Higher order quadratures and Gaussian Quadrature

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Recall: Last time, we came up with one way to create quadratures with a higher power of h (a higher order of accuracy) from a standard Newton-Cotes composite quadrature like Trapezoidal. We went through the general method (Richardson Extrapolation), which uses the fact that we have an asymptotic expansion of the error in powers of h. We then applied (and slightly modified) this procedure to the Trapezoidal rule, to find the set of Romberg quadratures; each application of Romberg gains 2 powers of h, so:

- Romberg 1, or R1(h), is Composite Trapezoidal and has an O(h^2) error.
- Romberg 2, or R2(h), was later revealed to be Simpsons rule (for h/2), and has an O(h^4) error.
- Romberg 3, or R3(h), was later revealed to be Boole (NC p=4), and has an O(h^6) error.
- Romberg k for k>3 onwards gives us non interpolation-based rules with O(h^{2k}) error.

We discussed two implementations of Romberg: one where we compute nodes and weights based on the rule, and one where we use a "Newton tableau" approach to compute R1(h) for h=h0, h0/2, … , h0/2^L, and then use the formulas to compute R2, R3, …, RL.

Today, we will discuss a more general approach to produce rules of higher order, given n+1 quadrature nodes. This will eventually take us to ask: what is the best set of n+1 points and nodes one can pick, and what is the best error we can get out of that? The answer is Gaussian quadrature, and it turns out the best way to compute its nodes and weights involves orthogonal polynomials.

NC → n+1 quad nodes (interpolation)

→ n+1 EVEN (Trapz) → exact for $p \in \mathcal{P}_n$
- $f^{(n+1)}(\eta)$
- $O(h^{n+2})$ error (one int)
- $O(h^{n+1})$ error (composite)

→ n+1 ODD (Simpson) → exact $p \in \mathcal{P}_{n+1}$
- $f^{(n+2)}(\eta)$
- $O(h^{n+3})$ one int
- $O(h^{n+2})$ composite.

In general, a quad rule w/ n+1 nodes

$$Q[f] = \sum_{j=0}^{n} \underbrace{\omega_j}_{\substack{n+1\\ \text{weights}}} f(\underbrace{x_j}_{\substack{n+1\\ \text{nodes}}}) \quad = \underline{2n+2 \text{ DOFs}}$$

What if I do not constrain x_j's?

→ Try make exact for $p \in \mathcal{P}_{2n+1}$

These are Gaussian Quadrature rules

These are Gaussian Quadrature rules

Interval: $[-1,1]$

$n=1$ (2 pts) $\to x_0, x_1, \omega_0, \omega_1$

$$\left\{\begin{aligned} 2 &= \int_{-1}^{1} 1\,dx = \omega_0 + \omega_1 \\ 0 &= \int_{-1}^{1} x\,dx = \omega_0 x_0 + \omega_1 x_1 \\ \frac{2}{3} &= \int_{-1}^{1} x^2\,dx = \omega_0 x_0^2 + \omega_1 x_1^2 \\ 0 &= \int_{-1}^{1} x^3\,dx = \omega_0 x_0^3 + \omega_1 x_1^3 \end{aligned}\right\}$$

$$\left\{ \omega_0 = \omega_1 = 1,\ x_0 = -1/\sqrt{3},\ x_1 = 1/\sqrt{3} \right\}$$

2 pts, error one int $\sim h^5$

comp $\sim h^4$

NOTE: $n=0$ 1pt $\to x_0, \omega_0$

$[-1,1]$ $\quad 2 = \omega_0$

$0 = 2x_0 \to x_0 = 0$

Error $\sim h^3$, Comp $\sim h^2$.

- If you set nodes $\{x_j\}_{j=0}^n$, first $n+1$ eqs $\rightarrow$ linear system of eqs.
- Gen. of quad rules

$$Q[f] = \sum_{j=0}^{n} \omega_j f(x_j) + \sum_{k=0}^{m} \mu_k f'(x_k)$$

$[-1,1]$,

$$Q[f] = \omega_0 f(x_0) + \omega_1 f'(x_1)$$

$$\left\{ \begin{aligned} 2 &= \int_{-1}^{1} 1\,dx = \omega_0 \\ 0 &= \int_{-1}^{1} x\,dx = \omega_0 x_0 + \omega_1 \\ 2/3 &= \omega_0 x_0^2 + 2\omega_1 x_1 \\ 0 &= \omega_0 x_0^3 + 3\omega_1 x_1^2 \end{aligned} \right\}$$

GAUSS-LEGENDRE (n+1 pt)

$\rightarrow [-1,1]$, $\int_{-1}^{1} f(x)\,dx$

$n=0 \rightarrow x_0 = 0$

$n=1 \rightarrow x_0 = -1/\sqrt{3}$, $x_1 = 1/\sqrt{3}$

$n=1 \longrightarrow x_0 = -1/\sqrt{3}, \; x_1 = 1/\sqrt{3}$

$P_0(x) = 1, \; P_1(x) = x, \; P_2(x) = x^2 - 1/3, \ldots$

Claim: Gauss-Legendre nodes $\{x_j\}_{j=0}^{n}$ are the zeroes of $P_{n+1}(x)$.

Let $p \in \mathcal{P}_{2n+1}$.

Divide p by P_{n+1}:

$$\begin{array}{r} q(x) \\ P_{n+1} \overline{\big) \, p(x)} \\ \vdots \\ \hline r(x) \end{array}$$

$$p(x) = \underbrace{q(x)}_{\in \mathcal{P}_n} \, \underline{P_{n+1}(x)} + \underbrace{r(x)}_{\in \mathcal{P}_n}$$

$$\int_{-1}^{1} p(x)\,dx = \underbrace{\cancel{\int_{-1}^{1} q(x) P_{n+1}(x)\,dx}}_{\langle q, P_{n+1}\rangle = 0} + \int_{-1}^{1} r(x)\,dx$$

- Given $\{x_j\}_{j=0}^{n} \longrightarrow \omega_j$ s.t. they integrate poly up to degree n.

Apply quad rule to p:

$$\underbrace{\sum_{j=0}^{n} \omega_j \, p(x_j)}_{} = \underbrace{\sum_{j=0}^{n} \omega_j \, q(x_j) \boxed{P_{n+1}(x_j)}}_{} + \underbrace{\sum_{j=0}^{n} \omega_j \, r(x_j)}_{}$$

$= 0$ for all $q \in \mathcal{P}_n$.

$\int_{-1}^{1} r(x)\,dx$

$$\boxed{P_{n+1}(x_j) = 0}$$

Formula for w_j:

$$w_j = \frac{2}{(1-x_j^2)\left[P_{n+1}'(x_j)\right]^2}$$

Gaussian Quadratures $(w(x) \geq 0)$

$$\int_a^b f(x)\, w(x)\,dx = \sum_{j=0}^{n} w_j f(x_j)$$

- $w(x)$ is the density function for a prob. dist. $\longrightarrow E[f(x)]$
- $w(x)$ is singular but integrable (e.g. $1/\sqrt{x}$)