



Limits Discretizations + Rectangles

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OUTLINE

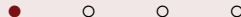
1. Riemann Integration Revisited
2. Illustrations and Numerical Experiments
3. Box, Midpoint, Trapezoidal, and Simpson Rules
4. Outlook on Advanced Numerical Integration

An implementation of the numerical examples can be found in the accompanying Python notebook `sinsm2023.ipynb`*

*Link: <https://github.com/grperalta/upbsinsm/tree/main/2023>



Riemann Integration Revisited



PARTITIONS

Let $a, b \in \mathbb{R}$ and $a < b$. A finite collection of points $\{x_k\}_{k=0}^n$ is called a **partition** of the closed interval

$$[a, b] := \{x \in \mathbb{R} : a \leq x \leq b\}$$

if the following inequalities hold:

$$a = x_0 < x_1 < x_2 < \cdots < x_{n-1} < x_n = b.$$

The **norm** of a partition is the largest length of the subinterval induced by it, i.e.

$$\|\{x_k\}_{k=0}^n\| = \max_{k=1, \dots, n} (x_k - x_{k-1}).$$

Example. The collection $P := \{0, \frac{1}{3}, \frac{1}{2}, 1\}$ is a partition of $[0, 1]$ with norm

$$\|P\| = \max \left\{ \frac{1}{3}, \frac{1}{6}, \frac{1}{2} \right\} = \frac{1}{2}.$$



BOUNDED FUNCTIONS

A function $f : [a, b] \rightarrow \mathbb{R}$ is said to be **bounded** if there exist $l, u \in \mathbb{R}$ such that

$$l \leq f(x) \leq u \quad \text{for all } x \in [a, b].$$

The numbers l and u are called **lower bound** and **upper bound** of f , respectively

Example. The function $f : [0, 2] \rightarrow \mathbb{R}$ given by

$$f(x) = \begin{cases} \frac{1}{4} & \text{if } 0 \leq x \leq \frac{1}{2}, \\ \frac{1}{\sqrt{x}} & \text{if } \frac{1}{2} < x \leq 2, \end{cases}$$

is bounded since we can take $l = \frac{1}{4}$ and $u = \sqrt{2}$.

Example. Every continuous function on a closed interval is bounded.

Extreme Value Theorem: If $f : [a, b] \rightarrow \mathbb{R}$ is continuous, then there exist $y, z \in [a, b]$ such that $f(y) \leq f(x) \leq f(z)$ for every $x \in [a, b]$.



RIEMANN SUMS

Given a function $f : [a, b] \rightarrow \mathbb{R}$, a partition $\{x_k\}_{k=0}^n$ of $[a, b]$, and a collection of representative points $\{x_k^*\}_{k=1}^n$ with $x_k^* \in [x_{k-1}, x_k]$ for $k = 1, 2, \dots, n$, a sum of the form

$$\sum_{k=1}^n f(x_k^*)(x_k - x_{k-1})$$

is called a **Riemann Sum**.



RIEMANN INTEGRABLE FUNCTIONS

A bounded function $f : [a, b] \rightarrow \mathbb{R}$ is said to be **Riemann integrable** if the limit of Riemann sums as the norm of the partition vanishes exists, i.e. there exists a $I \in \mathbb{R}$ such that

$$\lim_{\|\{x_k\}_{k=0}^n\| \rightarrow 0} \sum_{k=1}^n f(x_k^*)(x_k - x_{k-1}) = I.$$

Equivalently, given $\varepsilon > 0$ there exists $\delta = \delta(\varepsilon) > 0$ such that for every partition $\{x_k\}_{k=0}^n$ of $[a, b]$ such that $\|\{x_k\}_{k=0}^n\| < \delta$ and every collection of representative points $\{x_k^*\}_{k=1}^n$ with $x_k^* \in [x_{k-1}, x_k]$ for $k = 1, 2, \dots, n$, we have

$$\left| \sum_{k=1}^n f(x_k^*)(x_k - x_{k-1}) - I \right| < \varepsilon.$$

The number I is called the **Riemann integral** of f and is denoted by

$$I := \int_a^b f(x) dx.$$



SOME REMARKS ON RIEMANN INTEGRABILITY

- There is at most one Riemann integral.
- A continuous function on a closed interval is Riemann integrable.

Proof Idea: *Apply Extreme Value Theorem and the fact that a continuous function on a bounded and closed interval is uniformly continuous.*

- The function $f : [0, 1] \rightarrow \mathbb{R}$ defined by $f(x) = 1$ if x is rational and $f(x) = 0$ if x is irrational is **not Riemann integrable** since for any partition of $\{x_k\}_{k=0}^n$ of $[a, b]$

$$\sum_{k=1}^n f(x_k^*)(x_k - x_{k-1}) = 1 \quad \text{if } x_k^* \text{ is rational,}$$
$$\sum_{k=1}^n f(x_k^*)(x_k - x_{k-1}) = 0 \quad \text{if } x_k^* \text{ is irrational.}$$

- $\|\{x_k\}_{k=0}^n\| \rightarrow 0$ versus passing $n \rightarrow \infty$ in $\{x_k\}_{k=0}^n$?



Illustrations and Numerical Experiments



AN ALGORITHM FOR COMPUTING SUMS

Given a list of numbers s_0, s_1, \dots, s_n , the sum $\sum_{k=0}^n s_k$ can be computed as follows:

Algorithm: Sum(s_0, s_1, \dots, s_n)

Input: Numbers s_0, s_1, \dots, s_n

Output: The sum $s_0 + s_1 + \dots + s_n$

```
1. s = 0 // initialize sum to 0
2. for k = 0, 1, ..., n do // loop over all terms
3.     s = s + sk // update value of sum
4. end for // end of the for loop
5. return s // return value of sum
```



AN ALGORITHM FOR COMPUTING RIEMANN SUMS

The following algorithm computes the Riemann sum

$$\sum_{k=1}^n f(x_k^*)(x_k - x_{k-1}) \quad (\text{RS})$$

using a random partition and random points as representatives:

Algorithm: RiemannSum(f , a , b , n)

Input: A function f , left endpoint a , right endpoint b , and n as the number of points in the partition

Output: The Riemann sum (RS)

1. select random points $x_0 < x_1 < \dots < x_n$ on $[a, b]$
2. set $x_0 = a$ and $x_n = b$
3. set $rs = 0$
4. for $k = 1, \dots, n$ do
5. select a random point x_k^* on $[x_{(k-1)}, x_k]$
6. $rs = rs + [f(x_k^*) \times (x_k - x_{(k-1)})]$
7. end for
8. return rs



RIEMANN SUMS WITH RANDOM PARTITIONS

Example 1. Calculate the Riemann sums for the function $f(x) = x^2$ for $0 \leq x \leq 1$ using random partitions $\{x_k\}_{k=0}^n$ and with the following type of representative points:

a. left endpoint

$$x_k^* = x_{k-1}$$

b. right endpoint

$$x_k^* = x_k$$

c. midpoint

$$x_k^* = (x_{k-1} + x_k)/2$$

d. random point

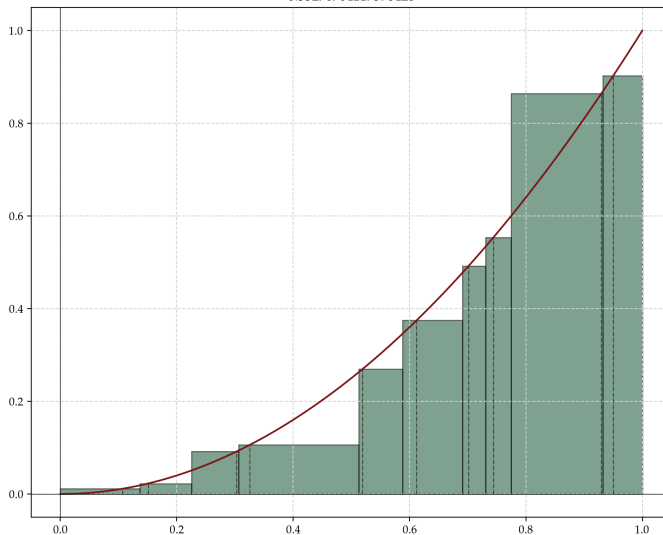
$$x_{k-1} \leq x_k^* \leq x_k$$

Use $n = 10^N$ for $N = 1, 2, 3, 4, 5, 6$.



A RIEMANN SUM WITH RANDOM PARTITION

Riemann Sum Using Random Partition with Random Points as Samples:
0.33290704119596426



RIEMANN SUMS WITH UNIFORM PARTITIONS

A partition $\{x_k\}_{k=0}^n$ of $[a, b]$ is called **uniform** if

$$x_k = a + kh \quad \text{for } k = 0, 1, \dots, n \quad \text{where } h = \frac{b-a}{n}$$

Specific versions of Riemann Sums:

- Left endpoints as representatives

$$\sum_{k=1}^n f(x_{k-1})(x_k - x_{k-1}) = h \sum_{k=1}^n f(a + (k-1)h) \quad (\text{RSUL})$$

- Right endpoints as representatives

$$\sum_{k=1}^n f(x_k)(x_k - x_{k-1}) = h \sum_{k=1}^n f(a + kh) \quad (\text{RSUR})$$

- Midpoints as representatives

$$\sum_{k=1}^n f\left(\frac{x_{k-1} + x_k}{2}\right)(x_k - x_{k-1}) = h \sum_{k=1}^n f\left(a + \frac{(2k-1)h}{2}\right) \quad (\text{RSUM})$$



AN ALGORITHM FOR COMPUTING RSUM

Algorithm: `RiemannSumUniformMid(f, a, b, n)`

Input: A function f , left endpoint a , right endpoint b , and n as the number of points in the partition

Output: The Riemann sum (RSUM)

```
1. set  $h = (b-a)/n$ 
1. set  $x = a - h/2$ 
3. set  $rs = 0$ 
4. for  $k = 1, \dots, n$  do
5.    $x = x + h$ 
6.    $rs = rs + f(x)$ 
7. end for
8. return  $h \times rs$ 
```



RIEMANN SUMS WITH UNIFORM PARTITIONS

Example 2. Repeat **Example 1** using uniform partitions.

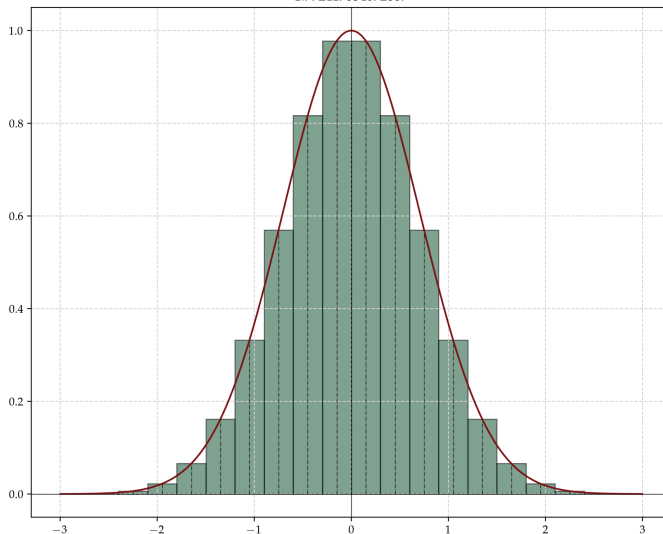
Example 3. Compute the Riemann sums for $f(x) = e^{-x^2}$ for $-3 \leq x \leq 3$ using uniform partitions and midpoints as representatives with $n = 10^N$ for $N = 1, 2, 3, 4, 5, 6$.



A RIEMANN SUM WITH UNIFORM PARTITION

Riemann Sum Using Uniform Partition with Midpoints as Samples:

1.772419834092869



Box, Midpoint, Trapezoidal, and Simpson Rules



BOX AND MIDPOINT RULES

For the rest of the lecture, we use a uniform partition $\{x_k\}_{k=0}^n$ of $[a, b]$ where

$$x_k = a + kh \quad \text{for } k = 0, 1, \dots, n \quad \text{where } h = \frac{b-a}{n}.$$

Specific versions of Riemann Sums:

- **Box Rule (Left Endpoint)**

$$h \sum_{k=1}^n f(x_{k-1})$$

- **Box Rule (Right Endpoint)**

$$h \sum_{k=1}^n f(x_k)$$

- **Midpoint Rule**

$$h \sum_{k=1}^n f\left(\frac{x_{k-1} + x_k}{2}\right)$$



QUADRATURE RULES

Let $f : [a, b] \rightarrow \mathbb{R}$ be continuous, $\{z_k\}_{k=0}^n$ be a partition of $[a, b]$, and $\{w_k\}_{k=0}^n$ be a finite sequence of real numbers. A formula of the form

$$\sum_{k=0}^n w_k f(z_k)$$

is called a **quadrature rule** for the integral $\int_a^b f(x) dx$.

The collections $\{z_k\}_{k=0}^n$ and $\{w_k\}_{k=0}^n$ are called **quadrature nodes** and **quadrature weights**, respectively.



BOX RULE (RIGHT ENDPOINT)

Example 4. Consider the function $f(x) = x^4 - 3x + 1$ for $-2 \leq x \leq 2$.

- a. Use the box rule with right endpoints to compute the Riemann sums (S_N) for $n = 2^N$ for $N = 0, 1, \dots, 15$.
- b. Plot the norms of partitions versus the Riemann sums in log scales.
- c. Denote the **numerical absolute errors** by $e_N := |S_N - S_{15}|$. Compute the following log error ratios:

$$\frac{\log(e_{N-1}/e_N)}{\log(2)} \quad \text{for } N = 1, 2, \dots, 14$$

Plot the norms of partitions versus the **log error ratios** in log scales. Discuss your observations.

- d. Repeat items **a**, **b**, and **c** using left endpoints and midpoints.



ORDER OF CONVERGENCE

Let $I(h)$ be an approximation of I where $h > 0$ is the norm of some partition and

$$e(h) := |I - I(h)|$$

be the absolute error. Suppose that for some constant $C > 0$ and $p > 0$ (**order of convergence**)

$$e(h) \approx Ch^p.$$

Let $\eta > 0$ be the norm of another partition so that $e(\eta) \approx C\eta^p$. Then,

$$\frac{e(h)}{e(\eta)} \approx \left(\frac{h}{\eta}\right)^p \quad \implies \quad p \approx \frac{\log(e(h)/e(\eta))}{\log(h/\eta)}.$$

If $\eta = h/2$ (**bisection**), then

$$p \approx \frac{\log(e(h)/e(h/2))}{\log(2)}.$$



LINEAR CONVERGENCE OF BOX RULES

Error with a single subinterval. By **Taylor's Theorem**, for each $x \in [a, b]$

$$f(x) = f(b) + f'(\xi)(x - b) \quad \text{for some } \xi = \xi(x) \in (a, b)$$

$$E[a, b] := \int_a^b f(x) dx - f(b)(b - a) = \int_a^b f'(\xi)(x - b) dx.$$

If $|f'(x)| \leq M_1$ for every $x \in [a, b]$, then

$$|E[a, b]| \leq \int_a^b M_1(x - b) dx = \frac{M_1}{2}(b - a)^2.$$

Cumulative errors for all subintervals. Write

$$\begin{aligned} I - I(h) &:= \int_a^b f(x) dx - h \sum_{k=1}^n f(x_k) \\ &= \sum_{k=1}^n \int_{x_{k-1}}^{x_k} f(x) dx - \sum_{k=1}^n f(x_k)(x_k - x_{k-1}) = \sum_{k=1}^n E[x_{k-1}, x_k] \end{aligned}$$

By the triangle inequality and $hn = b - a$, we have

$$e(h) \leq Ch \quad \text{where } C := \frac{M_1(b - a)}{2}.$$



QUADRATIC CONVERGENCE OF MIDPOINT RULE

Error with a single subinterval. Let $m = \frac{a+b}{2}$. For each $x \in [a, b]$

$$f(x) = f(m) + f'(\xi)(x - m) + \frac{1}{2}f''(\xi)(x - m)^2 \quad \text{for some } \xi = \xi(x) \in (a, b)$$

$$E[a, b] := \int_a^b f(x) dx - f(m)(b - a) = \frac{1}{2} \int_a^b f''(\xi)(x - m)^2 dx.$$

If $|f''(x)| \leq M_2$ for every $x \in [a, b]$, then

$$|E[a, b]| \leq \frac{1}{2} \int_a^b M_2(x - m)^2 dx = \frac{M_2}{24} (b - a)^3.$$

Cumulative errors for all subintervals. If $m_k = \frac{x_{k-1} + x_k}{2}$, then

$$I - I(h) := \int_a^b f(x) dx - h \sum_{k=1}^n f(m_k) = \sum_{k=1}^n E[x_{k-1}, x_k]$$

As before, this implies

$$e(h) \leq Ch^2 \quad \text{where } C := \frac{M_2(b - a)}{24}.$$



TRAPEZOIDAL RULE

Trapezoidal Rule on a single interval. Let $\ell : [a, b] \rightarrow \mathbb{R}$ be the linear function passing through the points $(a, f(a))$ and $(b, f(b))$, i.e.

$$\ell(x) = \frac{f(b) - f(a)}{b - a}(x - a) + f(a).$$

Then,

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

Composite Trapezoidal Rule. If $\{x_k\}_{k=0}^n$ is a uniform partition of $[a, b]$ with norm $h = (b - a)/n$, then

$$\begin{aligned} \int_a^b f(x) dx &= \sum_{k=1}^n \int_{x_{k-1}}^{x_k} f(x) dx \\ &\approx \sum_{k=1}^n \frac{x_k - x_{k-1}}{2} (f(x_k) + f(x_{k-1})) \\ &= h \left(\frac{1}{2}f(a) + \sum_{k=1}^{n-1} f(a + kh) + \frac{1}{2}f(b) \right). \end{aligned}$$

Example 5. Repeat **Example 4** using the composite trapezoidal rule.



QUADRATIC CONVERGENCE OF TRAPEZOIDAL RULE

Error with a single subinterval. Let $g(x) = f(x) - \ell(x)$. Then, $g(a) = g(b) = 0$. By **Rolle's Theorem**, there exists $\xi \in (a, b)$ such that $g'(\xi) = 0$.

$$\begin{aligned} E[a, b] &:= \int_a^b f(x) dx - \frac{b-a}{2}(f(a) + f(b)) \\ &= \int_a^b g(x) dx = \int_a^b \int_a^x \int_{\xi}^y g''(z) dz dy dx \end{aligned}$$

Note that $g'' = f''$. If $|f''(x)| \leq M_2$ for every $x \in [a, b]$, then

$$|E[a, b]| \leq \frac{M_2}{6}(b-a)^3.$$

Cumulative errors for all subintervals. As in the case of the midpoint rule

$$e(h) \leq Ch^2 \quad \text{where } C := \frac{M_2(b-a)}{6}.$$



SIMPSON RULE

Simpson Rule on a single interval. Let $q : [a, b] \rightarrow \mathbb{R}$ be the quadratic function passing through the points $(a, f(a))$, $(b, f(b))$, and $(m, f(m))$ where $m = \frac{a+b}{2}$. Then,

$$\int_a^b f(x) dx \approx \int_a^b q(x) dx = \frac{b-a}{6} (f(a) + 4f(m) + f(b)).$$

Composite Simpson Rule. If $\{x_k\}_{k=0}^n$ is a uniform partition of $[a, b]$ with norm $h = (b-a)/n$, then

$$\begin{aligned} \int_a^b f(x) dx &\approx \sum_{k=1}^n \frac{x_k - x_{k-1}}{6} (f(x_{k-1}) + f(x_{k-1/2}) + f(x_k)) \\ &= \frac{h}{6} \sum_{k=1}^n \left(f(a + (k-1)h) + f\left(a + \frac{(2k-1)h}{2}\right) + f(a + kh) \right). \end{aligned}$$

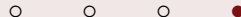
Example 6. Repeat **Example 4** using the composite Simpson rule.

It can be shown that the absolute error satisfies

$$e(h) \leq Ch^4.$$



Outlook on Advanced Numerical Integration



OUTLOOK ON ADVANCED NUMERICAL INTEGRATION

- Higher-Order Polynomial Approximations:
Closed Newton–Cotes Formulas
- Higher-Order Polynomial Approximations not Using the Endpoints:
Open Newton–Cotes Formulas
- Other Quadrature Rules:
Using Orthogonal Polynomials: **Gaussian Integration**
Using Derivatives: **Hermite Integration**
- Adaptive Methods:
Richardson Extrapolation, Romberg Integration
- Multi-Dimensional Problems:
Iterated Integrals
Integrals on General Domains Using Polygonal Shapes
(e.g. triangles, quadrilaterals, hexagons)



Thank you for your attention!

