Phys 305

Prof. Elisabeth Krause (she/her)

TAs: Marco Jimenez (he/him)
Maria Mutz (she/her)

Today's Lecture

- Announcements
  - Please submit either python code or notebook, not a mix!
  - Please follow naming conventions for python code!
  - **Problem Set 2** due 9/14/2020 at 5:00 pm (on D2L)
    - Note: Submitting zip (instead of tar.gz) folder will not result any point deductions!
- Today's lecture: intro to term projects, numerical integration examples, intro to term projects
- Outlook: Gaussian Quadrature integration, numerical differentiation

Improving over the Trapezoidal Rule

Richardson Extrapolation (cancellation of error terms):
Let $N_1(h)$ provide an estimate for M, with error of order h:

$$M = N_1(h) + K_1 h + K_2 h^2 + K_3 h^3 + \cdots . \quad (1)$$

$$M = N_1\left(\frac{h}{2}\right) + K_1 \frac{h}{2} + K_2 \frac{h^2}{4} + K_3 \frac{h^3}{8} + \cdots . \quad (2)$$

2*(2)-(1)

$$M = \underbrace{\boxed{N_1\left(\frac{h}{2}\right) + \left[N_1\left(\frac{h}{2}\right) - N_1(h)\right]}}_{\mathbf{N_2(h)}} + K_2\left(\frac{h^2}{2} - h^2\right) + K_3\left(\frac{h^3}{4} - h^3\right) + \cdots$$

$$M = \boxed{N_2(h)} - \frac{K_2}{2} h^2 - \frac{3K_3}{4} h^3 - \cdots .$$

By combining estimates with different step size, we cancelled the leading order error term, and gain an order in convergence!

Improving over the Trapezoidal Rule

Romberg Integration:
Apply Richardson Extrapolation to Trapezoidal rule

$$I_n = h_n\left(\frac{1}{2}f(a) + \sum_{k=1}^{2^n-1} f(a+kh) + \frac{1}{2}f(b)\right) \text{ with } N = 2^n \text{ and } h_n = (b-a)/2^n.$$

It can be shown that $\int_a^b f(x)dx = \sum_{i=1}^{N} \frac{1}{2}h(f_i + f_{i+1}) - \sum_{k=1}^{\lfloor 2p \rfloor} C_k h^{2k}$, apply to I_n

$$I_{n-1} = I + C_1 h_{n-1}^2 + \mathcal{O}(h^4)$$

$$I_n = I + C_1(\frac{1}{2}h_{n-1})^2 + \mathcal{O}(h^4)$$

Now, use Richardson Extrapolation to cancel leading error term

$$I_{n,1} = \frac{4I_{n,0} - I_{n-1,0}}{3} + \mathcal{O}(h^4)$$

$$I_{n+1,1} = \frac{4I_{n+1,0} - I_{n,0}}{3} + \mathcal{O}(h^4)$$

$$I_{n,1} = I + C_2(h_n)^4 + \mathcal{O}(h^6)$$

$$I_{n+1,1} = I + C_2(\frac{1}{2}h_n)^4 + \mathcal{O}(h^6)$$

$$I_{n+1,2} = \frac{16I_{n+1,1} - I_{n,1}}{15} + \mathcal{O}(h^6)$$

Romberg Integration Example

Use the Composite Trapezoidal rule to find approximations to $\int_0^{\pi} \sin x \, dx$ with $n = 1, 2, 4,$ 8, and 16. Then perform Romberg extrapolation on the results.

The Composite Trapezoidal rule for the various values of n gives the following approximations to the true value 2.

$$I_{1,0} = \frac{\pi}{2}[\sin 0 + \sin \pi] = 0;$$

$$I_{2,0} = \frac{\pi}{4}\left[\sin 0 + 2\sin\frac{\pi}{2} + \sin \pi\right] = 1.57079633;$$

$$I_{3,0} = \frac{\pi}{8}\left[\sin 0 + 2\left(\sin\frac{\pi}{4} + \sin\frac{\pi}{2} + \sin\frac{3\pi}{4}\right) + \sin \pi\right] = 1.89611890;$$

$$I_{4,0} = \frac{\pi}{16}\left[\sin 0 + 2\left(\sin\frac{\pi}{8} + \sin\frac{\pi}{4} + \cdots + \sin\frac{3\pi}{4} + \sin\frac{7\pi}{8}\right) + \sin \pi\right] = 1.97423160;$$

$$I_{4,0} = \frac{\pi}{32}\left[\sin 0 + 2\left(\sin\frac{\pi}{16} + \sin\frac{\pi}{8} + \cdots + \sin\frac{7\pi}{8} + \sin\frac{15\pi}{16}\right) + \sin \pi\right] = 1.99357034.$$

The $O(h^4)$ approximations are

$$I_{2,1} = I_{2,0} + \frac{1}{3}(I_{2,0}-I_{1,0}) = 2.09439511; \quad I_{3,1} = I_{3,1} + \frac{1}{3}(I_{3,0}-I_{2,0} \ {}_1) = 2.00455976;$$

$$I_{4,1} = I_{4,0} + \frac{1}{3}(I_{4,0}-I_{3,0}) = 2.00026917; \quad I_{5,1} = I_{5,1} + \frac{1}{3}(I_{5,0}-I_{4,0}) = 2.00001659;$$

Romberg Integration Example

The $O(h^6)$ approximations are

$$I_{3,2} = I_{3,1} + \frac{1}{15}(I_{3,1} - I_{2,1}) = 1.99857073; \quad I_{4,2} = I_{4,1} + \frac{1}{15}(I_{4,1} - I_{3,1}) = 1.99998313;$$

$$I_{5,2} = I_{5,1} + \frac{1}{15}(I_{5,1} - I_{4,1}) = 1.99999975.$$

The two $O(h^8)$ approximations are

$$I_{4,3} = I_{4,2} + \frac{1}{63}(I_{4,2} - I_{3,2}) = 2.00000555; \quad I_{5,3} = I_{5,2} + \frac{1}{63}(I_{5,2} - I_{4,2}) = 2.00000001,$$

and the final $O(h^{10})$ approximation is

$$I_{5,4} = I_{5,3} + \frac{1}{255}(I_{5,3} - I_{4,3}) = 1.99999999.$$

Romberg Integration

```
nextTrapezoidal(f, x_min, x_max, n):
    """
    Return the difference between the trapezoidal rule approx-
    imation for 2^n intervals and one-half the trapezoidal
    rule for 2^(n-1) intervals.
    """
    N = 2^n
    h = (x_max - x_min)/N
    I_n = 0
    for j = 1 to N/2:
        I_n = I_n + f(x_min + (2j - 1)h)

    return h I_n
```

$N = 2^n$

$h = (x_{max} - x_{min})/N$

$I_n = 0$

for $j = 1$ to $N/2$:

$I_n = I_n + f(x_{min} + (2j-1)h)$

return hI_n

Romberg Integration

```
romberg(f, x_min, x_max, n_max, ε):
    """
    Use Richardson extrapolation to compute the integral of f(x)
    from x_min to x_max with a relative error less than epsilon,
    using trapezoidal rules with up to 2^n_max intervals.
    """
    I_{0,0} = 1/2 (x_max - x_min)(f(x_min) + f(x_max))

    for n = 1 to n_max:
        I_{n,0} = 1/2 I_{n-1,0} + nextTrapezoidal(f, x_min, x_max, n)

        for k = 1 to n:
            q = 4^k
            I_{n,k} = (q I_{n,k-1} - I_{n-1,k-1})/(q - 1)

        if |I_{n,n} - I_{n,n-1}| < ε |I_{n,n-1}|:
            return I_{n,n}

    print "failured to converge!"
```

$$I_{0,0} = \frac{1}{2}(x_{max} - x_{min})(f(x_{min}) + f(x_{max}))$$

$$I_{n,0} = \frac{1}{2} I_{n-1,0} + \text{nextTrapezoidal}(f, x_{min}, x_{max}, n)$$

$$q = 4^k$$

$$I_{n,k} = (qI_{n,k-1} - I_{n-1,k-1})/(q-1)$$

$$|I_{n,n} - I_{n,n-1}| < \epsilon\,|I_{n,n-1}|$$

Your Turn!

- Calculate the unit disk and unit ball area using Monte Carlo Integration
- Determine the convergence rate of Monte Carlo Integration in two and three dimensions