

Lecture 11 - A

§5.1, 5.3 Numerical Integration

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Goals

We will answer these questions:

- What is numerical integration, and why do we care?
- What are Riemann sums and how are they insufficient for numerical integration?
- What is Trapezoid method and how accurate is it?
- What is Simpson's rule and how accurate is it?
- What are Newton-Cotes rules and how are they related to splines?



Why Numerical Integration?



What is Numerical Integration?

Definition: Numerical Integration

Numerical integration refers to a method which approximates the integral

$$\int_{\Omega} f(X) dX.$$

- For this class, we will only cover 1D integrals

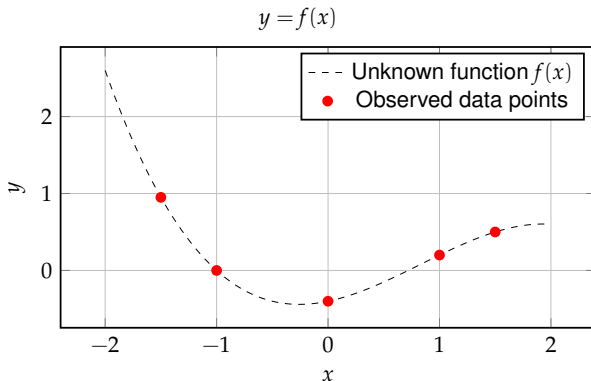
$$\int_a^b f(x) dx$$

- All 1D numerical integration discussed do carry over to higher dimensions



Motivation for Numerical Integration

- Suppose you observe data points (x_i, y_i) that come from an unknown function



- We can approximate the integral

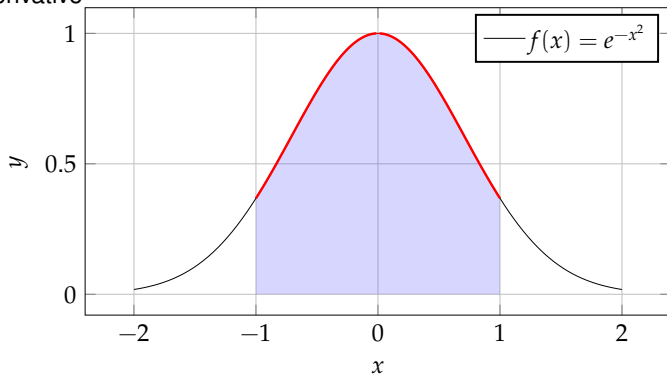
$$\int_a^b f(x) dx$$

even when $f(x)$ is unknown



Motivation for Numerical Integration

- Suppose you did know $f(x)$ but you had no way of finding the antiderivative



- We can approximate the value of

$$\int_a^b f(x) dx$$

even when the anti-derivative does not exist in closed form.



More Examples

There are many more examples:

- $\int e^{-x^3} dx$
- $\int \sin(x^2) dx$
- $\int e^{\sin x} dx$
- $\int \sqrt{1+x^3} dx$
- $\int \frac{\tan x}{x} dx$
- $\int \ln \ln x dx$
- $\int x^x dx$

Key Idea

There's no closed-form solution but we still want to evaluate them.



Why?

Integrals have meaningful information:

- Total distance traveled
- Total work done
- Total mass
- Center of mass
- Total revenue
- Total anything
- $\vdots$
- Differential equations



Riemann Sum



Riemann Sums

Definitions

Definition: Partition

- The **partition** of $[a, b]$ is a set of $n + 1$ distinct and ordered points

$$P = \{x_0 = a, x_1, x_2, \dots, x_i, x_{i+1}, \dots, x_n = b\}$$

- The **subinterval** $[x_i, x_{i+1}]$ has a width of $\Delta x_i = x_{i+1} - x_i$.
- The **sample point** $x_i^* \in [x_i, x_{i+1}]$ acts as a representative of the subinterval.

Definition: Riemann Sum

- Let $y = f(x)$ be defined over $[a, b]$ that is divided into a partition P .
- Then the **Riemann sum** of $f(x)$ over the partition P is defined to be

$$R(f, P) = \sum_{i=0}^{n-1} f(x_i^*) \Delta x_i$$

Upper and Lower Riemann Sums

Let P be a partition of $[a, b]$.

Definition: Upper and Lower Sums

- Let m_i be the **lower bound** of f on $[x_i, x_{i+1}]$
- Let M_i be the **upper bound** of f on $[x_i, x_{i+1}]$
- The **Lower Sum** of f on P is

$$L(f; P) = \sum_{i=0}^{n-1} m_i \Delta x_i$$

- The **Upper Sum** of f on P is

$$U(f; P) = \sum_{i=0}^{n-1} M_i \Delta x_i$$



The definition of an Integral

- In most cases, the lower and upper sums are equal in the limit

$$\lim_{n \rightarrow \infty} L(f; P) = \int_a^b f(x) dx = \lim_{n \rightarrow \infty} U(f; P)$$

Definition: The Integral

The integral $\int_a^b f(x) dx$ is the limit

$$\lim_{n \rightarrow \infty} L(f; P)$$

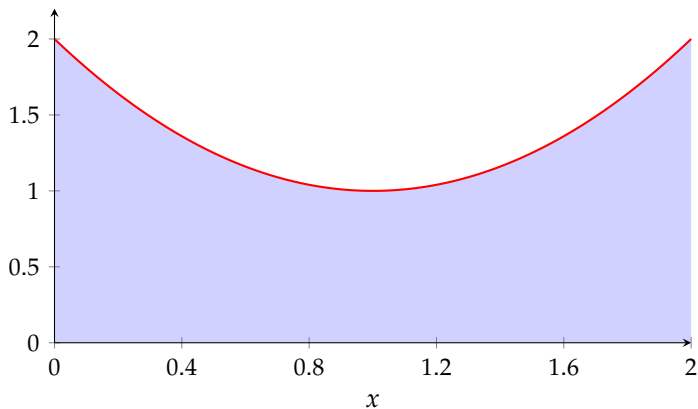
and

$$\lim_{n \rightarrow \infty} U(f; P)$$

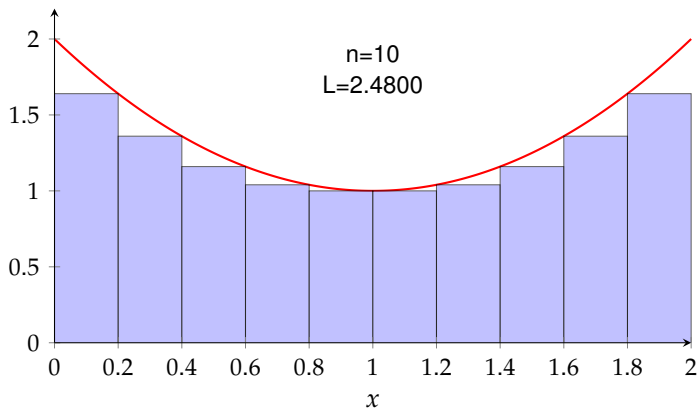
when they both agree.



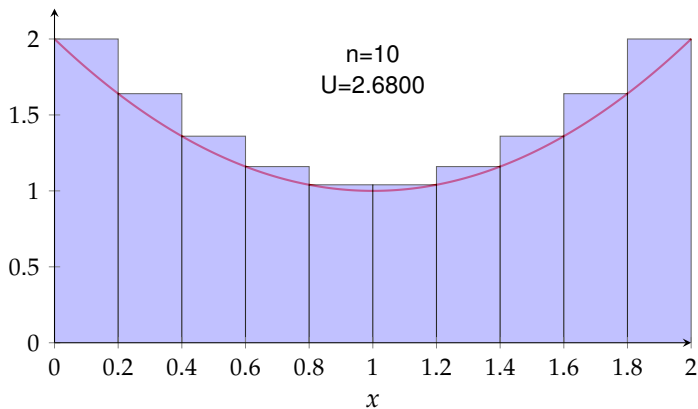
Graphically: Integral



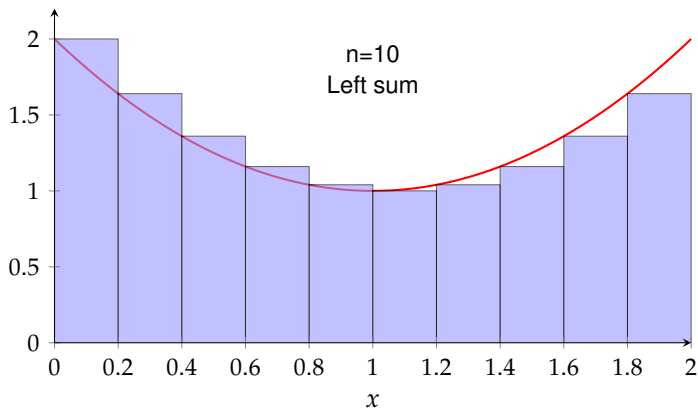
Graphically: Lower sum



Graphically: Upper sum



Graphically: Left-endpoint Riemann sum



Other Riemann Sums

There are specific names for sums depending on how we select the sample point

$$R(f, P) = \sum_{i=0}^{n-1} f(\underbrace{x_i^*}_{\text{sample point}}) \Delta x_i$$

- $x_i^* = \max_{x \in [x_i, x_{i+1}]} f(x) \implies$ upper sum
- $x_i^* = \min_{x \in [x_i, x_{i+1}]} f(x) \implies$ lower sum
- $x_i^* = x_i \implies$ **Left Riemann Sum**
- $x_i^* = x_{i+1} \implies$ **Right Riemann Sum**
- $x_i^* = \frac{x_{i+1} + x_i}{2} \implies$ **Midpoint rule**



Approximating the Integral

- In general, we have

$$\lim_{n \rightarrow \infty} R(f, P) = \lim_{n \rightarrow \infty} \sum_{i=0}^{n-1} f(x_i^*) \Delta x_i = \int_a^b f(x) dx$$

- Thus, for a finite n we have

$$\sum_{i=0}^{n-1} f(x_i^*) \Delta x_i \approx \int_a^b f(x) dx$$



Method: Riemann Integration

- **Given:** Function $f(x)$ continuous on $[a, b]$, partition P , way of choosing sample point
 - **Output:** Approximation to $\int_a^b f(x) dx$
 - **Idea:** Approximate the integral with a finite sum of rectangles.
-
- The basic Riemann sums are
 - Upper sum
 - Lower sum
 - Right Riemann
 - Left Riemann
 - Middle Riemann
 - Middle is the best one out of the five
 - But we can do better



Overview

Understand why some algorithms are better than others.

Understand how to evaluate the algorithm performance.

Learn how to implement them.

List of algorithms:

- Trapezoid Rule
- Composite Trapezoid Rule
- Simpson's Rule
- Composite Simpson's Rule
- General Newton-Cotes Rules



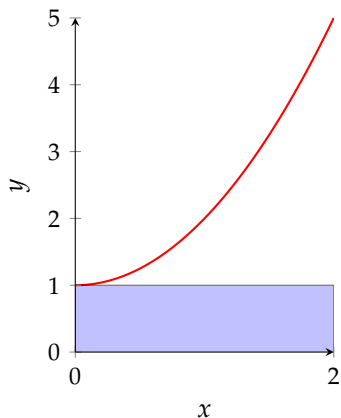
Trapezoid Rule



Improvement over Rectangles

Question

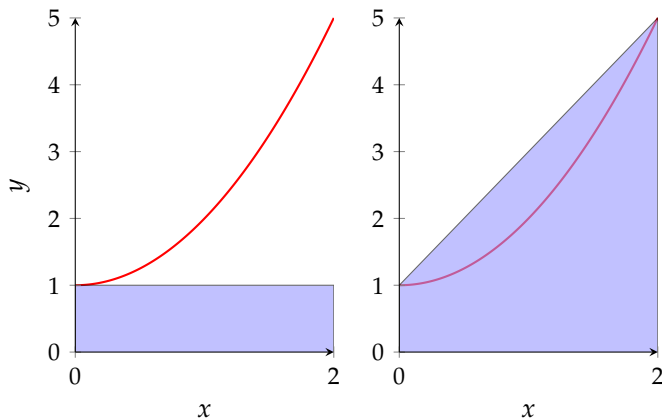
What's better than a rectangle?



Improvement over Rectangles

Question

What's better than a rectangle?



A trapezoid



Trapezoids > Rectangles

Goal: Approximate

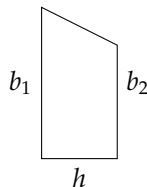
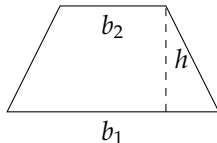
$$\int_a^b f(x) dx$$

Geometrically, the definite integral is related to the area under $f(x)$.

- Simple Idea: Riemann integration says:
Approximate the area under $f(x)$ with a sum of areas of rectangles.
- Better Idea: Trapezoidal rule says:
Approximate the area under $f(x)$ with a sum of areas of trapezoids.



Area of a Trapezoid



- These are both trapezoids
- The upright trapezoid is the one we care about

Area Formula

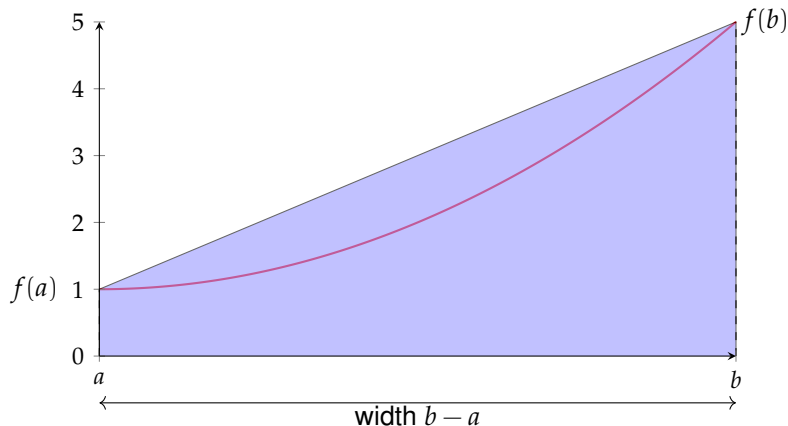
$$A = \frac{b_1 + b_2}{2}h$$



Basic Trapezoid

Formula for the Basic Trapezoid Rule

$$\int_a^b f(x) dx \approx \frac{f(a) + f(b)}{2} (b - a)$$



Example

Example

Approximate the integral

$$I = \int_1^2 (x^2 + 1) dx$$

using the basic trapezoid rule.

- The formula is

$$\int_a^b f(x) dx \approx \frac{f(a) + f(b)}{2} (b - a),$$

where $a = 1$, $b = 2$, and $f(x) = x^2 + 1$

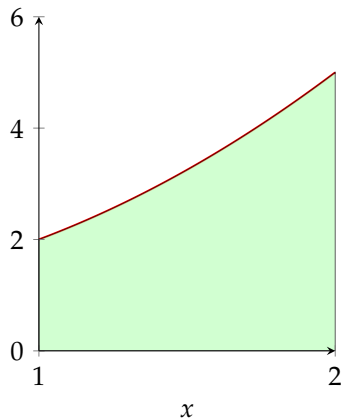
- We get

$$\int_1^2 (x^2 + 1) dx \approx \frac{(2^2 + 1) + (1^2 + 1)}{2} (2 - 1) = \frac{5 + 2}{2} = 3.5$$

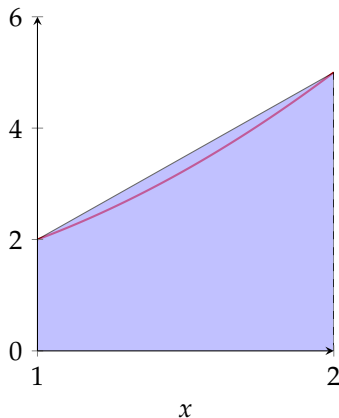


Example Visualization

Exact Integral



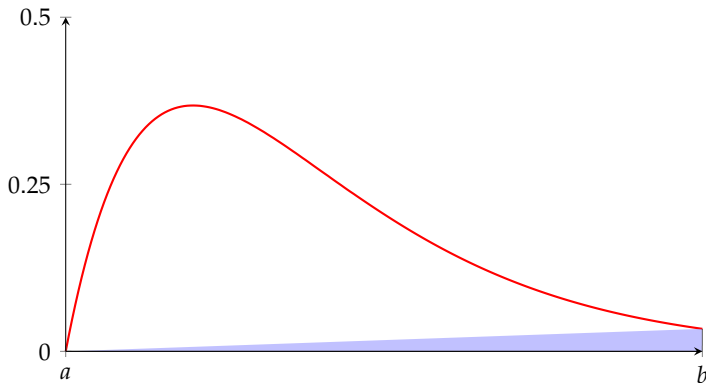
Trapezoid Approximation



- Left: $I = \frac{10}{3} \approx 3.3333$
- Right: $I \approx \frac{7}{2} = 3.5$



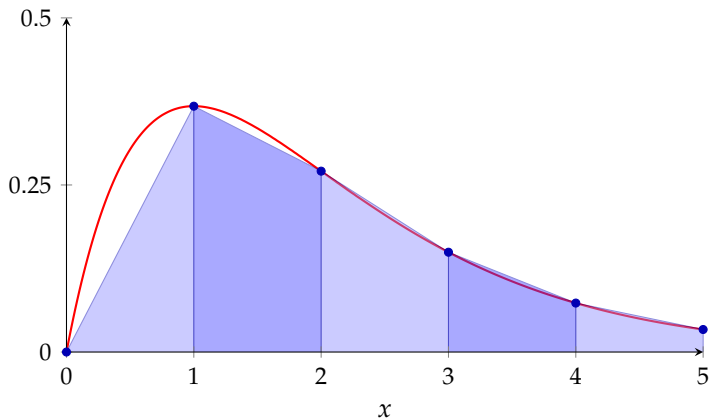
One Trapezoid is Not Enough



Question

How do you resolve this issue?

Use Multiple Trapezoids



Add up multiple trapezoids.

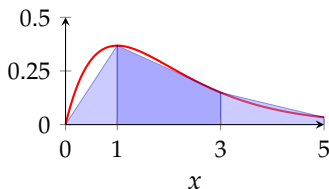


General Composite Trapezoid

- 1 Consider a partition $P = \{x_0 = a, x_1, x_2, \dots, x_n = b\}$ of $[a, b]$.
- 2 In each interval $[x_i, x_{i+1}]$ of width h_i , use the basic Trapezoid:

$$\int_a^b f(x) dx \approx \sum_{i=0}^{n-1} \frac{f(x_i) + f(x_{i+1})}{2} h_i$$

- 3 **Composite Trapezoid** adds the area of n trapezoids



The trapezoids do not have to have equal width.



Question

Suppose each interval width h_i is the same size. How does that affect the formula?

$$\begin{aligned}\int_a^b f(x) dx &\approx \sum_{i=0}^{n-1} \frac{f(x_i) + f(x_{i+1})}{2} h_i \\ &= \sum_{i=0}^{n-1} \frac{f(x_i) + f(x_{i+1})}{2} h \\ &= \frac{h}{2} \sum_{i=0}^{n-1} f(x_i) + f(x_{i+1}) \\ &= \frac{h}{2} (f(x_0) + 2f(x_1) + 2f(x_2) + \cdots + 2f(x_{n-1}) + f(x_n))\end{aligned}$$

$f(x_i)$ terms for interior nodes are weighted by 2



Composite Trapezoid with constant h

Formula

- The uniform composite trapezoid formula:

$$\begin{aligned}\int_a^b f(x) dx &\approx \frac{h}{2} (f(x_0) + 2f(x_1) + 2f(x_2) + \cdots + 2f(x_{n-1}) + f(x_n)) \\ &= h \left(\frac{1}{2}f(x_0) + f(x_1) + f(x_2) + \cdots + f(x_{n-1}) + \frac{1}{2}f(x_n) \right)\end{aligned}$$

- You can save on FLOPs by distributing $\frac{1}{2}$

```
1 h = (b - a)/n
2 sum = (f(a) + f(b))/2 % first and last heights
3 for i = 1 to n - 1
4     sum = sum + f(x_i) % interior hieghts
5 end
6 sum = sum * h % scale by h
```

Cost

- Let n = the number of subintervals
- Let FLOP be any operation
- Let FEVAL be any evaluation of $f(x)$

```
1  $h = (b - a)/n$  % 2 FLOPs
2  $sum = (f(a) + f(b))/2$  % 2 FEVAL + 2 FLOPs
3 for  $i = 1$  to  $n - 1$ 
4      $sum = sum + f(x_i)$  % 1 FEVAL + 1 FLOP
5 end
6  $sum = sum \cdot h$  % 1 FLOP
```

- Total: $n + 4$ FLOPs and $n + 1$ FEVALs



Uniform Composite Trapezoid Formula

Method: Uniform Composite Trapezoidal Method

- **Given:** Continuous function $f(x)$, interval $[a, b]$, number of subintervals n
- **Output:** Approximation to $\int_a^b f(x) dx$
- **Idea:** Using trapezoids instead of rectangles leads to a better approximation.

- Let $h = \frac{b-a}{n}$ and $x_i = a + ih$ for $i = 0$ to n
- We have an efficient formula

$$\int_a^b f(x) dx \approx h \left(\frac{1}{2}f(x_0) + f(x_1) + f(x_2) + \cdots + f(x_{n-1}) + \frac{1}{2}f(x_n) \right)$$

- Constant h simplifies the formula and saves FLOPs



Composite Trapezoid

Example

Approximate the integral

$$\int_0^4 \sqrt{x} dx$$

using composite trapezoidal method with $n = 2$ subintervals.

$$\begin{aligned}\int_0^4 \sqrt{x} dx &\approx T_1 + T_2 \\ &= h \frac{b_1 + b_2}{2} + h \frac{b_2 + b_3}{2} \\ &= (2) \frac{f(0) + f(2)}{2} + (2) \frac{f(2) + f(4)}{2} \\ &= \sqrt{0} + \sqrt{2} + \sqrt{2} + \sqrt{4} \\ &= 2\sqrt{2} + 2 \approx 4.28\end{aligned}$$



Example: trap_int_test.m

- Test composite trapezoid for

$$\int_0^5 xe^{-x}$$

- The exact solution is known: $\int_0^5 xe^{-x} = 1 - 6e^{-5}$

What is the order of accuracy?

- Find h^p numerically with the test

$$p \approx \frac{\log(err^{(k)} / err^{(k-1)})}{\log(h^{(k)} / h^{(k-1)})}$$

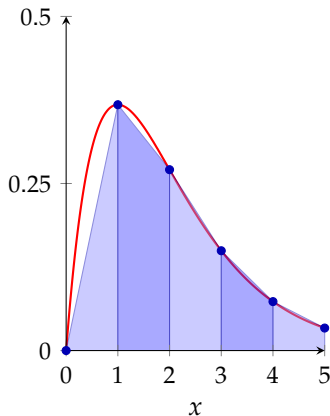
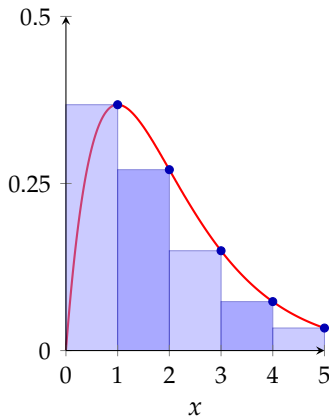
- Run trap_int_test.m



Summary



Trapezoids are Better than Rectangles



- The Riemann sum is a very basic way to approximate integrals
- Adding up trapezoids leads to a better approximation



- The formula is

$$\int_a^b f(x) dx \approx h \left(\frac{1}{2}f(x_0) + f(x_1) + f(x_2) + \cdots + f(x_{n-1}) + \frac{1}{2}f(x_n) \right)$$

- The experimental result is

$$E = \mathcal{O}(h^2)$$

- The trapezoid method has **quadratic accuracy**



Moving Forward

- Mathematical proof that $E = \mathcal{O}(h^2)$
- Simpson's Method - improvement over trapezoid method
- Newton-Cotes methods - a generalization of numerical integration

