quad i = 0, \dots n \quad \equiv n+1$ " " "

<u>Total</u>: $2n+2$ dof ... So maybe we can get a formula that is exact for polynomials of degree $\leq 2n+1$?

<u>Idea</u>: adjust coefficients and nodes so that we get more accuracy!

Where should we place nodes?

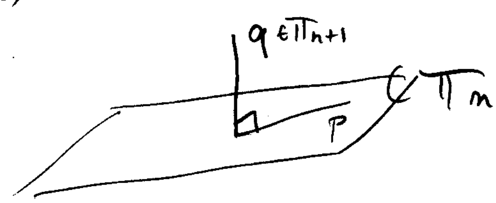
Recall notation: $\Pi_n =$ poly of degree $\leq n$

$= \text{span}\{1, x, x^2, \dots, x^n\}$

Theorem on Gaussian quadrature

Let $w(x) > 0$ be a weight function and let q be a non-zero poly $\in \Pi_{n+1}$ which is w-orthogonal to Π_n, i.e.:

$$\forall p \in \Pi_n \quad \int_a^b q(x)\, p(x)\, w(x)\, dx = 0.$$



Let $x_0, x_1, \dots x_n$ be the roots of q, then the quadrature formula $(*)$ with coeff $(**)$ is <u>exact</u> for poly in Π_{2n+1}.

~~proof~~: Take $f \in \Pi_{2n+1}$ then by remainder theorem:

$$f = qp + r \quad \text{where } r \in \Pi_n \text{ and } p \in \Pi_n$$

Since x_i are roots of q: $\quad f(x_i) = r(x_i) \quad i = 0, \dots, n.$

Now:
$$\int_a^b f w\, dx = \underbrace{\int_a^b qpw\, dx}_{\substack{= 0 \\ \text{by orthogonality}}} + \int_a^b r w\, dx$$

$$= \sum_{i=0}^{n} A_i\, r(x_i) \quad \text{because } r \in \Pi_n \text{ and formula is exact for such polynomials}$$

$$= \sum_{i=0}^{n} A_i\, f(x_i) \quad \text{since } r(x_i) = f(x_i)$$

QED

Wait a second. How do we know that roots of q, i.e. The nodes in Gaussian quadrature are real and distinct?

<u>Theorem on number of sign changes</u>

Let $w \in C[a,b]$ be a positive weight function. Let f be a nonzero element of $C[a,b]$ that is w-orthogonal to Π_n, then f changes sign at least $n+1$ times on (a,b).

<u>pause</u> why is this helpful? because if $f \in \Pi_{n+1}$ and is w-$\perp$ to Π_n it must have $n+1$ sign changes $=$ $n+1$ <u>real distinct roots</u>

<u>Proof</u>:

Since $1 \in \Pi_n$: $\int_a^b 1 \cdot f(x) w(x) dx = 0$

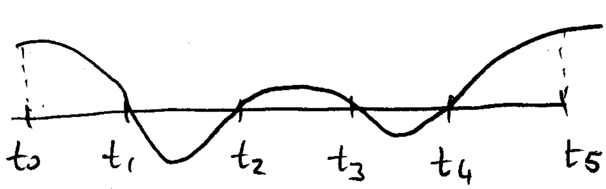
$\Rightarrow$ f must change signs on $[a,b]$ at <u>least once</u>.

Suppose for contradiction that f changes sign r times on $[a,b]$ with $r \le n$.

then we can find nodes: $a = t_0 < t_1 < t_2 < \dots < t_r < t_{r+1} = b$

such that function has same sign on each (t_i, t_{i+1}) interval.

e.g.:



$r = 4$, f has 4 sign changes

Let $p(x) = \prod_{i=1}^{r} x - t_i$, has r roots at the t_i, so it must have same sign on each (t_i, t_{i+1})

$$\Rightarrow \int_a^b f(x)\,p(x)\,w(x)dx = \sum_{i=1}^{r+1} \underbrace{\int_{t_{i-1}}^{t_i} f(x)\,p(x)\,w(x)}_{>0} > 0$$

contradiction!

QED

Gauss considered case where $w(x)=1$ and interval $[-1,1]$ (although one can always transform this interval to another interval by C.O.V):

$\underline{n=1}$ $$\int_{-1}^{1} f(x)\,dx \approx f(-\alpha)+f(\alpha), \quad \alpha = \frac{1}{\sqrt{3}}$$

$\underline{n=2}$ $$\int_{-1}^{1} f(x)\,dx \approx \frac{1}{9}\left[5f\left(-\sqrt{\tfrac{3}{5}}\right)+8f(0)+5f\left(\sqrt{\tfrac{3}{5}}\right)\right]$$

expressions become more complicated for larger n and we may not even have a fixed formulas.

As seen from Gaussian quadrature theorem all we need to define a Gaussian quadrature is a polynomial q_{n+1} s.t.

i) $q_{n+1} \in \Pi_{n+1}$

ii) q_{n+1} is w- orthogonal to Π_n

The coefficients then follow from formula ($\ast$-$\ast$).

Since for the Gaussian quadrature only zeros of q_{n+1} matter we may normalize q_{n+1} s.t. it is <u>monic</u> meaning coeff of x^{n+1} is one.

How to obtain these <u>orthogonal polynomials</u>? We can obtain them recursively by a procedure that amounts to <u>Gram-Schmidt orthogonalization</u>.

Let us denote by $(f,g) = \int_a^b f(x)\, g(x)\, w(x)\, dx$.

This an inner product which has properties analogous to the dot product in $\mathbb{R}^n$ namely: it is a <u>positive</u> <u>symmetric</u> <u>bilinear</u> form meaning:

$$(f,g) = (g,f) \quad \text{(symmetric)}$$

$$(f,f) \geq 0 \text{ and } (f,f) = 0 \Leftrightarrow f = 0 \quad \text{(positive)}$$

$$\left.\begin{array}{l}(\alpha f + \beta g, h) = \alpha(f,h) + \beta(g,h) \\ (f, \alpha g + \beta h) = \alpha(f,g) + \beta(f,g)\end{array}\right\} \quad \text{(bilinear)}$$

We prime recurrence with $\boxed{p_0(x) = 1}$ Then:

$$p_1 = x p_0 - \frac{(x p_0, p_0)}{(p_0, p_0)} p_0 \in \Pi_1; \text{ monic and } w\text{-orthogonal to } p_0 \text{ (check).}$$

$$p_2 = x p_1 - \frac{(x p_1, p_1)}{(p_1, p_1)} p_1 - \frac{(x p_1, p_0)}{(p_0, p_0)} p_0$$

$\in \Pi_2$; monic and w-orthogonal to p_0, p_1 | to Π_1.

$$p_3 = x p_2 - \frac{(x p_2, p_2)}{(p_2, p_2)} p_2 - \frac{(x p_2, p_1)}{(p_1, p_1)} p_1 - \underbrace{\frac{(x p_2, p_0)}{(p_0, p_0)}}_{= 0 \text{ why?}} p_0$$

$$(x p_2, p_0) = (p_2, x p_0) = 0.$$

$\vdots$

$$p_{i+1} = x p_i - \frac{(x p_i, p_i)}{(p_i, p_i)} p_i - \frac{(x p_i, p_{i-1})}{(p_{i-1}, p_{i-1})} p_{i-1}$$

We get a three term recurrence where by construction:

p_{i+1} is monic and in Π_{i+1}

p_{i+1} is w-$\perp$ to $p_0, p_1, p_2, \dots, p_i$

$\Leftrightarrow p_{i+1}$ ______ Π_i

In the case where $w = 1$ and on interval $[-1, 1]$ we get the so called Legendre polynomials:

$$\boxed{p_0(x) = 1}$$

$$\boxed{p_1(x) = x - \cancel{\frac{(x,1)}{(1,1)} 1} = x}$$

$$\boxed{p_2(x)} = x^2 - \cancel{\underbrace{\frac{(x^2,x)}{(x,x)}}_{=0}} x - \underbrace{\frac{(x^2,1)}{(1,1)}}_{=\frac{1}{3}} 1$$

$$\boxed{= x^2 - \frac{1}{3}}$$

and so on... The next Legendre polynomials are:

$$p_3(x) = x^3 - \frac{3}{5} x$$

$$p_4(x) = x^4 - \frac{6}{7} x^2 + \frac{3}{35}$$

$$p_5(x) = x^5 - \frac{10}{9} x^3 + \frac{5}{21} x$$

So when $w = 1$ the nodes for Gaussian quadrature are the roots of Legendre polynomials.

Here are some properties of Gaussian quadrature:

Lemma The coefficients A_i are positive and $\sum_{i=0}^{n} A_i = \int_a^b w(x)dx$.

proof: Let q_{n+1} be a poly in Π_{n+1} w-orthogonal to Π_n.

Let $x_0, x_1, \dots x_n$ be the $n+1$ distinct zeros of q_{n+1}.

Let $p(x) = \dfrac{q(x)}{(x-x_j)}$ for some $j = 0, \dots, n+1$

Since $p \in \Pi_n$, $p^2 \in \Pi_{2n}$ so Gaussian quad must be exact for p:

$$0 < \int_a^b p^2(x)\, w(x)\, dx = \sum_{i=0}^{n} A_i p^2(x) = A_j p^2(x_j)$$

$$\Rightarrow A_j > 0$$

Moreover Gaussian quad is exact for $f(x) \equiv 1$ thus:

$$\int_a^b w(x)\, dx = \sum_{i=0}^{n} A_i$$

Gaussian quadrature error formula:

Consider a Gaussian quadrature formula:

$$\int_a^b f(x)\, dx = \sum_{i=0}^{n-1} A_i f(x_i) + E, \text{ then}$$

if $f \in C^{2n}[a,b]$ then error term is: