Proof (last property)

For $r_k(x)$, let $\{\mu_1, \mu_2, \cdots \mu_m\}$ be the set of points in $[-1, 1]$ where $r_k(x)$ changes sign. It is clear that each μ_j is a zero of $r_k(x)$ and all simple zeros of $r_k(x)$ in $[-1, 1]$ must be in this set. We then have $m \leq k$ as the maximum number of zeros of a polynomial of degree k is k. Assume $m < k$. We then have,

$$\hat{q}_m(x) \equiv \prod_{i=1}^{m}(x - \mu_i),$$

is a polynomial of degree $m < k$ that changes sign at each μ_i and,

$$\int_{-1}^{1} \hat{q}_m(x) r_k(x) dx = 0.$$

But $\hat{q}_m(x)$ and $r_k(x)$ have the same sign for all x in $[-1, 1]$ (they change sign at the same locations). This implies a contradiction (the integrand is of one sign but the integral is zero)– our assumption must be false. We must therefore have $m = k$.

3-Term Recurrence

The $r_k(x)$ also satisfy,

$$r_{s+1}(x) = a_s(x - b_s)r_s(x) - c_s r_{s-1}(x),$$

for $s = 1, 2, \cdots k$, where the a_s are normalization constants, $r_{-1}(x) = 0$, and if $t_s = \int_{-1}^{1} r_s^2(x)dx$ then,

$$b_s = \frac{1}{t_s}\int_{-1}^{1} x r_s^2(x)dx, \quad c_s = \frac{a_s t_s}{a_{s-1}t_{s-1}}.$$

For example, we obtain the classical Legendre polynomials if we normalise so $r_s(-1) = 1$. This leads to,

$$a_s = \frac{2s+1}{s+1}, \quad b_s = 0, \quad c_s = \frac{s}{s+1}.$$

Orthogonal Polys on $[a, b]$

- To transform orthogonal polynomials defined on $[-1, 1]$ to $[a, b]$ consider the linear mapping from $[-1, 1] \rightarrow [a, b]$ defined by $x = \frac{b-a}{2}y + \frac{a+b}{2}$. The inverse mapping is $y = \frac{1}{b-a}[2x - b - a]$ and from calculus we know,

$$\int_a^b g(x)dx = (\frac{b-a}{2}) \int_{-1}^1 g(\frac{b-a}{2}y + \frac{a+b}{2})dy.$$

This relationship, combined with the properties of Legendre polynomials give a prescription for the choice of the x_i's for GQ:
For $i = 0, 1, \cdots n$, set y_i to the i^{th} zero of the Legendre Polynomial, $r_{n+1}(y)$. With this choice we note that $\prod_{j=0}^n (y - y_j) = K \ r_{n+1}(y)$ for some $K \neq 0$.

Choice of the x_i's for GQ

Then with the choice $x_i = \frac{b-a}{2} y_i + \frac{b+a}{2}$ we have,

$$
\begin{aligned}
\Pi_n(x) &= \Pi_n\left(\frac{b-a}{2} y + \frac{a+b}{2}\right) = \prod_{j=0}^{n} \left(\frac{b-a}{2} y + \frac{a+b}{2} - x_j\right) \\
&= \prod_{j=0}^{n} \left(\frac{b-a}{2} y + \frac{a+b}{2} - \left(\frac{b-a}{2} y_j + \frac{a+b}{2}\right)\right) \\
&= \prod_{j=0}^{n} \left[\frac{b-a}{2}(y - y_j)\right] = \left(\frac{b-a}{2}\right)^{n+1} \prod_{j=0}^{n} (y - y_j) \\
&= \left(\frac{b-a}{2}\right)^{n+1} K \; r_{n+1}(y).
\end{aligned}
$$

Choice of the x_i's (cont)

Therefore for any polynomial, $q(x)$ of degree at most n,

$$
\begin{aligned}
&\int_a^b \Pi_n(x) q(x) dx \\
= \quad & (\frac{b-a}{2}) \int_{-1}^{1} \Pi_n(x) q(\frac{b-a}{2} y + \frac{b+a}{2}) dy, \\
= \quad & (\frac{b-a}{2}) \int_{-1}^{1} \Pi_n(x) \hat{q}(y) dy, \\
= \quad & (\frac{b-a}{2})^{n+2} K \int_{-1}^{1} r_{n+1}(y) \hat{q}(y) dy \quad = \quad 0.
\end{aligned}
$$

since $\hat{q}(y)$ is a polynomial of degree at most n.

That is with the x_i's chosen as the 'transformed zeros' of the Legendre polynomial, $r_{n+1}(y)$, we have the property we need.

Composite Quadrature Rules

Approximating the integrand with a PP leads to the class of Composite Rules. Let $a = x_0 < \cdots x_M = b$ and $S(x)$ be a PP approximation to $f(x)$ (defined on this mesh). We can then use $\int_a^b S(x)dx$ as the approximation to $I(f) = \int_a^b f(x)dx$. Recall that $S(x) \equiv p_{i,n}(x)$ for $x \in [x_{i-1}, x_i] \;\; i = 1, \cdots M$. From calculus we have,

$$\int_a^b S(x)dx = \sum_{i=1}^{M} \int_{x_{i-1}}^{x_i} S(x)dx \quad = \sum_{i=1}^{M} \int_{x_{i-1}}^{x_i} p_{i,n}(x)dx,$$

–A sum of basic interpolatory rules.

If we use equally spaced x_i's and low degree interpolation we obtain familiar rules.

Composite Trapezoidal Rule

- The composite trapezoidal rule, $T_M(f)$:

$$\begin{aligned}\int_{x_{i-1}}^{x_i} f(x)dx &= \frac{x_i - x_{i-1}}{2}\left[f(x_{i-1}) + f(x_i)\right] - \frac{f''(\eta_i)(x_i - x_{i-1})^3}{12} \\ &= \frac{h}{2}\left[f_{i-1} + f_i\right] - \frac{f''(\eta_i)h^3}{12}.\end{aligned}$$

Summing over all sub-intervals we obtain,

$$T_M(f) \equiv h\sum_{i=1}^{M-1} f_i + \frac{h}{2}(f_0 + f_M),$$

with the corresponding error expression,

$$E_M^T(f) \equiv I(f) - T_M(f) = -\sum_{i=1}^{M} \frac{h^3}{12} f''(\eta_i).$$

Error term for CT Rule

If $f^{''}(x)$ is continuous we can apply the MVT for sums to obtain the expression,

$$\begin{aligned} E_M^T(f) &= -f^{''}(\eta) \sum_{i=1}^{M} \frac{h^3}{12} = -f^{''}(\eta)\ M \frac{h^3}{12} \text{ for some } \eta \in (a,b), \\ &= -f^{''}(\eta)(b-a)\frac{h^2}{12} \text{ since } h = (b-a)/M. \end{aligned}$$

We therefore have:

$$\boxed{T_M(f) = h \sum_{i=1}^{M-1} f_i + h/2(f_0 + f_M)}$$

with

$$\boxed{E_M^T = -f^{''}(\eta)(b-a)\tfrac{1}{3}(\tfrac{h}{2})^2}.$$

Composite Simpsons Rule

- Similarly we can derive the Composite Simpsons Rule

$$\boxed{S_M(f) = h/6\left[f_0 + f_M + 2\sum_{i=1}^{M-1} f_i + 4\sum_{i=1}^{M} f_{i-1/2}\right]}$$

with the corresponding error expression,

$$\boxed{E_M^S(f) = \frac{-f^{(4)}(\eta)}{180}(b-a)(\frac{h}{2})^4}$$

and $f_{i-1/2}$ defined to be f evaluated at $(x_{i-1} + x_i)/2$.

Error Estimates

- Composite Trapezoidal rule: The contribution to the error from the i^{th} sub-interval is,

$$\begin{aligned} E^{(i)} &\equiv I^{(i)} - T_1^{(i)} = \int_{x_{i-1}}^{x_i} f(x)dx - \frac{h}{2}(f_{i-1} + f_i) \\ &= -(\frac{1}{12})h_i^3 f^{''}(\xi_i). \end{aligned}$$

Subdividing $[x_{i-1}, x_i]$ into two subintervals leads to,

$$\int_{x_{i-1}}^{x_{i-1/2}} f(x)dx \approx \frac{h_i}{4}(f_{i-1} + f_{i-1/2}), \text{err} = \frac{-1}{12}(\frac{h_i}{2})^3 f^{''}(\bar{\xi}_i),$$

$$\int_{x_{i-1/2}}^{x_i} f(x)dx \approx \frac{h_i}{4}(f_{i-1/2} + f_i), \text{err} = \frac{-1}{12}(\frac{h_i}{2})^3 f^{''}(\hat{\xi}_i).$$

Error Estimate for CT Rule

Summing these two terms we obtain,

$$I^{(i)}(f) \approx \frac{h_i}{4}(f_{i-1} + 2f_{i-1/2} + f_i) \equiv T_2^{(i)}(f),$$

with an associated error expression,

$$I^{(i)} - T_2^{(i)} = \frac{-1}{12}(\frac{h_i}{2})^3 \left[f^{''}(\bar{\xi}_i) + f^{''}(\hat{\xi}_i)\right] = \frac{-h_i^3}{48} f^{''}(\tilde{\xi}_i).$$

If h is 'small enough', (ie, $f^{''}(\bar{\xi}_i) \approx f^{''}(\hat{\xi}_i) \approx f^{''}(\tilde{\xi}_i)$) then subtracting these two error expressions we obtain,

$$(I^{(i)} - T_1^{(i)}) - (I^{(i)} - T_2^{(i)}) = T_2^{(i)} - T_1^{(i)}$$

$$\approx \frac{-h_i^3}{12} f^{''}(\xi_i) [1 - 1/4] = \frac{-3}{48} h_i^3 f^{''}(\xi_i).$$

Error Estimate for CT Rule (cont)

We can then estimate the error associated with $T_2^{(i)}$ as $1/3\left[T_2^{(i)} - T_1^{(i)}\right]$ and, after summing over all M subintervals,

$$\begin{aligned} EST_{2M} &\equiv \sum_{i=1}^{M} \frac{1}{3}(T_2^{(i)} - T_1^{(i)}), \\ &= \frac{1}{3}\left[\sum_{i=1}^{M} T_2^{(i)} - \sum_{i=1}^{M} T_1^{(i)}\right], \\ &= \frac{1}{3}\left[T_{2M} - T_M\right]. \end{aligned}$$

Furthermore by applying the MVT for sums, it can easily be shown that EST_{2M} also equals $\frac{-f^{''}(\xi)}{24}(\frac{h}{2})^2(b-a)$ for some $\xi\ \in (a,b)$.

Observations re Error Est

- This estimate is only justified for h_i sufficiently small so that $f^{''}$ is almost constant over each subinterval.
- The computation of EST_{2M} can be subject to large relative error as it involves the subtraction of ‘near equals’.
- A validity check is available based on monitoring the ratio $|EST_M/EST_{2M}|$ which should be close to 4.

Error Est for Comp Simpsons

- A similar analysis for Composite Simpsons rule justifies,

$$\begin{aligned} EST_{2M}^{S} &= \frac{1}{15}\left[S_{2M} - S_{M}\right], \\ &= -\frac{f^4(\eta)}{180}(\frac{h}{4})^4(b-a). \end{aligned}$$

  where the corresponding validity check is that $|EST_M^S/EST_{2M}^S| \approx 16$.

- Exercise: Show that $T_{2M} + EST_{2M}^T = S_M$.

An Example

Consider applying the Composite Trapezoidal and Composite Simpsons rules in single and double precision floating point arithmetic ($\beta = 16$ and $s = 5,\ s = 12$, respectively) to approximate $\int_0^1 e^{-x^2} dx$.

The numerical results are presented in the attached Table and they clearly indicate the ability of the validity check to reflect when the error estimate can be trusted. Note that we have only justified it in the limit as $h \to 0$ and in the situation where truncation error dominates round-off error.

An Example (cont)

M	Approximation	EST	True Err	Ratio
I) Composite Trapezoidal, T_M – single precision				
2	0.73136990000000	-.158E-01	-.155E-01	4.07
4	0.74298350000000	-.387E-02	-.384E-02	4.02
8	0.74586510000000	-.961E-03	-.959E-03	4.00
16	0.74658410000000	-.240E-03	-.240E-03	4.00
32	0.74676080000000	-.589E-04	-.632E-04	3.79
64	0.74680320000000	-.141E-04	-.208E-04	3.04
128	0.74681350000000	-.342E-05	-.106E-04	1.97
256	0.74681560000000	-.715E-06	-.840E-05	1.26
512	0.74676600000000	.165E-04	-.580E-04	0.15
II) Composite Trapezoidal, T_M – double precision				
2	0.7313702518257	-.158E-01	-.155E-01	4.07
4	0.7429840977975	-.387E-02	-.384E-02	4.02
8	0.7458656148428	-.961E-03	-.959E-03	4.01
16	0.7465845967854	-.240E-03	-.240E-03	4.00
32	0.7467642546494	-.599E-04	-.599E-04	4.00
64	0.7468091636350	-.150E-04	-.150E-04	4.00
128	0.7468203905388	-.374E-05	-.374E-05	4.00
256	0.7468231972433	-.936E-06	-.936E-06	4.00
512	0.7468238989181	-.234E-06	-.234E-06	4.00
III) Composite Simpson, S_M – single precision				
2	0.74685500000000	.217E-04	.310E-04	11.5
4	0.74682550000000	.197E-05	.143E-05	21.7
8	0.74682190000000	.234E-06	-.209E-05	.7
16	0.74682180000000	.795E-08	-.221E-05	.9
32	0.74682170000000	.119E-07	-.238E-05	.9
64	0.74681340000000	.552E-06	-.107E-04	.2
128	0.74679560000000	.118E-05	-.284E-04	.4
256	0.74678870000000	.457E-06	-.353E-04	.8
512	0.74678670000000	.139E-06	-.374E-04	.9
IV) Composite Simpson, S_M – double precision				
2	0.7468553797881	.217E-04	.312E-04	11.4
4	0.7468261205246	.195E-05	.199E-05	5.71
8	0.7468242574329	.124E-06	.125E-06	5.91
16	0.7468241406041	.779E-08	.779E-08	16.0
32	0.7468241332968	.487E-09	.487E-09	16.0
64	0.7468241328400	.305E-10	.305E-10	16.0
128	0.7468241328115	.190E-11	.196E-11	5.61
256	0.7468241328097	.119E-12	.173E-12	11.3
512	0.7468241328096	.748E-14	.611E-13	2.8