CSC436 Tutorial 6 – Numerical Integration II

QUESTION 1 *Study the efficiency of composite Simpson's, in its uniform and adaptive versions, applied to compute $\int_0^1 f(x)dx$, where $f(x) = \log(1+\eta x)\log(1+\eta(1-x))/\log^2(1+\eta)$, with $\eta = 100$.*

SOLUTION:

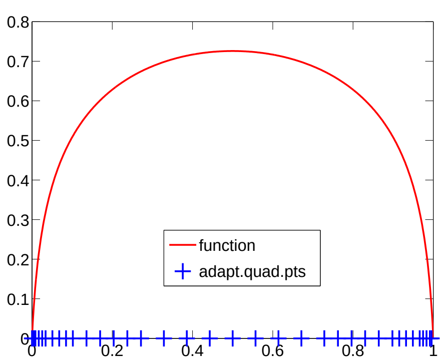
The first plot below shows that the function $f(x)$ increases and decreases sharply as $x \to 0$ and $x \to 1$, respectively, while it is fairly flat close to $x = 1/2$. We expect the adaptive quadrature rule to pick many more points close to $x = 0$ and $x = 1$, than close to $x = 1/2$.

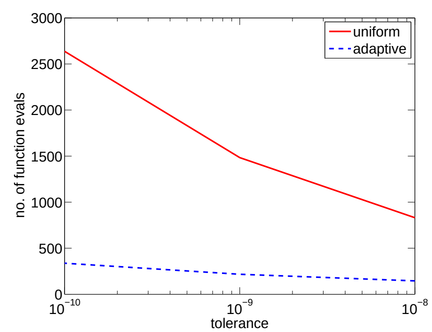
Using the adaptive quadrature MATLAB routine `quad` in the form

```
[q, nfcn] = quad(@(x)twolayer(x, eta), a, b, tol, 1);
```

we get, besides the approximate value of the integral, the number of function evaluations, as well as the trace of the location of panel nodes the adaptive routine chose. In the first plot below, we indicate by "+" the location of panel nodes as chosen by `quad` with $tol = 10^{-8}$. It is clear that the points become denser towards the endpoints where the function changes rapidly, and coarser towards the middle, when the function is relatively flat.

In the table, we see the number of function evaluations the uniform and adaptive Simpson's takes to reach the specified tolerances for this function.





tol	uniform	adaptive
10^{-8}	831	145
10^{-9}	1483	217
10^{-10}	2637	337

It is clear, that the uniform composite rule wastes a lot of function evaluations, compared to the adaptive one. We also see that, as the tolerance is divided by 10, the uniform rule requires approximately $10^{1/4} \approx 1.78$ more evaluations, which agrees with the theoretical bound for the number of panels s for Simpson's (i.e. $K(\frac{b-a}{s})^4 \le tol \Rightarrow s \ge (b-a)\frac{K^{1/4}}{tol^{1/4}}$).

For the adaptive rule, the factor by which the number of functions evaluations increases as the tolerance is divided by 10 is about 1.5. This is also seen in the second plot above, where

the adaptive rule has a better slope (as tol decreases, the number of functions evaluations increases at a slighlty lower rate compared to the uniform rule).

QUESTION 2 *Find x_0, x_1 and c_1 so that the quadrature formula*

$$I = \int_0^1 f(x)dx \approx \frac{1}{2}f(x_0) + c_1 f(x_1) = Q$$

has the highest degree of precision. What is the degree?

SOLUTION:

Since we have three unknowns, we setup three equations, in hope that they are uniquely solvable. Force the rule to be exact for

- $f(x) = 1$: $\int_0^1 dx = \frac{1}{2} + c_1 \Rightarrow 1 = \frac{1}{2} + c_1 \Rightarrow c_1 = \frac{1}{2}$.
- $f(x) = x$: $\int_0^1 x dx = \frac{1}{2}x_0 + \frac{1}{2}x_1 \Rightarrow \frac{1}{2} = \frac{1}{2}x_0 + \frac{1}{2}x_1 \Rightarrow x_0 + x_1 = 1$ (1)
- $f(x) = x^2$: $\int_0^1 x^2 dx = \frac{1}{2}x_0^2 + \frac{1}{2}x_1^2 \Rightarrow \frac{1}{3} = \frac{1}{2}x_0^2 + \frac{1}{2}x_1^2 \Rightarrow x_0^2 + x_1^2 = \frac{2}{3}$ (2)

From (1) and (2) we have $x_1 = 1 - x_0$ and

$$x_0^2 + (1-x_0)^2 = \frac{2}{3} \Rightarrow 6x_0^2 - 6x_0 + 1 = 0.$$

Thus $x_0 = \frac{6 \pm \sqrt{36-4\times6\times1}}{2\times6} = \frac{1}{2} \pm \frac{\sqrt{3}}{6}$ and $x_1 = 1 - x_0 = 1 - (\frac{1}{2} \pm \frac{\sqrt{3}}{6}) = \frac{1}{2} \mp \frac{\sqrt{3}}{6}$, i.e. $x_0 = \frac{3-\sqrt{3}}{6}$ and $x_1 = \frac{3+\sqrt{3}}{6}$. Note that x_0 and x_1 are symmetric w.r.t the midpoint of the interval. The rule

is

$$I = \int_0^1 f(x)dx \approx \frac{1}{2}f(\frac{3-\sqrt{3}}{6}) + \frac{1}{2}f(\frac{3+\sqrt{3}}{6}) = Q$$

The rule was constructed to be exact on x^i, $i = 0, 1, 2$. We now check the rule on a polynomial of degree 3:

Let $f(x) = x^3$, then $I = \int_0^1 x^3 dx = \frac{1}{4}$. Then

$$\begin{aligned} Q &= \frac{1}{2}(\frac{3-\sqrt{3}}{6})^3 + \frac{1}{2}(\frac{3+\sqrt{3}}{6})^3 = \frac{1}{2}\frac{1}{6^3}[(3-\sqrt{3})^3 + (3+\sqrt{3})^3)] \\ &= \frac{1}{2}\frac{1}{6^3}(2\times3^3 + 2\times3\times3\times3) = \frac{1}{2}\frac{1}{6^3}(4\times3^3) = \frac{1}{4} = \int_0^1 x^3 dx. \end{aligned}$$

So the rule is exact on x^3 as well, thus its polynomial degree is ≥ 3. We have to check for higher degree than 3. If we check on x^4, we see that the rule is NOT exact (calculations omitted), thus the degree is 3. This is expected, since we know we can't do better than degree $= 3$ with 2 data points. (See Gauss rules, in class.)

We can transform the rule we derived from $[0, 1]$ to a general interval $[a, b]$.

In general, the linear transformation from $[\alpha, \beta]$ to $[a, b]$ is $t = \frac{(b-a)x + a\beta - b\alpha}{\beta - \alpha}$ with $a \le t \le b$ and $\alpha \le x \le \beta$.

In this case, $\alpha = 0$ and $\beta = 1$. Thus the transformation is $t = (b-a)x + a$. The weights w_1 and w_2 are scaled by $\frac{b-a}{\beta-\alpha} = (b-a)$. Thus the rule for a general interval becomes

$$I = \int_a^b f(x)dx \approx (b-a)f((b-a)\frac{3-\sqrt{3}}{6} + a) + (b-a)f((b-a)\frac{3+\sqrt{3}}{6}) + a) = Q$$

As has been (or will be) seen, this is the two-point Gauss rule.

QUESTION 3 *Find x_0, x_1, c_0 and c_1 so that the quadrature formula*

$$I = \int_0^1 f(x)dx \approx c_0 f(x_0) + c_1 f(x_1) = Q$$

has the highest degree of precision. What is the degree?

SOLUTION:

Since we have four unknowns, we write four equations in hope that they are solvable. Force the rule to be exact for $f(x) = 1, x, x^2, x^3$. We get the equations $c_0 + c_1 = 1$, $c_0 x_0 + c_1 x_1 = 1/2$, $c_0 x_0^2 + c_1 x_1^2 = 1/3$ and $c_0 x_0^3 + c_1 x_1^3 = 1/4$. These four (nonlinear) equations are uniquely solvable, and their solution gives rise to the same (two-point Gauss) quadrature rule as Question 2. However, it is harder to manipulate these four equations to obtain their solution by hand than the three equations of Question 2, since the four equations in this question include cubic terms.

QUESTION 4 *Approximate $I = \int_1^2 x^4 dx$ using Simpson's, two-point and four-point Gauss rules with 1 and 2 panels. Compute the error for each rule.*

SOLUTION:

Exact value: $I = \int_1^2 x^4 dx = \frac{x^5}{5}\Big|_1^2 = \frac{32}{5} - \frac{1}{5} = \frac{31}{5} = 6.2$

With 1 panel:

Simpson's: $Q_{S,0} = \frac{2-1}{6}\big[f(1)+4f(\frac{3}{2})+f(2)\big] = \frac{1}{6}\big[1+4(\frac{3}{2})^4+16\big] = \frac{1}{6}\big[1+20.25+16\big] = 6.20833$

2-point Gauss: $Q_{G2} = \frac{2-1}{1-(-1)}\big[w_1 f(t_1) + w_2 f(t_2)\big] = \cdots = 6.19444$

The weights and points of the two-point Gauss rule in $[-1, 1]$ are

$w_1 = w_2 = 1$ and $x_1 = -x_2 = -\sqrt{3}/3 = -0.57735026919625$.

The weights in $[1, 2]$ are scaled by $\frac{1}{2}$. In order to obtain the points in $[1, 2]$, we use the linear transformation $t_i = \frac{(2-1)\times x_i + 1\times 1 - 2\times(-1)}{1-(-1)}$. In general, the linear transformation from $[\alpha, \beta]$ to $[a, b]$ is $t = \frac{(b-a)\times x + a\times\beta - b\times\alpha}{\beta-\alpha}$ with $a \le t \le b$ and $\alpha \le x \le \beta$.

4-point Gauss: $Q_{G4} = \frac{2-1}{1-(-1)}\Sigma_{i=1}^4 w_i f(t_i) = \cdots = 6.2$

The weights and points of the 4-point Gauss rule in $[1, -1]$ are

$w_1 = w_2 = 0.347854845137454$, $w_3 = w_4 = 0.652145154862546$,

$x_1 = -x_2 = -0.861136311594052$ and $x_3 = -x_4 = -0.339981043584856$. The same transformation and scaling as with the two-point Gauss is used.

Error for Simpson's: $6.2 - 6.20833 = -0.00833$

Error for 2-pt Gauss: $6.2 - 6.19444 = 0.00556$

Error for 4-pt Gauss: $6.2 - 6.2 = 0$

With 2 panels:

Simpson's: $Q_{S,1} = \frac{2-1}{12}\big[f(1) + 4f(1.25) + 2f(1.5) + 4f(1.75) + f(2)\big] = \cdots = 6.200520833$

2-point Gauss: $Q_{G2} = \frac{0.5}{1-(-1)}\big[w_1 f(t_{1,1}) + w_2 f(t_{2,1}) + w_1 f(t_{1,2}) + w_2 f(t_{2,2})\big] = \cdots = 6.199652778$

We have $w_1 = w_2 = 1$ and $x_1 = -x_2 = -\sqrt{3}/3 = -0.57735026919625$. The weights in $[1, 1.5]$ and $[1.5, 2]$ are scaled by $\frac{1}{4}$. In order to obtain the points in $[1, 1.5]$ and $[1.5, 2]$, we use the linear transformations $t_{i,1} = \frac{(1.5-1)\times x_i + 1\times 1 - 1.5\times(-1)}{1-(-1)}$, and $t_{i,2} = \frac{(2-1.5)\times x_i + 1.5\times 1 - 2\times(-1)}{1-(-1)}$, respectively.

4-point Gauss: $Q_{G4} = \frac{0.5}{1-(-1)}\Sigma_{j=1}^2 \Sigma_{i=1}^4 w_i f(t_{i,j}) = \cdots = 6.2$

Error for Simpson's: $6.2 - 6.200520833 = -5.20833 \times 10^{-4}$

Error for 2-pt Gauss: $6.2 - 6.199652778 = 3.47222 \times 10^{-4}$

Error for 4-pt Gauss: $6.2 - 6.2 = 0$

Results for $\int_1^2 x^4 dx$ with various rules:

rule	error formula	error	poly. degree
$s = 1$			
Simpson's	$-f^{(4)}(\eta)\frac{(b-a)^5}{2880}$	-0.00833	3
2-pt Gauss	$f^{(4)}(\eta)\frac{(b-a)^5}{4320}$	0.00556	3
4-pt Gauss	$f^{(8)}(\eta)\frac{(b-a)^9}{1778111926}$	0	7
$s = 2$			
Simpson's	$-f^{(4)}(\eta)\frac{(b-a)h^4}{2880}$	-5.2×10^{-4}	3
2-pt Gauss	$f^{(4)}(\eta)\frac{(b-a)h^4}{4320}$	3.5×10^{-4}	3
4-pt Gauss	$f^{(8)}(\eta)\frac{(b-a)h^8}{1778111926}$	0	7

Comments:

- The sign of error calculated numerically agrees with that of the error formula. Since $f(x) = x^4$, then $f^{(4)}(x) = 24 > 0$. Thus Simpson's error is negative, and two-point Gauss error is positive.
- The magnitude of the error of Simpson's with $s = 1$ and $s = 2$ panels is 1.5 times the magnitude of the 2-point Gauss rule error with $s = 1$ an $s = 2$ panels, respectively. By

the error formulae, we know that, if $f^{(4)}(x)$ does not vary a lot in $[1, 2]$, we expect the Simpson rule error to be approximately 1.5 (= 4320/2880) times in magnitude compared to the two-point Gauss rule error. For this integral, it turns out to be exactly 1.5 times, because the η's do not matter, since $f^{(4)}(x)$ is constant.

- The magnitudes of the errors of Simpson's and two-point Gauss decrease by a factor of 16 as the number of panels increases from $s = 1$ to $s = 2$. (Note that $\frac{-0.00833}{-5.20833\times10^{-4}} = \frac{0.00556}{3.47222\times10^{-4}} = 16$.) The above result is independent of η, since $f^{(4)}$ is constant.
- Not only the signs and relative magnitudes of the errors agree with those of the formulae, but we can actually (precisely) validate the error formula by each of the numerical experiments.

  Example: Simpson's with $s = 1$ panel. The error formula gives $-f^{(4)}(\eta)\frac{(b-a)^5}{2880}$ which is equal to $-24\frac{1^5}{2880} = -0.00833$, exactly what the numerical experiment gives.

  We can do this validation with each of the numerical results.
- Rules with polynomial degree higher than 3 are exact as expected.
- If the function was x^8 or a higher degree polynomial, none of the rules would be exact.