Lecture 5: Numerical integration

Discretizing the integral

In this lecture we will derive methods of computing integrals of functions that cannot be solved analytically. A typical function that cannot be solved analytically is the error function,

\[
\text{Erf}(y) = \frac{2}{\sqrt{\pi}} \int_0^y e^{-x^2} \, dx. \tag{1}
\]

To leave the analysis in its most general form, we will consider an evaluation of the integral

\[
\int_a^b f(x) \, dx. \tag{2}
\]

This integral is evaluated numerically by splitting up the domain \([a, b]\) into \(N\) equally spaced intervals as shown in Figure 1. Because we assume that the intervals are constant, then the interval width is given by

\[
h = \Delta x = x_{i+1} - x_i. \tag{3}
\]

Figure 1: Discretization of a function \(f(x)\) into \(N = 8\) equally spaced subintervals over \([a, b]\).

The idea behind the numerical integration formulas is to approximate the integral in each subinterval and add up the \(N\) approximate integrals to obtain the integral over \([a, b]\).
Trapezoidal rule

The Trapezoidal rule approximates the function within each subinterval using the first term in the Taylor series expansion about \( x_i \), such that, in the range \([x_i, x_{i+1}]\),

\[
f(x) = f_i + (x - x_i)f_i' + \frac{1}{2}(x - x_i)^2 f_i'' + \mathcal{O}((x - x_i)^3). \tag{4}
\]

Using this approximation, we can evaluate the integral over \([x_i, x_{i+1}]\) with

\[
\int_{x_i}^{x_{i+1}} f(x) \, dx = \int_{x_i}^{x_{i+1}} f_i + (x - x_i)f_i' + \frac{1}{2}(x - x_i)^2 f_i'' \, dx, \tag{5}
\]

where we have omitted the truncation error term since the last term will end up being the error term in the analysis. Making a change of variables such that

\[
s = \frac{x - x_i}{x_{i+1} - x_i} = \frac{x - x_i}{h}, \tag{6}
\]

we have

\[
\int_{x_i}^{x_{i+1}} f(x) \, dx = h \int_0^1 f_i + hs f_i' + \frac{1}{2}h^2 s^2 f_i'' \, ds, \]

\[
= hs f_i + \frac{1}{2}h^2 s^2 f_i' + \frac{1}{6}h^3 s^3 f_i'' \bigg|_0^1, \]

\[
= hf_i + \frac{1}{2}h^2 f_i' + \frac{1}{6}h^3 f_i''.
\]

Substituting in an approximation for the first derivative

\[
f_i' = \frac{f_{i+1} - f_i}{h} - \frac{h}{2} f_i'', \tag{7}
\]

we have

\[
\int_{x_i}^{x_{i+1}} f(x) \, dx = hf_i + \frac{1}{2}h^2 \left( \frac{f_{i+1} - f_i}{h} - \frac{h}{2} f_i'' \right) + \frac{1}{6}h^3 f_i'', \]

\[
= \frac{1}{2}h (f_i + f_{i+1}) - \frac{1}{12}h^3 f_i''. \tag{8}
\]

Which shows that the Trapezoidal rule approximates the integral of the function over the subinterval \([x_i, x_{i+1}]\) as the area of the trapezoid created by the function values at \( f_i \) and \( f_{i+1} \), as shown in Figure 2.

The integral over \([a, b]\) is evaluated by taking the sum of the approximate integrals evaluated in each subinterval as

\[
\int_a^b f(x) \, dx = \sum_{i=0}^{N-1} \int_{x_i}^{x_{i+1}} f(x) \, dx, \]

\[
= \sum_{i=0}^{N-1} \left[ \frac{1}{2}h (f_i + f_{i+1}) - \frac{1}{12}h^3 f_i'' \right], \]

\[
= \frac{1}{2}h (f_0 + 2f_1 + 2f_2 + \ldots + 2f_{N-2} + 2f_{N-1} + f_N) - \frac{h^3}{12} \sum_{i=0}^{N-1} f_i''.
\]
Figure 2: Depiction of how the trapezoidal rule approximates the integral on the subinterval \([x_i, x_{i+1}]\).

The error term is given by

\[
\text{Error} = -\frac{h^3}{12} \left( f''_0 + f''_1 + f''_2 + \ldots + f''_{N-1} \right),
\]

\[
= -\frac{Nh^3}{12} \left( \frac{f''_0 + f''_1 + f''_2 + \ldots + f''_{N-1}}{N} \right).
\]

If the mean value of \(f''_i\) is given by

\[
\left( \frac{f''_0 + f''_1 + f''_2 + \ldots + f''_{N-1}}{N} \right),
\]

then we know that it must lie within the bounds of \(f''(x)\), and hence it can be represented as \(f''(\xi)\) for some \(\xi\) such that

\[
f''(\xi) = \left( \frac{f''_0 + f''_1 + f''_2 + \ldots + f''_{N-1}}{N} \right).
\]

Therefore, since \(Nh = (b - a)\), the error becomes

\[
\text{Error} = -\frac{h^2}{12} (b - a) f''(\xi) = O(h^2),
\]

which shows that the trapezoidal rule is second order accurate.

**Simpson’s rules**

**Simpson’s 1/3 rule**

Simpson’s 1/3 rule approximates the function within the interval \([x_i, x_{i+2}]\) as a quadratic, as shown in Figure 3. This is done by writing the Taylor series expansion of \(f(x)\) about
Figure 3: Depiction of how the Simpson’s 1/3 rule approximates the function \( f(x) \) with a quadratic through \( x_i, x_{i+1}, \) and \( x_{i+2} \).

\[ x = x_{i+1} \] to obtain

\[
f(x) = f_{i+1} + (x - x_{i+1})f'_{i+1} + \frac{1}{2}(x - x_{i+1})^2 f''_{i+1} + \frac{1}{6}(x - x_{i+1})^3 f'''_{i+1} + \frac{1}{24}(x - x_{i+1})^4 f^{(iv)}_{i+1} + \mathcal{O} \left( (x - x_{i+1})^5 \right).
\]

The integral in the subinterval \([x_i, x_{i+2}]\) is then given by

\[
\int_{x_i}^{x_{i+2}} f(x) \, dx = \int_{x_i}^{x_{i+2}} f_{i+1} + (x - x_{i+1})f'_{i+1} + \frac{1}{2}(x - x_{i+1})^2 f''_{i+1} + \frac{1}{6}(x - x_{i+1})^3 f'''_{i+1} + \frac{1}{24}(x - x_{i+1})^4 f^{(iv)}_{i+1} \, dx,
\]

where the truncation error has been left off since the last term will end up being the error. Making a change of variables such that

\[
s = \frac{2(x - x_{i+1})}{x_{i+2} - x_i} = \frac{x - x_{i+1}}{h},
\]

we have

\[
\int_{x_i}^{x_{i+2}} f(x) \, dx = h \int_{-1}^{+1} f_{i+1} + h s f'_{i+1} + \frac{1}{2} h^2 s^2 f''_{i+1} + \frac{1}{6} h^3 s^3 f'''_{i+1} + \frac{1}{24} h^4 s^4 f^{(iv)}_{i+1} \, ds,
\]

which becomes

\[
\int_{x_i}^{x_{i+2}} f(x) \, dx = h s f_{i+1} + \frac{1}{2} h^2 s^2 f'_{i+1} + \frac{1}{6} h^3 s^3 f''_{i+1} + \frac{1}{24} h^4 s^4 f'''_{i+1} + \frac{1}{120} h^5 s^5 f^{(iv)}_{i+1} + \bigg|_{-1}^{+1},
\]

\[
= 2 h f_{i+1} + \frac{1}{3} h^3 f''_{i+1} + \frac{1}{60} h^5 f^{(iv)}_{i+1}.
\]
Using the second order accurate approximation to the second derivative

\[
\frac{f''_{i+1}}{h^2} = \frac{f_i - 2f_{i+1} + f_{i+2}}{h^2} - \frac{h^2}{12} f^{(iv)}_{i+1},
\]

the integral becomes

\[
\int_{x_i}^{x_{i+2}} f(x) \, dx = 2hf_{i+1} + \frac{1}{3} h^3 \left( \frac{f_i - 2f_{i+1} + f_{i+2}}{h^2} - \frac{h^2}{12} f^{(iv)}_{i+1} \right) + \frac{1}{60} h^5 f^{(iv)}_{i+1}.
\]

(14)

The integral over \([a, b]\) is taken by taking the sum of the approximate integrals, as in

\[
\int_a^b f(x) \, dx = \sum_{i=0}^{N/2} \int_{x_i}^{x_{i+2}} f(x) \, dx,
\]

\[
= \sum_{i=0}^{N/2} \left[ \frac{1}{3} h \left( f_i + 4f_{i+1} + f_{i+2} \right) - \frac{1}{90} h^5 f^{(iv)}_{i+1} \right].
\]

The sum is given by

\[
\frac{1}{3} h \left( f_0 + 4f_1 + f_2 + 4f_3 + f_4 + 4f_5 + f_6 + \ldots + f_{N-6} + 4f_{N-5} + f_{N-4} + 4f_{N-3} + f_{N-2} + 4f_{N-1} + f_N \right),
\]

which becomes

\[
\int_a^b f(x) \, dx = \frac{1}{3} \left( f_0 + 4f_1 + 2f_2 + 4f_3 + \ldots + 4f_{N-3} + 2f_{N-2} + 4f_{N-1} + f_N \right)
\]

\[
- \frac{1}{90} h^5 \sum_{i=0}^{N/2} f^{(iv)}_{i+1}.
\]

The error term is given by

\[
\text{Error} = -\frac{1}{90} h^5 \sum_{i=0}^{N/2} f^{(iv)}_{i+1},
\]

(16)

which, using the same arguments as those for the Trapezoidal rule, becomes

\[
\text{Error} = -\frac{1}{180} (b-a) h^4 f^{(iv)}(\xi) = O \left( h^4 \right),
\]

(17)

which shows that Simpson’s 1/3 rule is fourth order accurate.
Simpson’s 3/8 rule

Simpson’s 3/8 rule approximates the function within the subinterval \([x_i, x_{i+3}]\) using a quartic. The Taylor series expansion is performed about \(x_{i+3/2}\) to obtain

\[
f(x) = f_{i+3/2} + (x - x_{i+3/2})f'_{i+3/2} + \frac{1}{2}(x - x_{i+3/2})^2f''_{i+3/2} + \frac{1}{6}(x - x_{i+3/2})^3f'''_{i+3/2} \\
+ \frac{1}{24}(x - x_{i+3/2})^4f^{(iv)}_{i+3/2} + \mathcal{O}\left((x - x_{i+3/2})^5\right).
\]

Integrating this function in a similar manner to that used for the 1/3 rule yields

\[
\int_a^b f(x) \, dx = \frac{3}{8}h\left(f_0 + 3f_1 + 3f_2 + 2f_3 + 3f_4 + 3f_5 + \ldots \right) \\
+ 2f_{N-3} + 3f_{N-2} + 3f_{N-1} + f_N) \\
- \frac{1}{80}(b - a)h^4f^{(iv)}(\xi).
\]

Summary of integration formulas and pseudocodes

Trapezoidal rule

\[
\int_a^b f(x) \, dx = \frac{1}{2}h\left(f_0 + 2f_1 + 2f_2 + \ldots + 2f_{N-2} + 2f_{N-1} + f_N\right) + \text{Error}
\]
\[
\text{Error} = -\frac{1}{12}(b - a)h^2f''(\xi) = \mathcal{O}\left(h^2\right)
\]

1. If \(f_i\) and \(h\) are already known discretely on an equispaced grid with \(N + 1\) points, then proceed to step 2.

   Otherwise, choose interval \([a, b]\) and set \(h = (b - a)/N\).
   for \(i = 1\) to \(N + 1\)
   Set \(x_i = a + h(i - 1)\)
   Set \(f_i = f(x_i)\)
   end

2. Set \(I = 0\)
   for \(i = 2\) to \(N\)
   Set \(I = I + hf_i\)
   end
   Set \(I = I + \frac{1}{2}h(f_1 + f_{N+1})\)

3. The integral is given by \(I\).
Simpson’s 1/3 rule (N divisible by 2)

\[
\int_a^b f(x) \, dx = \frac{1}{3} (f_0 + 4f_1 + 2f_2 + 4f_3 + \ldots + 4f_{N-3} + 2f_{N-2} + 4f_{N-1} + f_N) + \text{Error}
\]

\[
\text{Error} = -\frac{1}{180} (b - a) h^4 f^{(iv)}(\xi) = O(h^4)
\]

1. If \( f_i \) and \( h \) are already known discretely on an equispaced grid with \( N + 1 \) points, where \( N \) is even, then proceed to step 2.

2. Set \( I = 0 \)

   for \( i = 1 \) to \( \frac{N}{2} \)

   Set \( I = I + \frac{1}{3} hf_{2i} \)

   end

   for \( i = 1 \) to \( \frac{N}{2} - 1 \)

   Set \( I = I + \frac{2}{3} hf_{2i+1} \)

   end

   Set \( I = I + \frac{1}{3} h(f_1 + f_{N+1}) \)

3. The integral is given by \( I \).
Simpson’s 3/8 rule (N divisible by 3)

\[
\int_a^b f(x) \, dx = \frac{3}{8} h (f_0 + 3f_1 + 3f_2 + 2f_3 + 3f_4 + 3f_5 + \ldots \\
+ 2f_{N-3} + 3f_{N-2} + 3f_{N-1} + f_N) \\
+ \text{Error}
\]

\[
\text{Error} = -\frac{1}{80} (b-a) h^4 f^{(iv)}(\xi).
\]

1. If \( f_i \) and \( h \) are already known discretely on an equispaced grid with \( N + 1 \) points, where \( N \) is divisible by 3, then proceed to step 2.
   Otherwise, choose interval \([a, b]\) and set \( h = (b - a)/N \), with \( N \) divisible by 3.
   for \( i = 1 \) to \( N + 1 \)
   \>
   Set \( x_i = a + h(i - 1) \)
   \>
   Set \( f_i = f(x_i) \)
   \>
   end

2. Set \( I = 0 \)
   for \( i = 2 \) to \( N \)
   \>
   Set \( I = I + \frac{3}{8} h f_i \)
   \>
   end
   for \( i = 1 \) to \( \frac{N}{3} - 1 \)
   \>
   Set \( I = I - \frac{3}{8} h f_{3i+1} \)
   \>
   end
   \>
   Set \( I = I + \frac{3}{8} h (f_1 + f_{N+1}) \)

3. The integral is given by \( I \).