Queens College, CUNY, Department of Computer Science

Numerical Methods

CSCI 361 / 761

Fall 2018

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6 Homework lecture 6: numerical integration

If you write the code to implement the midpoint, trapezoid and Simpson rules, this homework assignment will be much easier.

It is then simply a matter of substituting different functions for $f(x)$.

Value of π to machine precision on any computer.

1. Some compilers support the constant `M_PI` for π, in which case you can write

```
const double pi = M_PI;
```

2. If your compiler does not support `M_PI`, the value of π can be computed via

```
const double pi = 4.0*atan2(1.0,1.0);
```

- Please email your solution, as a file attachment, to `Sateesh.Mane@qc.cuny.edu`.
- Please submit one zip archive with all your files in it.
  1. The zip archive should have either of the names (CS361 or CS761):

     `StudentId_first_last_CS361_hw6.zip`

     `StudentId_first_last_CS761_hw6.zip`

  2. The archive should contain one "text file" named "hw6.[txt/docx/pdf]" and one cpp file per question named "Q1.cpp" and "Q2.cpp" etc.
  3. Note that not all homework assignments may require a text file.
  4. Note that not all questions may require a cpp file.

6.1 Proper/improper integrals

- **Question: Which of the integrals below are proper integrals?**

  1. **Note: other authors may have a different definition of a proper integral.**
  2. We want the domain of integration to be finite, the function (integrand) to be bounded and well–defined, including at the endpoints (not all authors may agree with this), we also exclude integrands which evaluate to 0/0 (but are finite) at one or more points in the integration domain (not all authors may agree with this).
  3. In other words, we want to be able to compute the integral without any difficulties.

- In each case where you believe the integral is **improper**,
  explain **why you consider the integral is improper.**

- **Note: the value of an improper integral does not need to be infinite.**
  An improper integral could have a finite value.

- **Do not attempt to perform mathematical transformations on the integrals,**
  e.g. change of variable.

- **Do not compute the values of the integrals.**

$$I_1 = \int_{-\infty}^{\infty} e^{-x^2/2}\,dx\,, \tag{6.1.1}$$

$$I_2 = \int_0^5 (x-1)(x-2)(x-3)\,dx\,, \tag{6.1.2}$$

$$I_3 = \int_0^5 \frac{1}{(x-1)(x-2)(x-3)}\,dx\,, \tag{6.1.3}$$

$$I_4 = \int_0^{1/\sqrt{2}} \frac{1}{\sqrt{1-x^2}}\,dx\,, \tag{6.1.4}$$

$$I_5 = \int_0^1 \frac{1}{\sqrt{1-x^2}}\,dx\,, \tag{6.1.5}$$

$$I_6 = \int_0^{\infty} \frac{1}{\sqrt{1-x^2}}\,dx\,, \tag{6.1.6}$$

$$I_7 = \int_{-1}^1 \frac{1}{x}\,dx\,, \tag{6.1.7}$$

$$I_8 = \int_0^2 \frac{\sin(\pi x)}{1-x^2}\,dx\,, \tag{6.1.8}$$

$$I_9 = \int_0^{\pi} \sin(\frac{1}{x})\,dx\,, \tag{6.1.9}$$

$$I_{10} = \int_0^1 \arcsin(x)\,dx\,. \tag{6.1.10}$$

6.2 Integrand with parameter

- In the questions below, α and β are constants and their values are real numbers.
- **The values of α and β need not be positive.**
- **Question: Is the integral below a proper integral?**

$$I(\alpha) = \int_0^1 \frac{1}{\sqrt{1-\alpha^2 x^2}}\,dx\,, \tag{6.2.1}$$

- **Question: Is the integral below a proper integral?**

$$I(\beta) = \int_0^1 \frac{1}{\sqrt{1-\beta x^2}}\,dx\,, \tag{6.2.2}$$

6.3 Math library functions for numerical integration

- **Write functions to implement the midpoint, trapezoid and Simpson's rules.**
- Add extra functions to the math library from the root finding lectures.
- The abstract base class is the same as before. We use the function $f(x)$.

```
class MathFunction {
  virtual double f(double x) const { return 0; }
  // etc., same as before
};

class MathLibraryCPP {
public:
  // new functions
  static double midpoint (const MathFunction &mf, double a, double b, int n);
  static double trapezoid(const MathFunction &mf, double a, double b, int n);
  static double Simpson  (const MathFunction &mf, double a, double b, int n);

  // (root finding algorithms from previous work)
};
```

- **You may also implement Java versions of the above functions.**

6.4 Triangle function: higher order does not always imply higher accuracy

- You are given the following 'triangle' function, for $0 \le x \le 1$:

$$f_{\rm tri}(x) = \begin{cases} 4x & (0 \le x \le \frac{1}{2})\,, \\ 4(1-x) & (\frac{1}{2} < x \le 1)\,. \end{cases} \tag{6.4.1}$$

- Hence $f_{\rm tri}(x)$ describes a triangle with base 1 and height 2. The area of the triangle is 1.
- Let us calculate the area of the triangle by computing the following integral.

$$I_{\rm tri} = \int_0^1 f_{\rm tri}(x)\,dx\,. \tag{6.4.2}$$

- **Compute the above integral numerically using the following:**
  (a) midpoint rule, (b) trapezoid rule, (c) Simpson's rule.
- **Fill the tables below for n subintervals.**
  If the answer is not exactly 1, write it 4 decimal places.
  I have filled in a few values for you, which you should confirm.

n	midpoint	trapezoid	Simpson
2	**1**	**1**	**4/3**
4			4 d.p.
6			4 d.p.
8			4 d.p.
10			4 d.p.
12			4 d.p.
14			4 d.p.
16			4 d.p.
18			4 d.p.
20			4 d.p.

n	Simpson−1.0	$4/(3n^2)$
2	**1/3**	**1/3**
6	4 d.p.	**1/27**
10	4 d.p.	**1/75**
14	4 d.p.	**1/147**
18	4 d.p.	**1/243**

- *If you have done your work correctly, you should find that the midpoint and trapezoid rules yield exactly 1 for all even values of n.*
- This is because $f_{\rm tri}(x)$ is a piecewise linear function.
- *However, you should find Simpson's rule does not yield exactly 1 for all values of n.*
- This is because Simpson's rule fits the function with a quadratic, and $f_{\rm tri}(x)$ is not differentiable at $x = \frac{1}{2}$, the peak of the triangle.
- *If you have done your work correctly, the numbers in the second table should be an exact match. This demonstrates that the rate of convergence is $O(1/n^2)$, not $O(1/n^4)$.*
- *Actually, the midpoint and trapezoid rules do not yield exactly 1 for if you use odd values of n. You should obtain midpoint $= 1 + (1/n^2)$ and trapezoid $= 1 - (1/n^2)$. Try it and see, $n = 1, 3, 5, 7$.*
- **These are things to bear in mind, in real–life applications. The integrand may not behave well at all points in the domain of integration.**

6.5 Computation of integral

- You are given the following integral

$$I = \int_0^1 \frac{1+x^2}{\sqrt{1-\frac{1}{2}x^2}}\,dx\,. \tag{6.5.1}$$

- Let I_n be the value of the computation using n subintervals.
- **Compute the above integral numerically using the following:**
  1. midpoint rule
  2. trapezoid rule
  3. Simpson's rule
- **Question: For each technique, determine the value of n such that $|I_n - I_{n-2}| < 10^{-4}$.**
- **Use even values of n because of Simpson's rule and fill the table below.**
- You might have to go up to about $n \simeq 20$.

n	midpoint	trapezoid	Simpson
2			
4			
6			
8			
10			
12			
14			
16			
18			
20			
⋮			

- **Question: What is the value of the integral to 4 decimal places?**

6.6 Computation of integration with parameter

- **The function $f(x)$ can depend on a parameter, say γ.**
  1. **In that case the value of the integral will also depend on that parameter.**
  2. There is nothing wrong or unusual about this. It happens all the time.
  3. For example the integral could be the air pressure in some region.
  4. The parameter could be the temperature.
- You are given the following integral.

$$I(\gamma) = \int_0^1 \frac{1+x^2}{\sqrt{1-\gamma^2 x^2}}\,dx\,. \tag{6.6.1}$$

- **Use only Simpson's rule to answer this question. Use $n = 10$ subintervals.**
- **Question: Compute the value of the integral in eq. (6.6.1) for $\gamma = 0, 0.1, 0.2, \ldots, 0.9$ and fill the table below. State your results to 4 decimal places.**

γ	I_{Simpson}
0.1	4 d.p.
0.2	4 d.p.
0.3	4 d.p.
0.4	4 d.p.
0.5	4 d.p.
0.6	4 d.p.
0.7	4 d.p.
0.8	4 d.p.
0.9	4 d.p.

- **Not a question. For your information, Fig. 1 displays a graph of $I(\gamma)$ for $-1 < \gamma < 1$.**

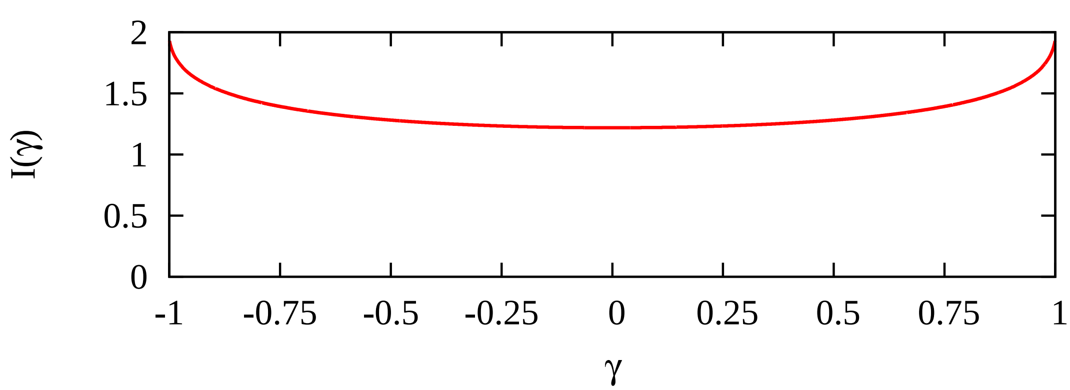

Figure 1: Graph of $I(\gamma)$ as a function of γ for $-1 < \gamma < 1$.

6.7 Integral representation of Bessel function

- The Bessel function $J_m(x)$ $(m = 0, 1, 2, \dots)$ can be computed by evaluating the following integral:
$$J_m(x) = \frac{1}{\pi} \int_0^{\pi} \cos(x \sin(\theta) - m\theta)\, d\theta\,. \tag{6.7.1}$$
- Plots of the Bessel functions $J_0(x)$, $J_1(x)$ and $J_2(x)$ are displayed in Fig. 2, for $0 \le x \le 20$.
- For any integer $m \ge 0$, $J_m(x)$ oscillates forever and has infinitely many roots.
- **Set $m = 1$ and $x = 200$ in the calculations below.**
- **Compute the integral in eq. (6.7.1) using:**
  1. midpoint rule = J_{mid}
  2. trapezoid rule = J_{trap}
  3. Simpson's rule = J_{Simp}
- **Fill the table below. State your results to 6 decimal places.**
  The answer is a negative number.

n	J_{mid}	J_{trap}	J_{Simp}
1	6 d.p.	6 d.p.	—
2	6 d.p.	6 d.p.	6 d.p.
4	6 d.p.	6 d.p.	6 d.p.
8	6 d.p.	6 d.p.	6 d.p.
16	6 d.p.	6 d.p.	6 d.p.
32	6 d.p.	6 d.p.	6 d.p.
64	6 d.p.	6 d.p.	6 d.p.
128	6 d.p.	6 d.p.	6 d.p.
256	6 d.p.	6 d.p.	6 d.p.

- For the trapezoid rule you may, if you wish, employ the extended trapezoid rule.
- *If you have done your work correctly, the midpoint and trapezoid rules should converge to 6 d.p. by $n = 128$.*
- *Curiously, Simpson's rule is the slowest to converge and requires $n = 256$. I do not know why.* **(But see below.)**
- **Use Romberg integration with inputs from the trapezoid rule.**
  1. The $R(j, 0)$ values are obtained from the trapezoid rule.
  2. **Compute $R(j, 1)$ from the $R(j, 0)$ numbers.**
  3. *If you have done your work correctly, the $R(j, 1)$ values should match the results from Simpson's rule (up to rounding).*
  4. **STOP. Do not compute the next level $R(j, 2)$.**

6.7.1 Why does Simpson's rule converge slower than midpoint or trapezoid?

- **This is not a homework question for you.**
- It is a homework assignment *for me*.
- The midpoint and trapezoid rules are $O(1/n^2)$ algorithms, and Simpson's rule is $O(1/n^4)$.
- The integrand in eq. (6.7.1) is smooth and infinitely differentiable. It has no kinks, etc.
- And yet Simpson's rule converges more slowly than the midpoint and trapezoid rules.
- I stated above that I do not know why this is.
- *But I* **should** *know.*
- In fact the Romberg integration results for $R(j,2)$, $R(j,3)$, etc. behave *very* poorly.
- That is why I told you to stop the Romberg integration at $R(j,1)$.
- *But why is this happening? Why does the Romberg integration behave poorly?*
- Here is my answer.
- It is more of a speculation really. You can critique it and offer your own analysis.
- Recall that Romberg integration derives originally from the extended trapezoid rule.
- Recall also (from the lectures) that the error terms for the trapezoid rule have the property

$$I = h\left[\frac{f(x_0)}{2} + f(x_1) + f(x_2) + \cdots + f(x_{n-1}) + \frac{f(x_n)}{2}\right] - c_2h^2 - c_4h^4 - c_6h^6 - \cdots \qquad (6.7.2)$$

- The coefficients c_k, $k = 2, 4, \dots$ are proportional to numbers called **Bernoulli numbers** B_k

$$\begin{aligned} c_2 &= \frac{B_2}{2!}(f'(b) - f'(a))\,, \\ c_4 &= \frac{B_4}{4!}(f'''(b) - f'''(a))\,, \\ &\vdots \\ c_k &= \frac{B_k}{k!}(f^{(k-1)}(b) - f^{(k-1)}(a)) \qquad\qquad (k = 2, 4, 6, \dots)\,. \end{aligned} \qquad (6.7.3)$$

- However, the Bernoulli numbers are just constants. They do not depend on the function $f(x)$.
- The explanation must lie in the derivatives $f'(a)$ and $f'(b)$, etc.
- Ignoring the factor of $1/\pi$, the integrand in eq. (6.7.1) is

$$f(\theta) = \cos(x\sin(\theta) - m\theta)\,. \qquad (6.7.4)$$

- Then f' and f'' mean $df/d\theta$, $d^2f/d\theta^2$, etc.
- Now make a list of derivatives:

$$\frac{df}{d\theta} = -(x\cos(\theta) - m)\,\sin(x\sin(\theta) - m\theta)\,, \tag{6.7.5a}$$

$$\frac{d^3f}{d\theta^3} = \quad (x\cos(\theta) - m)^3\,\sin(x\sin(\theta) - m\theta) + \cdots\,, \tag{6.7.5b}$$

$$\frac{d^5f}{d\theta^5} = -(x\cos(\theta) - m)^5\,\sin(x\sin(\theta) - m\theta) + \cdots\,. \tag{6.7.5c}$$

- There are additional terms in the derivatives which I have neglected.
- Note that $|\sin(x\sin(\theta) - m\theta)| \le 1$ and is not important.
- What *is* important, and I think is the key, is that $x = 200$, so (setting $\theta = 0$ or π)

$$\left|\frac{df}{d\theta}\right| = O(x) = O(10^2)\,, \tag{6.7.6a}$$

$$\left|\frac{d^3f}{d\theta^3}\right| = O(x^3) = O(10^6)\,, \tag{6.7.6b}$$

$$\left|\frac{d^5f}{d\theta^5}\right| = O(x^5) = O(10^{10})\,. \tag{6.7.6c}$$

- *These are enormous values.*
- Hence, *I think*, although the remainder term of the trapezoid rule adds up overall to a small total (we know this is true numerically), the individual error terms *grow larger before they eventually become smaller* (because of the factorial denominators).
- Hence, *I think*, at each step of the Romberg integration, we cancel one error term of the series in eq. (6.7.2), ***and the next term is larger in magnitude.***
- Hence the cancellations of the Romberg integration (including Simpson's rule) actually make things worse before they will (eventually) get better.
- ***Why not assign you a problem with $|x| \lesssim 1$ for example $x = 1$?***
- The answer is simple: *because the answer converges too rapidly, after $n \le 10$ steps.*
- Then it would be impossible to give you practice with the extended trapezoid rule and Romberg integration.
- **Try computing $J(x)$ using eq. (6.7.1) with $x = 1$. You may obtain convergence to 4 decimal places after only $n \simeq 6$.**
- ***Why not choose a different function?***
- Yes, I could do that. I could dream up some meaningless function.

- It would produce a boring homework assignment.
- Bessel functions are important functions of mathematical physics.
- They have important practical applications.
- I try to assign you problems that have some connection to my career as a scientist or from the financial industry.
- But it does have side effects.
- The homework assignments can get weird.
- Then again, that is part of what makes me different from the rest.

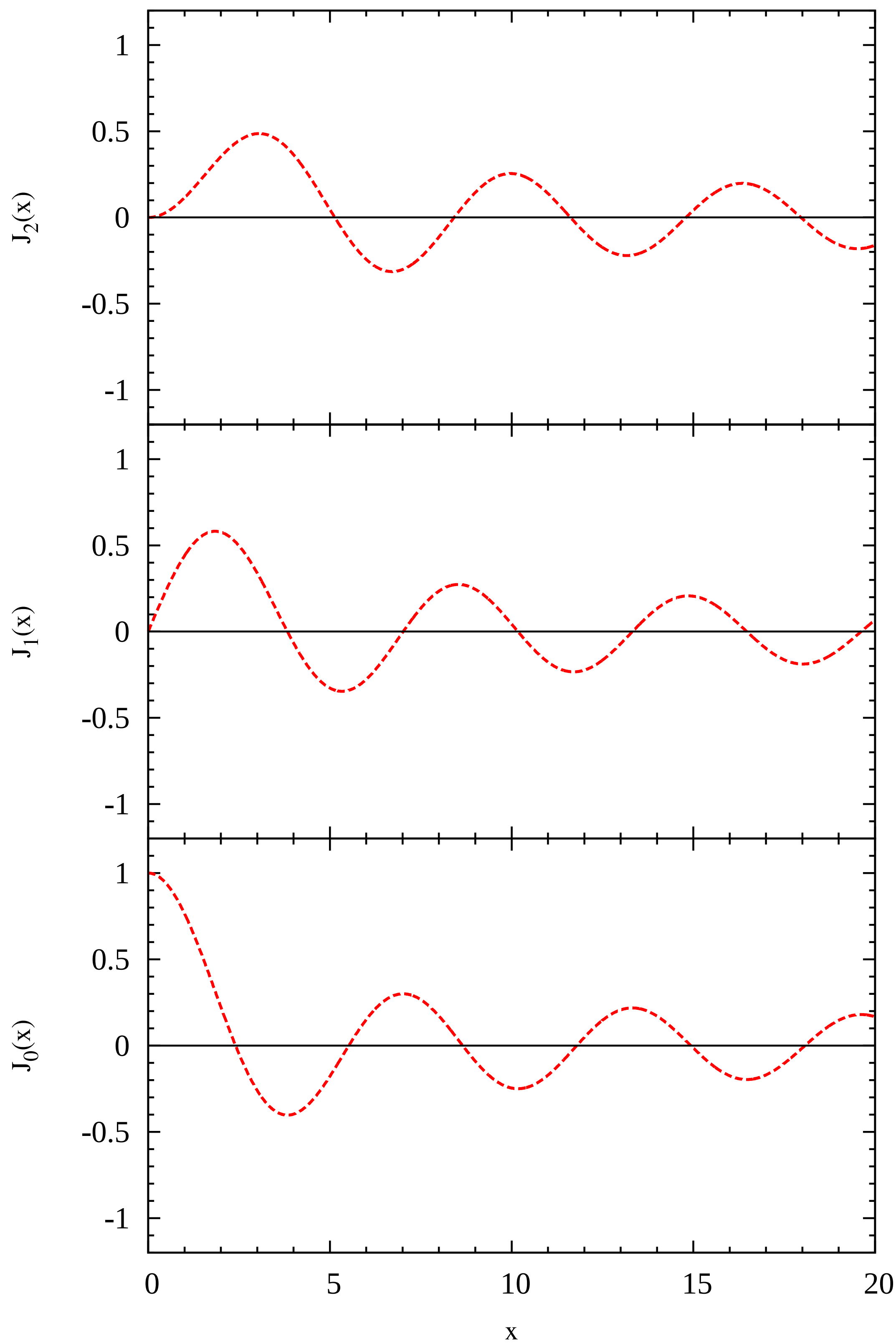

Figure 2: Plots of the Bessel functions $J_0(x)$, $J_1(x)$, $J_2(x)$ for $0 \leq x \leq 20$.