Numerical Calculus

Numerical Differentiation and Integration

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Taylor Expansion

- One basic tool that we will use in this class.

Taylor expansion of a function $f(x)$ around a point x_0

$$f(x) = f(x_0) + (x - x_0)f'(x_0) + \frac{(x - x_0)^2}{2!}f''(x_0) + \cdots \tag{1}$$

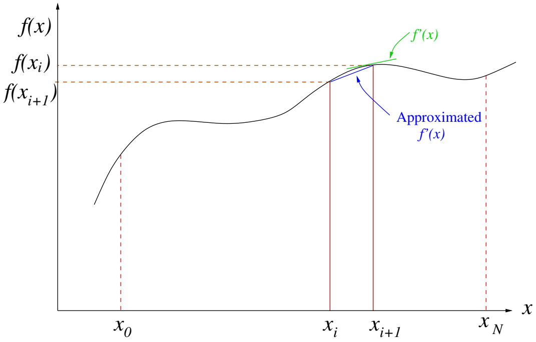
Taylor expansion of a mutivariable function $f(x, y, \cdots)$ around a point $(x_0, y_0, \cdots)$

$$\begin{aligned} f(x, y, \cdots) = \; & f(x_0, y_0, \cdots) + (x - x_0)f_x(x_0, y_0, \cdots) \\ & + (y - y_0)f_y(x_0, y_0, \cdots) + \cdots \\ & + \frac{(x-x_0)^2}{2!}f_{xx}(x_0, y_0, \cdots) \\ & + \frac{(y-y_0)^2}{2!}f_{yy}(x_0, y_0, \cdots) \\ & + \frac{(x-x_0)(y-y_0)}{2!}f_{xy}(x_0, y_0, \cdots) + \cdots \end{aligned}$$

First-Order Derivative: Single Variable, Two-Point Formula

- From the high school definition of the first-oder derivative.

$$f'(x_i) = \lim_{\Delta x \to 0} \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x} = \lim_{\Delta x \to 0} \frac{\Delta f_i}{\Delta x} \tag{2}$$



First-Order Derivative: Single Variable, Two-Point Formula

- Or more exactly, from the Taylor series (Eq. (1))
- Let $\Delta x = h$.

First order derivative: Two-Point Definition

$$\frac{df_i}{dx} = f_i' = \frac{f_{i+1} - f_i}{h} + \mathcal{O}(h^2) \tag{3}$$

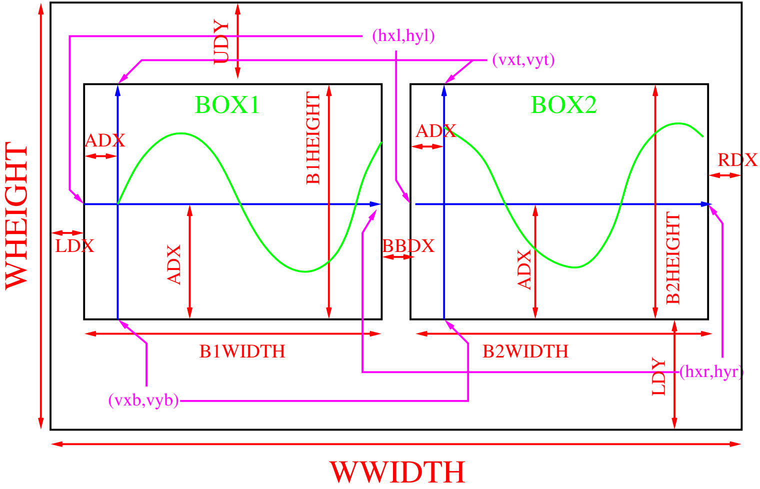
Accumulated Error

- For each step the largest error is proportional to h^2.
- At the end of the interval $[x_0, x_N]$, m steps of derivative has been made.
- The accumulated error becomes

$$\sum_i^m h^2 = mh^2 = \frac{x_N - x_0}{h} h^2 = (x_N - x_0)h = \mathcal{O}(h)$$

Example: $d\sin(x)/dx$

Design for the visualization



Improved Method: Three-Point Definition

Again from the Taylor series:

$$f(x+h) = f(x) + f'(x)h + \frac{1}{2}f''(x)h^2 + \frac{1}{6}f'''(x)h^3 + \cdots \tag{4}$$

$$f(x-h) = f(x) - f'(x)h + \frac{1}{2}f''(x)h^2 - \frac{1}{6}f'''(x)h^3 + \cdots \tag{5}$$

From Eq. (4) and Eq. (5)

$$f(x+h) - f(x-h) = 2f'(x)h + \mathcal{O}(h^3) \tag{6}$$

Therefore,

Three-Point Definition

$$f'(x_i) = \frac{f(x_i+h) - f(x_i-h)}{2h} + \mathcal{O}(h^3) \tag{7}$$

Accumulated error: $\mathcal{O}(h^2)$

Homework

Find the first order derivative numerically

$$f(x) = x^2$$

in the interval $x \in [-2, 2]$ using both two-point and three-point definitions.

Second Order Derivative

Again from the Taylor series for $f(x)$, add Eq. (4) and Eq. (5)

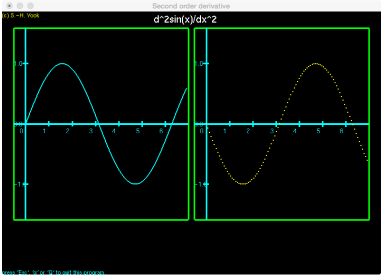
$$f(x+h) - 2f(x) + f(x-h) = h^2 f''(x) + \mathcal{O}(h^4) \quad (8)$$

Therefore,

Second Order Derivative:Three-Point Definition

$$f''(x_i) = \frac{f(x_i+h) - 2f(x) + f(x_i-h)}{h^2} + \mathcal{O}(h^2) \quad (9)$$

Example: Find $\frac{d^2 \sin(x)}{dx^2}$.



Homework

Find the second order derivative numerically

$$f(x) = x^2$$

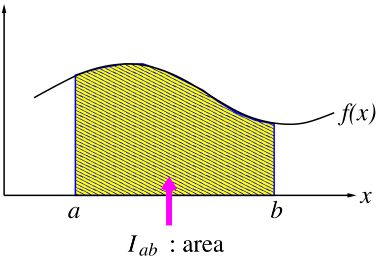
in the interval $x \in [-2, 2]$.

Numerical Integration

- Not all integrations are carried out analytically.
    - Ex. integrals including $\mathrm{erf}(x)$, $\Gamma(x)$, etc.
    - $\Rightarrow$ the results should be found numerically.
- Definite Integral

$$I_{[a,b]} = \int_a^b f(x)dx \qquad (10)$$

for simply assume that $f(x) > 0$ for $x \in [a,b]$ then $I_{[a,b]}$ is just the area enclosed by $f(x)$ [high school definition].



Basic Idea

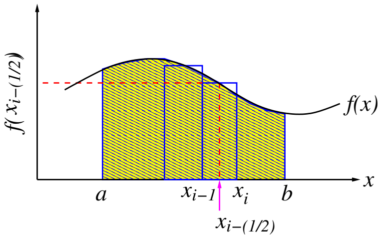
- Devide the interval $[a, b]$ into N sclices.
- For convenience, the width of each slice is identical, i.e. evenly spaced with intherval h.
- If we label the position (or the data points) as x_i, with $i = 1, 2, \cdots, N$, the integral Eq. (10) can be expressed as s summation of integrals over each slice.

Basic Idea

$$\int_a^b f(x)dx = \sum_{i=0}^{N-1} \int_{x_i}^{x_{i+1}} f(x)dx \tag{11}$$

- Find a numerical scheme that evaluates the summation over each slice.

Rectangular Method



- The most intuitive method
- For simplicity, let all subinterval has equal size, $h = x_i - x_{i-1}$.
- Divide the intreval $[a, b]$ into N subintervals: $Nh = b - a$.
- Let $\bar{f}_i \equiv \frac{1}{h}\int_{x_{i-1}}^{x_i} f(x)dx$.

Then

Rectangular Method

$$I_{[a,b]} = \int_a^b f(x)dx = \sum_{i=1}^{N}\int_{x_{i-1}}^{x_i} f(x)dx = h\sum_{i=1}^{N}\bar{f}_i. \quad (12)$$

For slow varying function $\bar{f}_i \approx f(x_{i-1/2})$ where $x_{i-1/2} = (x_{i-1} + x_i)/2$.

Rectangular Method–Error Estimation

Contribution of each interval

$$I_{[x_{i-1},x_i]} = \int_{x_{i-1}}^{x_i} f(x)dx \approx hf_{i-1/2}$$

$$f(x) = f_{i-\frac{1}{2}} + f'_{i-\frac{1}{2}}(x - x_{i-\frac{1}{2}}) + \frac{1}{2}f''_{i-\frac{1}{2}}(x - x_{i-\frac{1}{2}})^2 + \frac{1}{3!}f'''_{i-\frac{1}{2}}(x - x_{i-\frac{1}{2}})^3 + \cdots$$

$$\begin{aligned}\int_{x_{i-1}}^{x_i} f(x)dx = f_{i-\frac{1}{2}}\int_{x_{i-1}}^{x_i} dx &+ f'_{i-\frac{1}{2}}\int_{x_{i-1}}^{x_i}(x - x_{i-\frac{1}{2}})dx \\ &+ \frac{1}{2}f''_{i-\frac{1}{2}}\int_{x_{i-1}}^{x_i}(x - x_{i-\frac{1}{2}})^2dx \\ &+ \frac{1}{3!}f'''_{i-\frac{1}{2}}\int_{x_{i-1}}^{x_i}(x - x_{i-\frac{1}{2}})^3dx + \cdots\end{aligned}$$

Rectangular Method–Error Estimation

Thus,

$$\begin{aligned}\Delta I_{[x_{i-1},x_i]} &= \int_{x_{i-1}}^{x_i} f(x)dx - \int_{x_{i-1}}^{x_i} f'_{i-\frac{1}{2}}dx \\ &= \int_{x_{i-1}}^{x_i} f(x)dx - hf'_{i-\frac{1}{2}} \\ &\approx \frac{1}{2}f''_{i-\frac{1}{2}}\int_{x_{i-1}}^{x_i}(x-x_{i-\frac{1}{2}})^2dx\end{aligned}$$

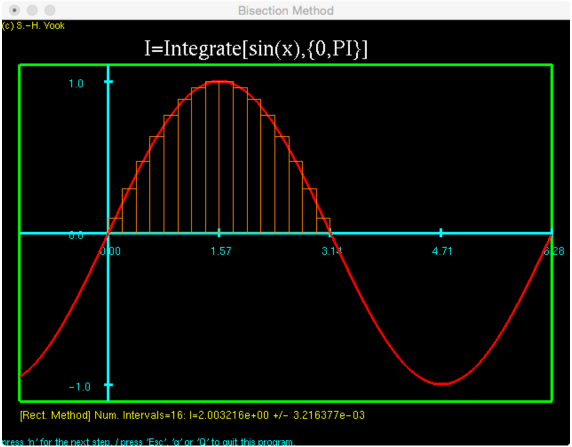
For over all interval $[a,b]$

$$\Delta I_{[a,b]} = \int_a^b f(x)dx - I_{[a,b]} \approx \frac{b-a}{24}h^2f''(\xi) = \frac{(b-a)^3}{24N^2}f''(\xi)$$

where $f''(\xi)$ is the average value of the second derivative of $f(x)$

Rectangular Method–Example

$$\int_0^{\pi} \sin(x)dx$$



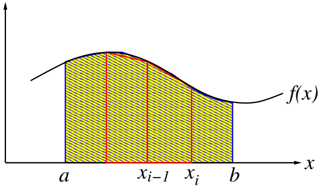
Homework

Integrate

$$f(x) = \exp(x)$$

over the interval $x \in [0, 2.5]$ using the rectangular method.

Trapezoidal Method



- Simply replace the rectangles by trapezoids.
- Or simply from the Taylor series ,Eq. (1),

$$f(x) = f(x_i) + (x - x_i)f'(x_i) + \mathcal{O}(h^2) \tag{13}$$

- Replace $f'(x_i)$ by $\frac{f(x_{i+1})-f(x_i)}{h}$, then

$$f(x) \simeq f(x_i) + (x - x_i)\frac{f(x_{i+1}) - f(x_i)}{h} \tag{14}$$

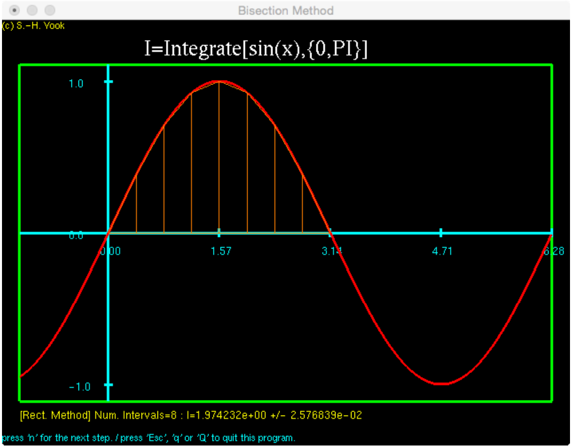
Integrate over every interval with this linear function to obtain

Trapezoidal Method

$$I_{[a,b]} = \frac{h}{2}\sum_{i=0}^{N-1}(f(x_i) + f(x_{i+1})) + \mathcal{O}(h^2) \tag{15}$$

Trapezoidal Method–Example

$$\int_0^{\pi} \sin(x)dx$$



Homework

Integrate

$$f(x) = \exp(x)$$

over the interval $x \in [0, 2.5]$ using the trapezoidal method.

Simplson's Rule

If all interval have the same length, i.e.,

$$x_{i+1} - x_i = h = const., \qquad \forall i,$$

to improve the accuracy (from the Taylor series (Eq. (1)))

$$\begin{aligned} I_{[x_{i-1},x_{i+1}]} &= \int_{x_{i-1}}^{x_{i+1}} f(x)dx \\ &= f_i \int_{x_{i-1}}^{x_{i+1}} dx + f' \int_{x_{i-1}}^{x_{i+1}} (x - x_i)dx + \frac{1}{2} f_i'' \int_{x_{i-1}}^{x_{i+1}} (x - x_i)^2 dx \\ &\quad + \frac{1}{3} f_i''' \int_{x_{i-1}}^{x_{i+1}} (x - x_i)^3 dx \\ &= 2hf_i + 0 + \frac{1}{2} f_i'' \frac{2}{3} h^3 + 0 + \mathcal{O}(h^5) \end{aligned} \tag{16}$$

Simplson's Rule

Now use the discretized second order derivative (Eq. (9))

$$f_i'' = \left.\frac{d^2 f(x)}{dx^2}\right|_{x=x_i} = \frac{1}{h^2}\left(f_{i+1} - 2f_i + f_{i-1}\right).$$

Then Eq. (16) can be rewritten as

$$\begin{aligned} I_{[x_{i-1},x_{i+1}]} &= 2hf_i + \frac{1}{3}h\left(f_{i+1} - 2f_i + f_{i-1}\right) + \mathcal{O}(h^5) \\ &= \frac{h}{3}\left(f_{i+1} + 4f_i + f_{i-1}\right) + \mathcal{O}(h^5) \end{aligned} \quad (17)$$

Simpson's Rule

$$I_{[a,b]} = \sum_{i=0}^{N/2-1} \frac{h}{3}\left(f_{2i} + 4f_{2i+1} + f_{2i+2}\right) \quad (18)$$

Simpson's $3/8$ Rule

Simpson's $3/8$ Rule (Newton-Cotes formula with $n = 3$)

$$\int_a^b f(x)dx = \sum_{i=1}^{N/3} \frac{3h}{8} \left(f_i + 3f_{i+1} + 3f_{i+2} + f_{i+3}\right) \qquad (19)$$

Verification of Simpson's $3/8$ rule: Let an integral of any function $f(x)$ over an interval $[a, a+3h]$ can be approximated as

$$\int_a^{a+3h} f(x)dx \approx c_0 f(a) + c_1 f(a+h) + c_2 f(a+2h) + c_3 f(a+3h)$$

Replace x by $x - a - \frac{3h}{2}$ then

$$\int_{-\frac{3h}{2}}^{\frac{3h}{2}} f(x)dx = c_0 f\left(-\frac{3h}{2}\right) + c_1 f\left(-\frac{h}{2}\right) + c_2 f\left(\frac{h}{2}\right) + c_3 f\left(\frac{3h}{2}\right) \qquad (20)$$

Simpson's 3/8 Rule

Since there are four unknowns, c_0, c_1, c_2, c_3, we need four equations to obtain the unknown parameters.
Since Eq. (20) is satisfied by any function, we consider four different types of $f(x)$: $f(x) = 1$, $f(x) = x$, $f(x) = x^2$, and $f(x) = x^3$ for simplicity.

$$\int_{-\frac{3h}{2}}^{\frac{3h}{2}} dx = 3h = c_0 + c_1 + c_2 + c_3 \tag{21}$$

$$\int_{-\frac{3h}{2}}^{\frac{3h}{2}} x dx = 0 = c_0 \left(-\frac{3h}{2}\right) + c_1 \left(-\frac{h}{2}\right) + c_2 \left(\frac{h}{2}\right) + c_3 \left(\frac{3h}{2}\right) \tag{22}$$

$$\int_{-\frac{3h}{2}}^{\frac{3h}{2}} x^2 dx = \frac{9h^3}{4} = c_0 \left(\frac{9h^2}{4}\right) + c_1 \left(\frac{h^2}{4}\right) + c_2 \left(\frac{h^2}{4}\right) + c_3 \left(\frac{9h^2}{4}\right) \tag{23}$$

$$\int_{-\frac{3h}{2}}^{\frac{3h}{2}} x^3 dx = 0 = c_0 \left(-\frac{27h^3}{8}\right) + c_1 \left(-\frac{h^3}{8}\right) + c_2 \left(\frac{h^3}{8}\right) + c_3 \left(\frac{27h^3}{8}\right) \tag{24}$$

Simpson's $3/8$ Rule

From Eqs. (21)-(24), we obtain

$$c_0 = c_3 = \frac{3h}{8}$$

and

$$c_1 = c_2 = \frac{9h}{8}$$

Thus,

$$\int_{-\frac{3h}{2}}^{\frac{3h}{2}} f(x)dx \approx \frac{3h}{8}\left[f\left(-\frac{3h}{2}\right) + 3f\left(-\frac{h}{2}\right) + 3f\left(\frac{h}{2}\right) + f\left(\frac{3h}{2}\right)\right]$$

or equivalently

$$\int_{a}^{a+3h} f(x)dx \approx \frac{3h}{8}\left[f\left(a\right) + 3f\left(a+h\right) + 3f\left(a+2h\right) + f\left(a+3h\right)\right] \qquad (25)$$

By summing over all interval, we obtain Eq. (19).

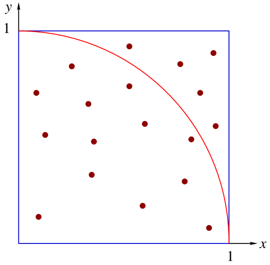
Homework

Integrate

$$f(x) = \exp(x)$$

over the interval $x \in [0, 2.5]$ using the Simpson's rule.

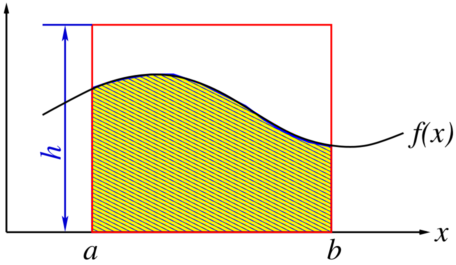
Monte Carlo Integration



- Find π.
- Use the area of the unit quarter circle.
- Area of the blue square: $A = 1$.
- Area of the quarter circle: $A' = \pi/4$
- The probability that a dart lands in any particular region is proportional to the area of that region.

1. Generate a pair of random numbers x and y $(0 \leq x \leq 1$ and $0 \leq y \leq 1)$
2. If $y \leq \sqrt{1 - x^2}$ then increase N_{circle} by one.
3. Repeat process (1) and (2) for N times.
4. Calculate the probability $p = N_{circle}/N$.
5. From the relation $p = \frac{\frac{\pi}{4}}{1} = \frac{N_{circle}}{N}$, we obtain $\pi = 4N_{circle}/N$.

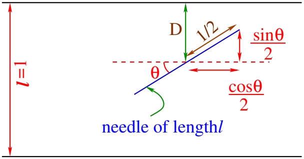
Monte Carlo Integral



- The most basic concept of Monte Carlo method is the important sampling.
- sample the value of $f(x)$

$$\int_a^b f(x)dx = \frac{b-a}{N}\sum_{i=1}^{N} f(x_i) \quad \text{for large } N \tag{26}$$

Monte Carlo Method – Buffon's Needle



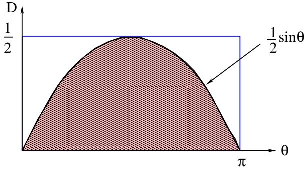
- Throw a needle to locate at a random position.
- Use the probability that the needle touch or cross the lines.
- Two random variables: D and θ.

$$0 \leq D \leq \frac{1}{2}, \qquad 0 \leq \theta \leq \pi \tag{27}$$

Monte Carlo Method – Buffon's Needle

Condition that the needle touch or cross the black lines:

$$D \leq \frac{1}{2}\sin\theta \tag{28}$$



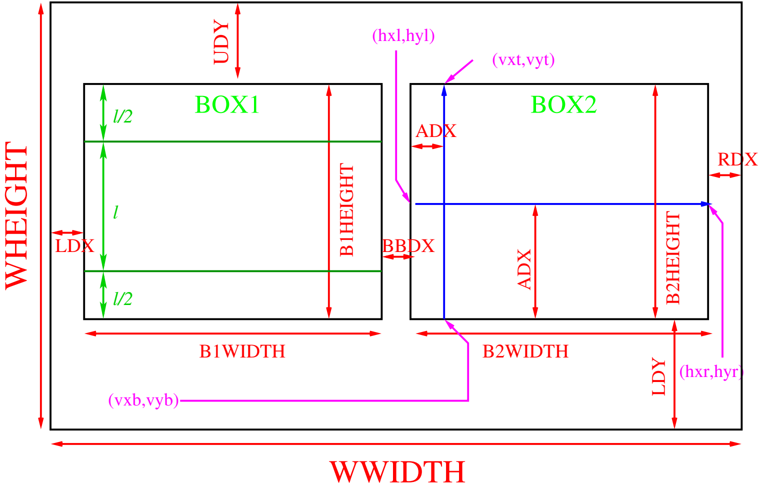
Then we just obtain the area of the shaded region.

1. Generate two random numbers $0 \leq D \leq 1/2$ and $0 \leq \theta \leq \pi$.
2. If $D \leq \frac{1}{2}\sin\theta$ then increase N_{count} by 1.
3. Repeat (1) and (2) by N times.

Then the area of the shaded region becomes $A = \int_0^\pi \frac{1}{2}\sin\theta = 1$. Thus,

$$p = \frac{N_{count}}{N} = \frac{1}{\frac{\pi}{2}} \Rightarrow \pi = \frac{2}{p}$$

Design the Window for Buffon's Needle



Multidimensional Integral

- Basic idea: extension of the algorithms for single variable functions
- Monte Carlo Method: more efficient!

$$\int_a^b \int_c^d \int_e^f F(x, y, z) dxdydz = \sum_{i=1}^{N} F(x_i, y_i, z_i) \Delta v$$

where $\Delta v = \frac{(b-a)(d-c)(f-e)}{N}$ for large N.

Homework

Integrate

$$f(x, y, z) = x + y + z$$

over the interval $x \in [0, 1]$, $y \in [0, 1]$, and $z \in [0, 1]$ using the Monte Carlo method.

Improper Integral

- Types of improper integral
  - range of integral $\rightarrow$ infinite
  - Integrand contains a singularity within the integration range
    - integrable singularity: $\int_0^1 \frac{1}{\sqrt{1-x^2}}dx$
    - nonintegrable singularity: $\int_0^1 \frac{dx}{x}$
- Some special case:

$$\lim_{x\rightarrow 0}\frac{\sin x}{x} = 1$$

Take small ϵ then

$$\int_0^{\pi}\frac{\sin x}{x}dx = \epsilon + \int_{\epsilon}^{\pi}\frac{\sin x}{x}dx$$

Infinite range integration: in some cases

$$I = \int_0^b \exp(-x^2) \rightarrow \frac{\sqrt{pi}}{2} = 0.886227 \text{ as } b \rightarrow \infty$$

for $b = 3$, $I = 0.886207 \Rightarrow$ error might be reasonably small.