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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



Riemann Integration Revisited



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

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

if the following inequalities hold:

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

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

$$l \le f(x) \le u$$
 for all $x \in [a, b]$.

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

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

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

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Example. Every continuous function on a closed interval is bounded. **Extreme Value Theorem:** If $f:[a,b]\to\mathbb{R}$ is continuous, then there exist $y,z\in[a,b]$ such that $f(y)\leq f(x)\leq f(z)$ for every $x\in[a,b]$.

Given a function $f:[a,b]\to\mathbb{R}$, 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 $k=1,2,\ldots,n$, 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 $f:[a,b]\to\mathbb{R}$ 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

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

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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 $k=1,2,\ldots,n$, we have

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

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

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

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

• There is at most one Riemann integral.



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



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



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• The function $f : [0,1] \to \mathbb{R}$ defined by f(x) = 1 is 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]

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

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

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• $\|\{x_k\}_{k=0}^n\| \to \text{o versus passing } n \to \infty \text{ in } \{x_k\}_{k=0}^n\|$?

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Illustrations and Numerical Experiments

An Algorithm for Computing Sums

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

An Algorithm for Computing Riemann Sums

The following algorithm computes the Riemann sum

$$\sum_{k=1}^{n} f(x_k^*)(x_k - x_{k-1})$$
 (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 x0 < x1 < ... < xn on [a, b]
- 2. set x0 = a and xn = b
- 3. set rs = 0
- 4. for k = 1, ..., n do
- 5. select a random point xk^* on [x(k-1), xk]
- $rs = rs + [f(xk^*) \times (xk x(k-1))]$
- 7. end for
- 8. return rs

c.

RIEMANN SUMS WITH RANDOM PARTITIONS

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

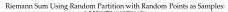
$$x_k^* = x_{k-1}$$
$$x_k^* = x_k$$

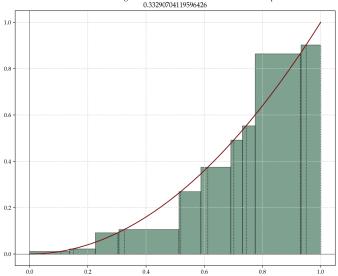
$$x_k^* = (x_{k-1} + x_k)/2$$

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

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

A RIEMANN SUM WITH RANDOM PARTITION







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

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

Specific versions of Riemann Sums:

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Specific versions of Riemann Sums:

Left endpoints as representatives

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

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$$\sum_{k=1}^{n} f(x_{k-1})(x_k - x_{k-1}) = h \sum_{k=1}^{n} f(a + (k-1)h)$$
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Right endpoints as representatives

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

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Right endpoints as representatives

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

Midpoints as representatives

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

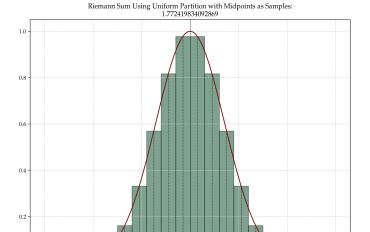
- 1. set h = (b-a)/n
- 1. set x = a h/2
- 3. set rs = 0
- 4. for k = 1, ..., n do
- $5. \qquad x = x + h$
- 6. rs = rs + f(x)
- 7. end for
- 8. return hxrs

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



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



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Box, Midpoint, Trapezoidal, and Simpson Rules

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

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

Specific versions of Riemann Sums:

Box and Midpoint Rules

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

$$x_k = a + kh$$
 for $k = 0, 1, ..., n$ 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

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

Let $f:[a,b]\to\mathbb{R}$ 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 $-2 \le x \le 2$.

- **a.** Use the box rule with right endpoints to compute the Riemann sums (S_N) for N = 0, 1, ..., 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:

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

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)

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

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

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

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

28 Apr 2023

LINEAR CONVERGENCE OF BOX RULES

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

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

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

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

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

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Cumulative errors for all subintervals. Write

$$I - I(h) := \int_{a}^{b} f(x) dx - h \sum_{k=1}^{n} f(x_{k})$$

$$= \sum_{k=1}^{n} \int_{x_{k-1}}^{x_{k}} f(x) dx - \sum_{k=1}^{n} f(x_{k})(x_{k} - x_{k-1}) = \sum_{k=1}^{n} E[x_{k-1}, x_{k}]$$

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

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

Ouadratic Convergence of Midpoint Rule

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

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

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

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

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

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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

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

Trapezoidal Rule

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

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

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Then,

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

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

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

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

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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) = o. By **Rolle's Theorem**, there exists $\xi \in (a,b)$ such that $g'(\xi) = o$.

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

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

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

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

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

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 $g'(\xi) = o$. Then,

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

Note that g'' = f''. If $|f''(x)| \le M_2$ 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

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

Simpson Rule on a singe interval. Let $q:[a,b]\to\mathbb{R}$ 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

$$\int_{a}^{b} f(x) dx \approx \sum_{k=1}^{n} \frac{x_{k} - x_{k-1}}{6} (f(x_{k-1}) + f(x_{k-1/2}) + f(x_{k}))$$

$$= \frac{h}{6} \sum_{k=1}^{n} \left(f(a + (k-1)h) + f\left(a + \frac{(2k-1)h}{2}\right) + f(a+kh) \right).$$

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

 Higher-Order Polynomial Approximations: Closed Newton-Cotes Formulas



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- Higher-Order Polynomial Approximations not Using the Endpoints:
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- Multi-Dimensional Problems:

Iterated Integrals Integrals on General Domains Using Polygonal Shapes (e.g. triangles, quadrilaterals, hexagons)

Thank you for your attention!

