Numerical Analysis – Lab 9

1 Newton-Cotes quadrature rules

How Regularity Influences Convergence. Recall the composite Trapezoidal Rule and Simpson's Rule with error forms:

$$\int_a^b f(x)dx = \frac{h}{2}\left[f(a) + 2\sum_{j=1}^{n-1} f(x_j) + f(b)\right] - \frac{b-a}{12}h^2 f''(\mu),$$

$$\int_a^b f(x)dx = \frac{h}{3}\left[f(a) + 2\sum_{j=1}^{(n/2)-1} f(x_{2j}) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + f(b)\right] - \frac{b-a}{180}h^4 f^{(4)}(\mu) \quad (n \text{ is even}),$$

where $x_i - x_{i-1} = h = (b-a)/n$, $i = 1, \ldots, n$. Apparently, both the Trapezoidal and Simpson's rules require the integrand f to be some times differentiable with bounded derivatives. What happens if the integrand does not have the required regularity? Let us do some numerical experiments. First, we implement the composite quadrature rules as follows.

```
function I = trapez(f,a,b,n)
% assume f is vectorized
h = (b-a)/n;
x = linspace(a,b,n+1);
I = f(a) + f(b);
I = I + 2*sum(f(x(2:end-1)));
I = I*h/2;
```

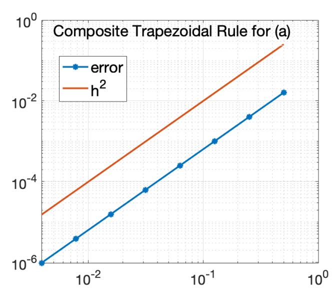
```
function I = simpson(f,a,b,n)
% n must be an even number
% f must be a vectorized function
h = (b-a)/n;
x = linspace(a,b,n+1);
I = f(a)+f(b)+2*sum(f(x(3:2:n-1)))+4*sum(f(x(2:2:n)));
I = I*h/3;
```

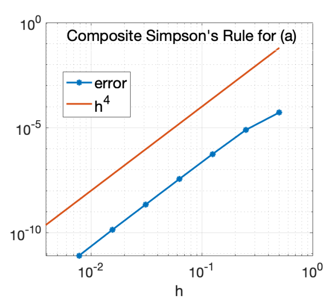
Next, we experiment with the two rules on the following integrals:

$$\text{(a)} \int_0^1 \mathrm{e}^{-\sin x}\, \mathrm{d}x \qquad \text{(b)} \int_0^1 x^{\frac{5}{2}}\, \mathrm{d}x = \frac{2}{7} \qquad \text{(c)} \int_0^1 x^{\frac{3}{2}}\, \mathrm{d}x = \frac{2}{5} \qquad \text{(d)} \int_0^1 x^{\frac{1}{2}}\, \mathrm{d}x = \frac{2}{3}.$$

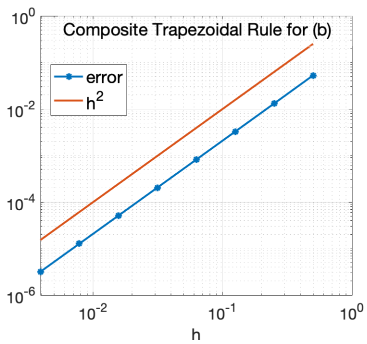
To measure the convergence, we compute the integral with $n = 2, 2^2, 2^3, \ldots$ until the result changes very little. In other words, for $b - a = 1$, we have $h = 2^{-1}, 2^{-2}, 2^{-3}, \ldots$. This allows us to check whether the error goes down as $O(h^\alpha)$ and find α. For the integral (a), we take the final result as the exact value to compute the errors.

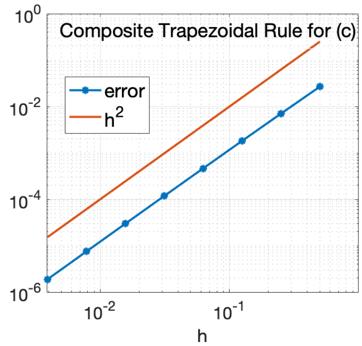
```
LW = 'linewidth'; lw = 2;
f = @(x) exp(-sin(x));
a = 0; b = 1; tol = 1e-10;
Q = zeros(50,1); m = 1;
while true
    Q(m) = trapez(f,a,b,2^m);
    if m>1 && abs(Q(m)-Q(m-1))<tol
        break;
    end
    m = m+1;
end
Q = Q(1:m); I = Q(end);
E = abs(Q(1:8)-I);
h = (b-a)./2.^(1:8);
loglog(h,E,'*-',LW,lw);
hold on; loglog(h,h.^2,LW,lw);
legend('error','h^2','fontsize',18);
xlabel('h'); shg;
```

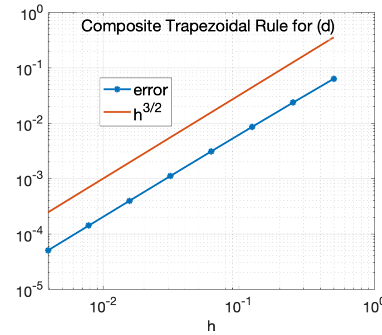




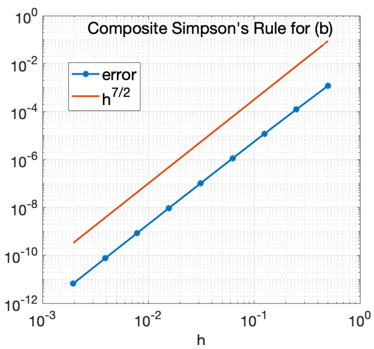
For the other experiments, one needs only to change the definition of `f`, the exact integral value, and/or `trapez` to `simpson` in the program, as well as `h.^2` to an appropriate power of h for `loglog` and `legend`. We see that the composite trapezoidal rule converges as $O(h^2)$ for (b) which is reasonable from the error form, and also as $O(h^2)$ for (c) with $f''(0) = \infty$, but slower as $O(h^{3/2})$ for (d) with $f'(0) = \infty$.

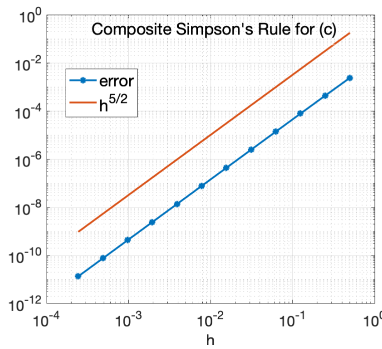


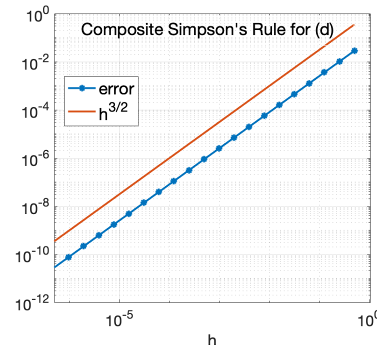




The composite Simpson's rule converges for (b) as $O(h^{7/2})$, for (c) as $O(h^{5/2})$, and for (d) as $O(h^{3/2})$.







Considering the regularity of x^β at $x = 0$, it seems that the actual convergence order of the composite quadrature rules for the integrand x^β is $O(h^\alpha)$ with $\alpha = \min\{p, 1+\beta\}$ where $O(h^p)$ is the convergence order for smooth integrands, e.g. $p = 2$ for the trapezoidal rule and $p = 4$ for Simpson's rule. It is then very tempting to compute the improper integral (**optional**)

$$\text{(e)}^1 \int_0^1 \frac{1}{\sqrt{x}}\, \mathrm{d}x = 2.$$

But the singularity of the integrand at $x = 0$ prohibits the use of composite trapezoidal or Simpson's rule which needs the integrand value at $x = 0$. By definition of the improper integral

$$\int_0^1 \frac{1}{\sqrt{x}}\, \mathrm{d}x = \lim_{\delta \to 0^+} \int_\delta^1 \frac{1}{\sqrt{x}}\, \mathrm{d}x,$$

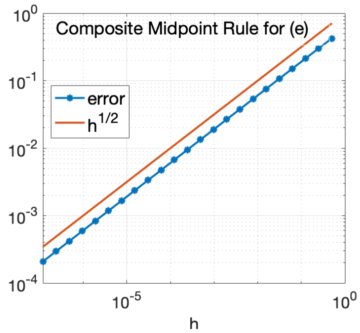
an apparent fix is simply to discard the first subinterval for the composite quadrature rules. But it was hopeless to get convergence with h-refinement in numerical experiments. So we turn to open quadrature rules which do not use the end-points of the interval. For example, the mid-point rule:

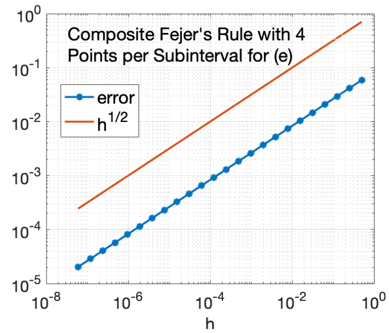
$$\int_{x_0}^{x_1} f(x)\, \mathrm{d}x = hf\left(\frac{x_0 + x_1}{2}\right) + \frac{f''(\mu)}{24} h^3.$$

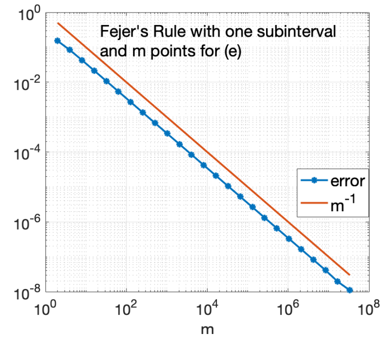
```
function I = mid(f,a,b,n)
h = (b-a)/n;
x = linspace(a,b,n+1);
I = sum(f((x(2:end)+x(1:end-1))/2));
I = I*h;
```

But I can only get the `tol` down to `1e-4` (i.e. 10^{-4}). The complexity for smaller tolerance is prohibitive. The uniform refinement of step size h throughout the interval $[0, 1]$ is inefficient. The only place that demands more points is around the singularity $x = 0$. The convergence is $O(h^{1/2})$.

[1] The example is obviously of only theoretical interest because the exact result can be found by calculus. But for the same reason, it is a good example to start with before going to a real-world problem.





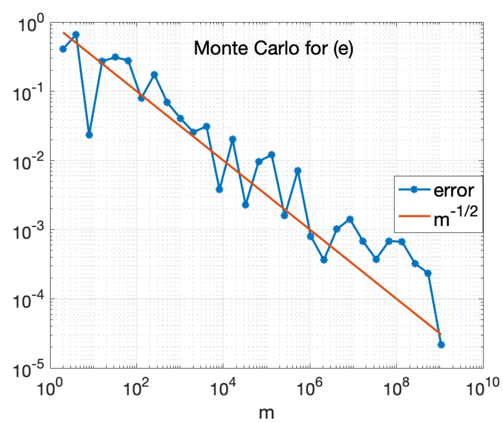


What about a higher-order open quadrature rule? We can use the zeros of a degree m Chebyshev polynomial as the quadrature points, for which the quadrature weights were found by the Hungrian mathematician Lipót Fejér (1880-1959). We can choose how many points m to be used on one subinterval and also how many subintervals `nsub` to be used. If we fix the degree m (e.g. $m = 4$) and still use the uniform h-refinement (i.e. split $[0, 1]$ into more equal subintervals), then the complexity will become prohibitive for some tolerance (e.g. `tol=1e-6`), and the convergence is $O(h^{1/2})$– the same as the mid-point rule. But if we use only one subinterval $[0, 1]$ and increase m which amounts to using higher-order rules (p-refinement), then it is easy to get the tolerance down to e.g. 10^{-8}, and the convergence order is $O(1/m)$ (the previous methods converge as the order of inverse square-root of the number of points).

```
function I = fejer1(f,a,b,nsub,m)
% nodes t and weight w on [-1,1]
t = cos((2*(1:m)-1)/2/m*pi);
N=(1:2:m-1)'; l = length(N); K=(0:m-1-l)';
v0=[2*exp(1i*pi*K/m)./(1-4*K.^2);zeros(l+1,1)];
v1=v0(1:end-1)+conj(v0(end:-1:2));
w=ifft(v1); % continue to the right
% map nodes to each subinterval
hsub = (b-a)/nsub; e=ones(size(t));
xsub = linspace(a,b,nsub+1)';
x = (xsub(1:end-1)+xsub(2:end))/2*e;
x = x+(xsub(2:end)-xsub(1:end-1))/2*t;
% sum all
I = sum(f(x)*w)*hsub/2;
```

We can also use the simple Monte Carlo method. We see that the Monte Carlo method converges as $O(m^{-1/2})$, which is typical. We note also that the points where the integrand is evaluated are sampled from the uniform distribution, which is inefficient because the singularity $x = 0$ demands more points around. So there is some room for improvement.

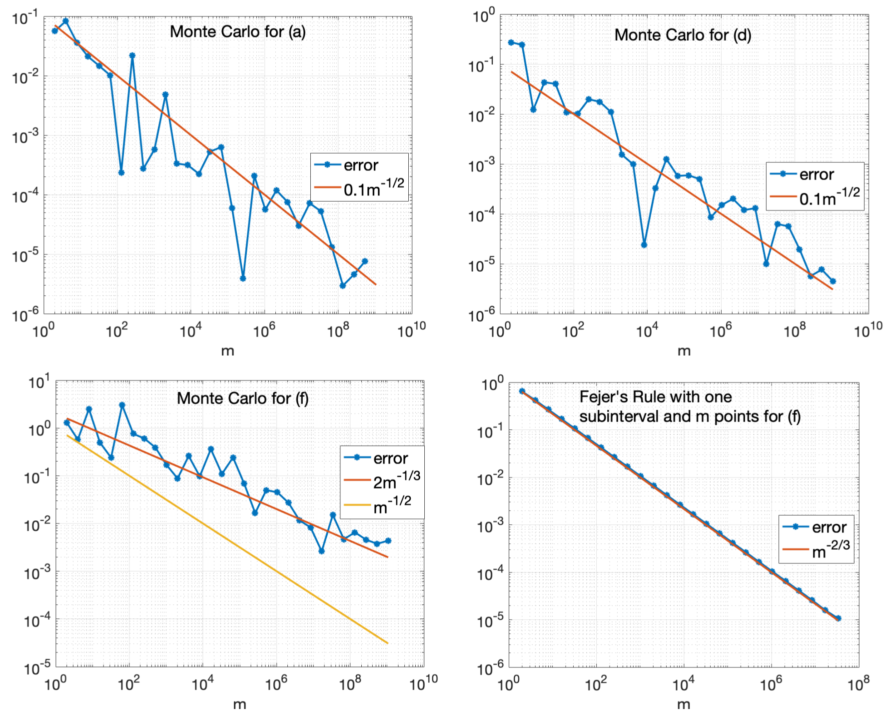
```
function I = monte(f,a,b,m)
s = 1e4; % maximum samples each time
if m<s
    x = a+(b-a)*rand(m,1);
    I = sum(f(x))/m;
else
    I = 0;
    for i=1:floor(m/s)
        x = a+(b-a)*rand(s,1);
        I = I + sum(f(x));
    end
    x = a+(b-a)*rand(mod(m,s),1);
    I= I + sum(f(x));
    I = I/m;
end
```



Does the Monte Carlo method relies on regularity of the integrand? We test it for (a), (d) and

$$\text{(f)} \int_0^1 \frac{1}{\sqrt[3]{x^2}} = 3.$$

For comparision, it is also interesting to test Fejer's rule for (f). What do you observe from the results? See the following figures.



Quadrature in Finance. Below is an excerpt from a book on financial models.

> Let us consider the pricing problem of a plain vanilla option in the Black–Scholes setting. The option price requires computing the following integral:
>
> $$c = \mathrm{e}^{-r\tau} \int_{\ln K}^{+\infty} (\mathrm{e}^{\xi} - K) h(\xi, \tau; z)\, \mathrm{d}\xi,$$
>
> where
>
> $$h(\xi, \tau; z) = \frac{1}{\sqrt{2\pi\sigma^2\tau}} \exp\left(-\frac{1}{2\sigma^2\tau}\left(\xi - z - \left(r - \frac{\sigma^2}{2}\right)\tau\right)^2\right),$$

where the strike price $K = 100$, time to maturity $\tau = 1$, the instantaneous volatility $\sigma = 0.2$, the risk-free interest rate $r = 0.1$, and the standing market price $x = 100$ for $z = \ln x$. The integral is on a semi-infinite interval. To deal with the infinity, one choice is to *transform* the interval to a bounded interval by change of variables. For example, setting $t = \mathrm{e}^{-\xi}$, then

$$c = \mathrm{e}^{-r\tau} \int_0^{1/K} \frac{1}{t^2}(1 - Kt) \frac{1}{\sqrt{2\pi\sigma^2\tau}} \mathrm{e}^{-\frac{1}{2\sigma^2\tau}\left(-\ln t - z - (r - \frac{\sigma^2}{2})\tau\right)^2}\, \mathrm{d}t.$$

It is found that as $t \to 0$ the integrand (the function to be integrated) tends to zero. Another choice is to *truncate* the infinite interval to a (sufficiently large) bounded interval. For example, to change the upper limit of the integral to $\ln 400$. Use the composite Simpson's rule to compute the transformed or truncated integral. Compare it to the Black–Scholes price 13.26967658466089.

When the Composite Trapezoidal Rule Converges Exponentially (optional). Read Trefethen's paper *The exponentially convergent trapezoidal rule* and try the examples therein.

2 Romberg integration (optional)

Read the relevant section of the textbook, and try it on the examples in the previos section.