Ch. 3 ~~Rung~~ Runge-Kutta Methods

Key Points : Quadrature (Newton-Cotes, Gaussian, ...)

weights, nodes

orthogonal polynomials (Jacobi, Legendre, Chebyshev, ...)

Runge-Kutta schemes.

- RK matrix
- RK weights
- RK nodes
- stages

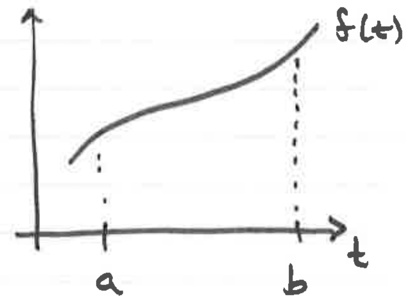
Can we tie this back to ideas used in multistep case even though these will be single-step methods

(i.e. interpolation used there for $\int p(t)dt$?

Numerical Quadrature (see also Heath, Ch. 8)

We've talked a little about ways to approximate an integral

$$I(f) \equiv \int_a^b f(t)\,dt$$



"Left endpoint"

$$\int_a^b f(t)\,dt \approx (b-a)\cdot f(a)$$

"right endpoint"

$$\int_a^b f(t)\,dt \approx (b-a)\cdot f(b)$$

midpoint rule

$$\int_a^b f(t)\,dt \approx (b-a)\, f\left(\frac{a+b}{2}\right)$$

These are exact for the case where $f(t) =$ polynomial of degree 0 (i.e. a constant function)

...

[redacted]

but midpoint is exact also for a polynomial of degree 1.

trapezoid rule

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

This is exact if the function is linear. (polynomial of degree one).

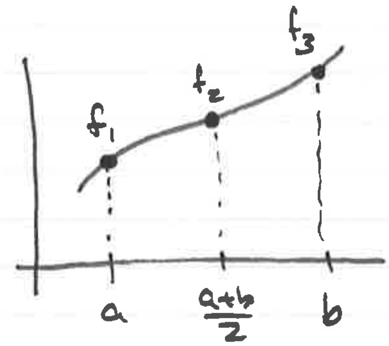
[redacted]

What about more general methods?

Here is an example — <u>Simpson's Method</u>

Approximate the integral

$$I(f) \equiv \int_a^b f(t)\,dt$$



using three equally-spaced points (3-pt. quadrature rule)

$f_1 = f(a)$

$f_2 = f\left(\frac{a+b}{2}\right)$

$f_3 = f(b)$

so

$$\int_a^b f(t)\,dt \approx w_1 f_1 + w_2 f_2 + w_3 f_3$$

where the <u>weights</u> w_1, w_2 and w_3 are chosen so that the quadrature rule integrates the first 3 polynomial basis functions exactly. We'll use monomial basis functions $(1, t, t^2)$ in this example.

$f(t) = 1$:

$$\int_a^b 1\,dt = (b-a) = w_1 \cdot 1 + w_2 \cdot 1 + w_3 \cdot 1$$

$f(t) = t$:

$$\int_a^b t\,dt = \frac{1}{2}t^2\Big|_a^b = \frac{1}{2}(b^2 - a^2) = w_1 a + w_2\left(\frac{a+b}{2}\right) + w_3 \cdot b$$

$f(t) = t^2$:

$$\int_a^b t^2\,dt = \frac{1}{3}t^3\Big|_a^b = \frac{1}{3}(b^3 - a^3) = w_1 a^2 + w_2\left(\frac{a+b}{2}\right)^2 + w_3 \cdot b^2$$

This leads to the linear system

$$\boxed{\begin{bmatrix} 1 & 1 & 1 \\ a & \frac{a+b}{2} & b \\ a^2 & \left(\frac{a+b}{2}\right)^2 & b^2 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ w_3 \end{bmatrix} = \begin{bmatrix} b-a \\ \frac{1}{2}(b^2-a^2) \\ \frac{1}{3}(b^3-a^3) \end{bmatrix}}$$

Solving for the weights gives

$$w_1 = \frac{1}{6}(b-a) \qquad w_2 = \frac{2}{3}(b-a) \qquad w_3 = \frac{1}{6}(b-a)$$

So

$$\boxed{\int_a^b f(t)\,dt = (b-a)\left[\frac{1}{6}f(a) + \frac{2}{3}f\left(\frac{a+b}{2}\right) + \frac{1}{6}f(b)\right]}$$

This is Simpsons Quadrature Rule.

~~(order 3)~~ For discussion of degree/order see

p. 49.2 in notes.

Consider the numerical quadrature case where we approximate the integral

$$I(f) \equiv \int_a^b f(t)\,dt$$

by the n-point quadrature rule

$$I(f) \approx Q_n(f) = \sum_{i=1}^{n} w_i f(t_i)$$

where $a \le t_1 < t_2 < \dots < t_n \le b$. The points t_i are called the nodes and the coefficients w_i are called the weights.

Plan: choose the nodes + weights for optimal performance (accuracy, computational cost, stability, ...)

Consider first the case where the nodes are specified (possibly equally-spaced but not necessarily).

Given $t_1, t_2, \dots, t_n$ find $w_1, w_2, \dots, w_n$ so that the quadrature rule integrates the first n basis functions exactly. Again, we'll use the monomial basis functions here

$$1, t, t^2, \dots, t^{n-1}$$

(As we shall note below, this gives a quadrature rule of order n.

$$\int_a^b 1\,dt = b-a = w_1 + w_2 + \dots + w_n$$

$$\int_a^b t\,dt = \frac{\cancel{(b-a)^2}\ b^2-a^2}{2} = w_1 t_1 + w_2 t_2 + \dots + w_n t_n$$

$$\vdots$$

$$\int_a^b t^{n-1}\,dt = \frac{\cancel{(b-a)^n}\ b^n-a^n}{n} = w_1 t_1^{n-1} + \dots + w_n t_n^{n-1}$$

This leads to the linear system

$$\underbrace{\begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ t_1 & t_2 & t_3 & \cdots & t_n \\ \vdots & \vdots & \vdots & \ddots & \\ t_1^{n-1} & t_2^{n-1} & t_3^{n-1} & \cdots & t_n^{n-1} \end{bmatrix}}_{\text{Vandermonde Matrix}} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix} = \begin{bmatrix} b-a \\ \cancel{\frac{1}{2}(b-a)^2}\ \frac{1}{2}(b^2-a^2) \\ \vdots \\ \frac{1}{n}\cancel{(b-a)^n}\,(b^n-a^n) \end{bmatrix}$$

~~fix~~ fix in notes...

- this nonsingular (although possibly not well-conditioned if n is large) can be solved to uniquely determine the weights $w_1, w_2, \dots, w_n$.

An alternative way to view this same problem is in terms of the Lagrangian basis functions. Basically, what we just did was to fit the function at n points to a polynomial of degree $n-1$ and then integrated that polynomial.

So in terms of the Lagrangian basis functions

$$l_j(t) = \frac{\prod_{k=1, k\neq j}^{n} (t-t_k)}{\prod_{k=1, k\neq j}^{n} (t_j-t_k)} \qquad j=1,2,\ldots,n$$

So

$$f(t) \approx p(t) = f_1 l_1(t) + f_2 l_2(t) + \ldots + f_n l_n(t)$$

Note: $l_j(t_i) = \begin{cases} 1 & \text{if } i=j \\ 0 & \text{if } i\neq j \end{cases}$ $\qquad f_j = f(t_j)$

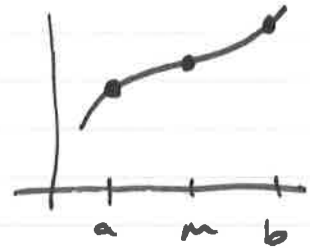
So

$$\int_a^b f(t)\,dt \approx \int_a^b p(t)\,dt = \sum_{j=1}^{n} f_j \underbrace{\int_a^b l_j(t)\,dt}_{w_j}$$

That is,

$$\boxed{w_j = \int_a^b l_j(t)\,dt} \qquad j=1,2,\ldots,n$$

EX (Simpson's Rule)



$m = \frac{a+b}{2}$

$$l_1(t) = \frac{(t-m)(t-b)}{(a-m)(a-b)}$$

$$l_2(t) = \frac{(t-a)(t-b)}{(m-a)(m-b)}$$

$$l_3(t) = \frac{(t-a)(t-m)}{(b-a)(b-m)}$$

... after some effort ...

$$w_1 = \int_a^b l_1(t)\,dt = \frac{1}{6}(b-a)$$

$$w_2 = \int_a^b l_2(t)\,dt = \frac{2}{3}(b-a)$$

$$w_3 = \int_a^b l_3(t)\,dt = \frac{1}{6}(b-a)$$

so

$$\int_a^b f(t)\,dt \approx w_1 f_1 + w_2 f_2 + w_3 f_3 .$$

Error in Quadrature Rules

(see also Heath, p. 344)

$$I(f) = \int_a^b f(t)\,dt$$

$$E(f) \equiv I(f) - Q_n(f)$$

$$Q_n(f) = \sum_{i=1}^{n} w_i f(t_i)$$

Suppose the quadrature rule is exact for a polynomial of degree $n-1$. That is,

$$Q_n(f) = I(p_{n-1})$$

Note: $Q_n(f) = Q_n(p_{n-1})$ since p_{n-1} interpolates f

Note that later we'll make more specific error estimates for midpoint, Simpson, trap. & in some cases get improved estimates

Then

$$
\begin{aligned}
|E(f)| &= |I(f) - Q_n(f)| \\
&= |I(f) - I(p_{n-1})| \\
&= |I(f - p_{n-1})| \\
&\le (b-a)\,\|f - p_{n-1}\|_{sup} \\
&\le \frac{(b-a)h^n}{4n}\,\|f^{(n)}\|_{sup} \\
&\le \frac{1}{4} h^{n+1}\,\|f^{(n)}\|_{sup}
\end{aligned}
$$

see notes p. 48.1

$f^{(n)}$ = nth deriv. of f.

$h = \frac{b-a}{n}$

$\begin{cases} h = \max h_i \\ h_i = t_{i+1} - t_i \end{cases}$

Def: A quadrature rule is order n if it is exact for every polynomial of degree $n-1$ but not exact for a polynomial of degree n

Iserles p. 33/34

Note: (p. 344)

Heath defines the <u>degree</u> of a quadrature rule..

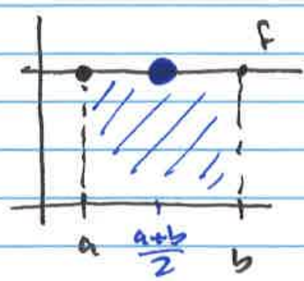
<u>Def:</u> A quadrature rule is said to be of <u>degree d</u> if it is exact for every polynomial of degree d but is not exact for some polynomial of degree d+1.

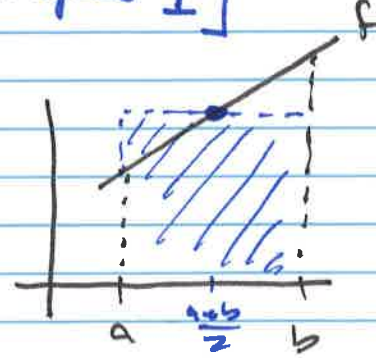
[i.e. the largest positive integer n such that the formula is exact for t^k, $k=0,1,\dots,n$

- An n-pt. interpolatory quadrature rule is of degree <u>at least</u> n−1.

<u>Observe:</u>

- <u>The Midpoint Rule</u> is a 1-pt. interpolatory quadrature rule. Note that it gets both constant functions (polynomial of degree 0) and linear functions (polynomial of degree 1) exact [Degree 1]





- <u>The Trapezoid Rule</u> is a 2-pt. interpolatory quadrature rule. It gets constant and linear functions exact. It does not get quadratic functions exact. [Degree 1]

Iserles refers to these as <u>Order 2</u>. ["Order" = "Degree" + 1]

(see Heath, p. 324)

Note: If a polynomial of degree $n-1$, $p_{n-1}(t)$, interpolates a sufficiently smooth function $f(t)$ at $t = t_1, t_2, \ldots, t_n$ distinct points, then

$$f(t) - p_{n-1}(t) = \frac{f^{(n)}(\theta)}{n!}(t-t_1)(t-t_2)\cdot\ldots\cdot(t-t_n)$$

where $\theta \in [t_1, t_n]$.

If $|f^{(n)}(t)| < M$ for $t \in [t_1, t_n]$

and $h = \max\{t_{i+1} - t_i \mid i = 1, 2, \ldots, n-1\}$ then

$$\| f(t) - p_{n-1}(t) \|_{sup} \leq \frac{Mh^n}{4n}$$

$$\| \cdot \|_{sup} = \sup\{ |\cdot| \mid t \in [t_1, t_n] \}$$ least upper bound

---

See also Iserles result p. 33 (written here for weighting function $w(t) = 1$.

$$\left| \int_a^b f(t)\,dt - \sum_{i=1}^{n} w_i f(t_i) \right| \leq c \max_{a \leq t \leq b} |f^{(p)}(t)|$$

(proved using Peano kernel theorem)

constant >0 indep. of f

order "p" quadrature rule.

Summarizing so far ... (Iserles Lemma 3.1)

Lemma 3.1

Given any distinct set of nodes $t_1, t_2, \dots, t_n$, it is possible to find a set of weights $w_1, w_2, \dots, w_n$ such that

$$\int_a^b f(t)\,dt \approx \sum_{i=1}^{n} w_i f(t_i)$$

is of order $p \geq n$. (so degree $\geq n-1$)

Proof: this uses the construction we've already examined using basis functions $(1, t, t^2, \dots, t^{n-1})$, Vandermonde matrix, etc.

Remark:

- Again recall the example of the midpoint rule that is an interpolatory quadrature rule (1-pt) (i.e. $n=1$) but has order 2 (degree 1) (i.e. $p=2$, $n=1$)

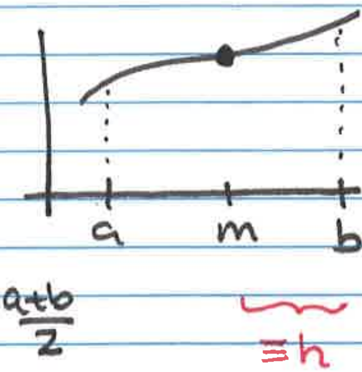
  $p \geq n$.

- Simpson's Rule, a 3-pt interpolatory quadrature rule, (i.e. $n=3$) has order 4 (degree 3) (i.e. $p=4$, $n=3$)
- Trapezoid Rule, a 2-pt interpolatory quadrature rule, (i.e. $n=2$) has order 2 (so here $p=2$, $n=2$)

Comment: In general, an n-pt N-C quadrature method with $\underline{\underline{n = \text{odd}}}$ has degree one higher than the interpolating polynomial.

Newton-Cotes (given equally spaced points)

Error in Midpoint Rule



$$I(f) = \int_a^b f(t)\,dt$$

$$Q_{MID}(f) = (b-a) f(m) \qquad m = \frac{a+b}{2}$$

$$E(f) = I(f) - Q_{MID}(f)$$

$$= \int_a^b f(t)\,dt - (b-a) f(m)$$

Let us expand $f(t)$ in a Taylor Series about $t = m$

$$f(t) = f(m) + f'(m)(t-m) + \frac{1}{2} f''(m)(t-m)^2 + \frac{1}{3!} f'''(m)(t-m)^3 + \frac{1}{4!} f^{(4)}(\theta)(t-m)^4$$

$$\int_a^b f(t)\,dt = f(m)(b-a) + f'(m) \cancelto{0}{\int_a^b (t-m)\,dt} + \frac{1}{2} f''(m) \int_a^b (t-m)^2\,dt$$

$$+ \frac{1}{3!} f'''(m) \cancelto{0}{\int_a^b (t-m)^3\,dt} + \frac{1}{4!} f^{(4)}(\theta) \int_a^b (t-m)^4\,dt$$

$$= f(m)(b-a) + \frac{1}{2} f''(m) \left[\frac{1}{3}(b-m)^3 - \frac{1}{3}(a-m)^3\right] + \frac{f^{(4)}(\theta)}{4!} \left[\frac{1}{5}(b-m)^5 - \frac{1}{5}(a-m)^5\right]$$

$$= f(m)(b-a) + \frac{1}{2} f''(m) \left[\frac{1}{3} h^3 - \frac{1}{3}(-h)^3\right] + O(h^5)$$

$$= f(m)(b-a) + \frac{1}{3} h^3 f''(m) + O(h^5)$$

So

$$E(f) = I(f) - Q_{MID}(f)$$

$$= \underbrace{\frac{1}{3} h^3 f''(m) + O(h^5)}$$

this formula suggests that $E = 0$ (method is exact)
for constant and linear functions (for which $f'' = 0$).

interpolating polynomial is degree 0

(ie. midpoint → degree [redacted], order [redacted])
1 2

• A similar calculation can be made (see Burden + Faires)
to show for Simpson's rule

$$E(f) = I(f) - Q_{SIMP}(f) \sim \underbrace{h^5 f^{(4)}(\theta)}$$

Simpson (3-pt quad.)
is exact for polynomials
of degree 0, 1, 2, 3.

interpolating polynomial is degree 2

(ie. Simpson's Rule → degree , order)
3 4

• Similarly, Trapezoid Rule has (Burden + Faires)

$$E(f) = I(f) - Q_{TRAP}(f) \sim h^3 f''(\theta)$$

interpolating polynomial is degree 1

(degree [redacted] , order)
1 2

(compare conditioning?) $\overset{\circ}{\times}$ ✓

Stability in Quadrature Rules

let $$Q_n(f) = \sum_{i=1}^{n} w_i f(t_i)$$

be some quadrature rule (n-pt.)

If there is a perturbation in the function — call it $\hat{f}$

$$\left| Q_n(\hat{f}) - Q_n(f) \right| = \left| \sum_{i=1}^{n} w_i \hat{f}(t_i) - \sum_{i=1}^{n} w_i f(t_i) \right|$$

$$= \left| \sum_{i=1}^{n} w_i \left(\hat{f}(t_i) - f(t_i) \right) \right|$$

triangle inequality

$$\leq \sum_{i=1}^{n} |w_i| \left| \hat{f}(t_i) - f(t_i) \right|$$

$$\leq \left(\sum_{i=1}^{n} |w_i| \right) \| \hat{f} - f \|_{sup}$$

For stability (i.e. output relatively insensitive to input)

we hope for $\left(\sum_{i=1}^{n} |w_i| \right)$ to not be large.

Note: if w_i's are all positive then $\sum_{i=1}^{n} |w_i| = \sum_{i=1}^{n} w_i$

and we know from the Vandermond matrix (row 1 eg.)

that $\sum_{i=1}^{n} w_i = (b-a)$

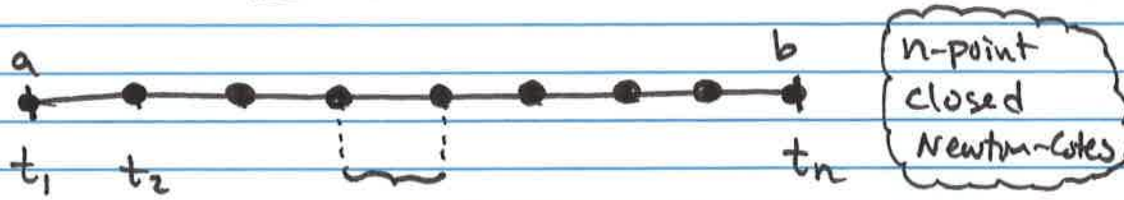
this is as good as you can expect as this is the condition # for integration (see Heath, p. 341)

If the w_i's have different signs then the quantity $\sum_{i=1}^{n} |w_i|$ could be considerably larger than $b-a$.

Types of Quadrature

- Newton-Cotes Quadrature:

  - here the nodes are equally-spaced on the interval $[a,b]$. These can be "closed"

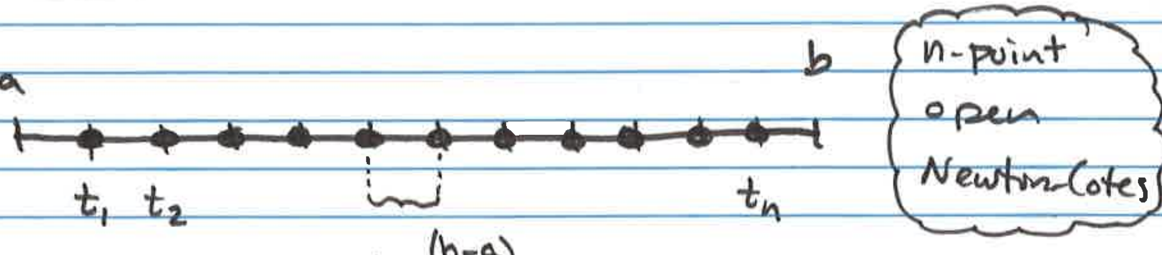


$$h = \frac{b-a}{n-1}$$

e.g. Trapezoid — 2pt. closed N-C.

Simpson — 3pt. closed N-C

or "open"



$$h = \frac{(b-a)}{(n+1)}$$

e.g. Midpoint Rule — 1 pt. open N-C

Further comments on Newton - Cotes

- polynomial "wiggle" becomes a problem as n increases
- infact, according to Heath (p. 350)

$$\sum_{i=1}^{n} |w_i| \to \infty \quad \text{as} \quad n \to \infty$$

indicating loss of stability.

- from an error point of view odd # of points (n) seems better than even.

↳ clue: maybe a careful choice of nodes can make things better!

Some of these issues can be addressed using quadrature rules involving

- orthogonal polynomials
- Gaussian quadrature

Orthogonal Polynomials

Suppose p and g are polynomial functions. Define the inner product of p and g with respect to a weight function $w(t)$ (nonnegative)

$$\langle p, g \rangle = \int_a^b w(t)p(t)g(t)\,dt$$

with $\left| \int_a^b t^j w(t)\,dt \right| < \infty$ for $j = 0, 1, 2, \ldots$ and $\int_a^b w(t)\,dt > 0.$

p and g are orthogonal with respect to the weighting function $w(t)$ if $\langle p, g \rangle = 0$

A set of polynomials $\{p_j\}$ is orthonormal if

$$\langle p_i, p_j \rangle = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

EX

Legendre Polynomials $\boxed{w(t) = 1}$ on $[-1, 1]$.

$P_0(t) = 1$

$P_1(t) = t$

$P_2(t) = \frac{1}{2}(3t^2 - 1)$

$P_3(t) = \frac{1}{2}(5t^3 - 3t)$

$\vdots$

Recurrence

$$(k+1)P_{k+1}(t) = (2k+1)tP_k(t) - kP_{k-1}(t)$$

inner product $\langle p, g\rangle = \int_a^b p(t)g(t)w(t)\,dt$

55.1

OP, 1

Orthogonal Polynomials $(P_0(t), P_1(t), P_2(t), P_3(t), \ldots)$

EX Legendre ... $[a, b]$ $[-1,1]$ $w(t) = 1$, $P_k(1) = 1$

normalization (note: not orthonormal by previous def.)

$P_0 = A$

$$\boxed{P_0(t) = A = 1}$$

$P_1 = At+B$ 1: $0 = \int_{-1}^{1} (At+B)\,1\cdot 1\,dt = \frac{1}{2}At^2+Bt\Big|_{-1}^{1} = (\frac{1}{2}A+B)-(\frac{1}{2}A-B) = 2B$ $\boxed{B=0}$

$P_1(t) = At$ $P_1(1)=1 \Rightarrow A=1$ $\boxed{P_1(t) = t}$

$P_2 = At^2+Bt+C$ 1: $0 = \int_{-1}^{1}(At^2+Bt+C)\cdot 1\,dt = \frac{1}{3}At^3+\frac{1}{2}Bt^2+Ct\Big|_{-1}^{1}$

$(\frac{1}{3}A+\frac{1}{2}B+C)-(-\frac{1}{3}A+\frac{1}{2}B-C)$

$$\boxed{0 = \frac{2}{3}A+2C}$$

t: $0 = \int_{-1}^{1}(At^2+Bt+C)\cdot t\,dt = \frac{1}{4}At^4+\frac{1}{3}Bt^3+\frac{1}{2}Ct^2\Big|_{-1}^{1} = \frac{2}{3}B$

$\boxed{B=0}$

$P_2(1) = 1 = A+C =$ $A = -3C$

$1 = -2C$

$C = -\frac{1}{2}$ $A = 3/2$

$P_2(t) = \frac{3}{2}t^2 - \frac{1}{2} = \boxed{\frac{1}{2}(3t^2-1) = P_2(t)}$

So in general, we can generate ~~these~~ $P_K(t)$

by requiring

$$\boxed{\begin{array}{ll} 0 = \int_{-1}^{1} t^j P_K(t)\,dt & \text{for } j=0,1,2,3,\dots,k-1 \\ & k = \text{degree } k \text{ polynomial.} \\ \text{and } P_K(1) = 1 & \end{array}}$$

(i.e. P_k is orthogonal wrt weight function $w(t)=1$ to all lower degree polynomials)

... but there is also a recurrence relation

$$\boxed{(k+1)P_{k+1}(t) = (2k+1)\,t\,P_k(t) - k\,P_{k-1}(t)}$$

so for example since we already have

$$P_0(t) = 1$$

$$P_1(t) = t$$

$$P_2(t) = \tfrac{1}{2}(3t^2-1)$$

[note: $2P_2(t) = 3tP_1(1) - P_0(t)$
$= 3t^2 - 1$]

$$3 \cdot P_3(t) = 5\,t\,P_2(t) - 2P_1(t)$$

$$= 5t\left(\tfrac{1}{2}(3t^2-1)\right) - 2t$$

$$= \tfrac{5}{2}\cdot(3t^3 - t) - 2t$$

$$\boxed{P_3(t) = \tfrac{5}{2}t^3 - \tfrac{3}{2}t}$$

more generally... (with $p_m \neq 0$) Def: of $\mathbb{P}_m$

really this should be interpreted as polynomials of degree less than or equal to m.

$\S 3.2$

We say $p_m \in \mathbb{P}_m$ ($\mathbb{P}_m$ = set of all real polynomials of degree m)

is an m^{th} orthogonal polynomial

see Iserles p.34/35

with respect to the weight function $w(t)$ if

"monic" means leading coefficient = 1.

$$\langle p_m, \hat{p} \rangle = 0$$

for every $\hat{p} \in \mathbb{P}_{m-1}$

That is, p_m is orthogonal to all lower degree polynomials.

(it follows easily...

$a t^{n-1}$

$a t^{n-1} + b t^{n-2}$

$a t^{n-1} + b t^{n-2} + c t^{n-3}$ ...

EX

Note: $\langle P_2, P_j \rangle = 0$ on $[-1,1]$ w.r.t. $w(t)=1$
$j=0,1.$

$$\int_{-1}^{1} \tfrac{1}{2}(3t^2-1)\cdot t \, dt = \int_{-1}^{1} \underbrace{\left(\tfrac{3}{2}t^3 - \tfrac{1}{2}t\right)}_{\text{odd function}} dt = 0 \checkmark$$

as noted on previous pages

and

$$\int_{-1}^{1} \tfrac{1}{2}(3t^2-1)\cdot 1 \, dt = \tfrac{1}{2}\left(t^3 - t\right)\Big|_{-1}^{1} = \tfrac{1}{2}(0-0) = 0 \checkmark$$

$\boxed{\text{See comment on uniqueness of monic orthogonal polynomials}}$

(Iserles, p. 35

EX Chebyshev $\boxed{w(t) = \frac{1}{(1-t^2)^{1/2}}}$ on $[-1,1]$

$T_0(t) = 1$

$T_1(t) = t$

$T_2(t) = 2t^2 - 1$

$T_3(t) = 4t^3 - 3t$

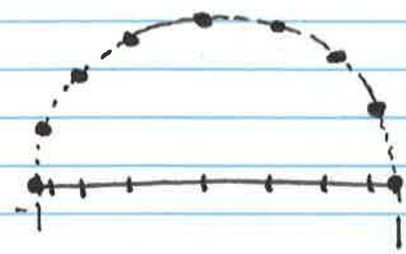
$\vdots$

Recurrence

$$T_{k+1}(t) = 2t\,T_k(t) - T_{k-1}(t)$$

also... $T_k(t) = \cos(k \arccos(t))$

zeros at... $t_i = \cos\left(\frac{(2i-1)\pi}{2k}\right) \quad i = 1, 2, \ldots, k$



— the zeros tend to bunch up near the ends -1 and 1.

How are these related to Gaussian Quadrature?

Gaussian Quadrature

Basic idea: Previously, we started with a given set of nodes t_j and then selected the weights w_j in order to maximize the number of polynomials (maximize the degree) that we could represent exactly. If we used an n-pt quadrature rule we were, in general, able to get a quadrature method of degree $n-1$ (maybe n in certain cases).

Here, for Gaussian Quadrature, we shall use the nodes as unknowns as well and ~~require that~~ use the requirements that additional polynomial degrees be exactly represented to determine the weights + nodes.

<u>EX</u> (Heath, p.351)

$$I(f) = \int_{-1}^{1} f(t)\,dt \approx \underbrace{w_1 f(t_1) + w_2 f(t_2)}_{\text{2-pt quadrature rule.}}$$

treat w_1, w_2 <u>AND</u> t_1, t_2 as "to be determined"

(using $w(t)=1$)

Require

$p(t) = 1$ $\qquad \int_{-1}^{1} 1\,dt = w_1 f(t_1) + w_2 f(t_2)$

$$\boxed{2 = w_1 \cdot 1 + w_2 \cdot 1}$$

$p(t) = t$ $\qquad \int_{-1}^{1} t\,dt = w_1 f(t_1) + w_2 f(t_2)$

$$\boxed{0 = w_1 t_1 + w_2 t_2}$$

$p(t) = t^2$ $\qquad \int_{-1}^{1} t^2\,dt = w_1 f(t_1) + w_2 f(t_2)$

$$\boxed{\frac{2}{3} = w_1 t_1^2 + w_2 t_2^2}$$

$p(t) = t^3$ $\qquad \int_{-1}^{1} t^3\,dt = w_1 f(t_1) + w_2 f(t_2)$

$$\boxed{0 = w_1 t_1^3 + w_2 t_2^3}$$

Solve these nonlinear equations for w_1, w_2, t_1, t_2

$$\Rightarrow \quad t_1 = -\frac{1}{\sqrt{3}} \qquad w_1 = 1$$
$$t_2 = \frac{1}{\sqrt{3}} \qquad w_2 = 1$$

$n = 2$ pts.

i.e. $2 \cdot n - 1$

In general, this method is degree 3 (order 4)

since $1, t, t^2, t^3$ are [redacted] integrated exactly.

Before connecting orthogonal polynomials to Gaussian Quadrature, let's go back and generalize slightly our definition of quadrature ... introducing a weight function $\omega(t)$

$$(*) \qquad \int_a^b \omega(t) f(t)\,dt \approx \sum_{i=1}^{n} w_i f(t_i)$$

where

$$0 < \int_a^b \omega(t)\,dt < \infty \quad , \quad \left| \int_a^b t^j w(t)\,dt \right| < \infty \quad j=1,2,\ldots$$

Here's the main Gaussian Quadrature Theorem [but see also Lemma 3.2 (p.36) for background]

Thm 3.3

Let $t_1, t_2, \ldots, t_n$ be the zeros of (orthogonal polynomial) $p_n \in \mathbb{P}_n$ (n^{th})

(set of all polynomials of degree n) "or less", and let $w_1, w_2, \ldots, w_n$ be the solution to the Vandermonde system

$$\sum_{j=1}^{n} w_j t_j^m = \int_a^b t^m \omega(t)\,dt \qquad m = 0,1,2,\ldots,n-1$$

$\omega(t)$ = given

(requiring the quadrature rule be exact for polynomials $1, t, t^2, \ldots, t^{n-1}$).

Then

(i) The quadrature method $(*)$ is of order $2n$ ("degree" $2n-1$)

(ii) No other quadrature (n-pt.) can exceed this order.

Proof: of (i)

Idea: Show that the coefficients (weights) w_j and the nodes t_j are such that the quadrature rule

$$Q_n(f) = \sum_{j=1}^{n} w_j f(t_j)$$

is exact for polynomials $\hat{p} \in \mathbb{P}_{2n-1}$ (all polynomials of degree $2n-1$ or less)

$$\left(\text{i.e.} \quad \int_a^b \hat{p}\, w(t)\, dt = \sum_{j=1}^{n} w_j \hat{p}(t_j)\right)$$

(not just $\mathbb{P}_{n-1}$)

Let $\hat{p} \in \mathbb{P}_{2n-1}$. Note that $\hat{p}$ can be expressed in terms of "quotient" "remainder" $\left[\dfrac{\hat{p}}{p_n} = g + \dfrac{r}{p_n}\right]$

$$\hat{p} = p_n g + r$$

where p_n is an n^{th} orthogonal polynomial of degree n and g, r are polynomials of degree $n-1$ or less. Consider

$\deg(g) \le n-1$
$\deg(r) \le n-1$

$$\int_a^b \hat{p}(t) w(t)\, dt = \int_a^b p_n(t) g(t) w(t)\, dt + \int_a^b r(t) w(t)\, dt$$

$$= \underbrace{\cancel{\langle p_n, g \rangle}}_{0} + \int_a^b r(t) w(t)\, dt$$

since p_n is an n^{th} orthogonal polynomial and $g \in \mathbb{P}_{n-1}$

Also

$$\sum_{j=1}^{n} w_j \hat{p}(t_j) = \sum_{j=1}^{n} w_j \underbrace{\cancel{p_n(t_j)}}_{0} g(t_j) + \sum_{j=1}^{n} w_j r(t_j) = \sum_{j=1}^{n} w_j r(t_j)$$

$p_n(t_j) = 0$ by definition of t_j.

We have already seen (Lemma 3.1), given nodes $t_1, t_2, \ldots, t_n$ it is possible to choose weights w_j $(j=1,\ldots,n)$ such that if $r \in \mathbb{P}_{n-1}$

$$\int_a^b w(t) r(t)\,dt = \sum_{j=1}^{n} w_j r(t_j)$$

So, choose the weights w_j based on these conditions.

Then

$$\int_a^b w(t)\hat{p}(t)\,dt = \int_a^b w(t) r(t)\,dt = \sum_{j=1}^{n} w_j r(t_j) = \sum_{j=1}^{n} w_j \hat{p}(t_j)$$

That is, our choice of t_j and w_j allow our quadrature scheme to integrate exactly any polynomial of degree $2n-1$. (i.e. it works for $\hat{p} \in \mathbb{P}_{2n-1}$). Therefore, the order of quadrature method (*) is $2n$ (degree $2n-1$).

$\Rightarrow$ So with a carefully selected set of nodes we basically double degree of the quadrature rule.

How does this not apply if $\hat{p} \in \mathbb{P}_{2n-1}$?

Proof of (ii)

Suppose the method integrates $\hat{p} \in \mathbb{P}_{2n}$ exactly.

In particular, consider the polynomial

$$\hat{p}(t) = \prod_{i=1}^{n} (t-t_i)^2 \geq 0.$$

(so $\hat{p}(t_i) = 0$ and $\hat{p}(t) \geq 0$). Note

$$\sum_{j=1}^{n} w_j \hat{p}(t_j) = 0$$

answer

if $\hat{p} = \prod_{i=1}^{n-1} (t-t_i)^2 \geq 0$ for example $\sum_{j=1}^{n} w_j \hat{p}(t_j) \neq 0$ since $\hat{p}(t_n) \neq 0$. so the argument does not apply

but, recalling that $w(t)$ is non-negative

$$\int_a^b w(t)\,\hat{p}(t)\,dt > 0$$

(note, this integral could be zero only if $w(t) = \begin{cases} 0 & t \neq t_i \\ \neq 0 & \text{elsewhere} \end{cases}$

but this function — indicator function — would have $\int_a^b w(t)\,dt = 0$.

Therefore, it is not possible that

$$\int_a^b w(t)\,\hat{p}(t)\,dt = \sum_{j=1}^{n} w_j \hat{p}(t_j)$$

So the method does not integrate $\hat{p} \in \mathbb{P}_{2n}$ exactly.

Therefore, the quadrature rule is order $2n$ (degree $2n-1$).

A generalization of this Thm is...

Thm 3.4 (Iserles, p. 37)

Let $r \in \mathbb{P}_n$ obey the orthogonality conditions

$$\langle r, \hat{p} \rangle = 0 \quad \text{for every } \hat{p} \in \mathbb{P}_{m-1}$$

and

$$\langle r, t^m \rangle \neq 0 \quad \text{for some } m \in \{0,1,2,\dots,n\}$$

Let $t_1, t_2, \dots, t_n$ be the zeros of the polynomial r.

Choose $w_1, w_2, \dots, w_n$ as in

$$\sum_{j=1}^{n} w_j t_j^m = \int_a^b t^m w(t)\,dt \qquad m = 0,1,2,\dots,n-1$$

Then the quadrature formula

$$\int_a^b w(t) f(t) \approx \sum_{j=1}^{n} w_j f(t_j)$$

has order $p = n+m$ (degree $n+m-1$).

Comments:
- $m \in \{0,1,2,\dots,n\}$ so $m \leq n$.

  and the order $p = n+m \leq 2n$
- r does not satisfy "full" orthogonality conditions ... only a partial set of conditions
- this gives a quadrature scheme with an order reduced from the original Gaussian quad. rule.