Introduction to Computation (CS2201)

Lecture 5

Kripabandhu Ghosh

CDS, IISER Kolkata

Numerical Integration

Numerical Integration

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

Problem

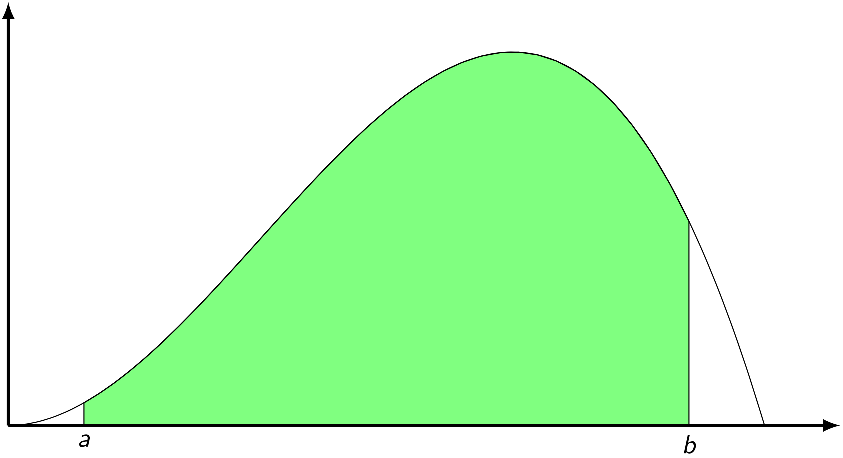
Find an indefinite integral or *primitive* $\phi(x)$ such that $\phi^{'}(x) = f(x)$

Multiple applications like area under a curve $(f(x))$ bounded by two points a, b (in a 2-D space)

Need for numerical integration

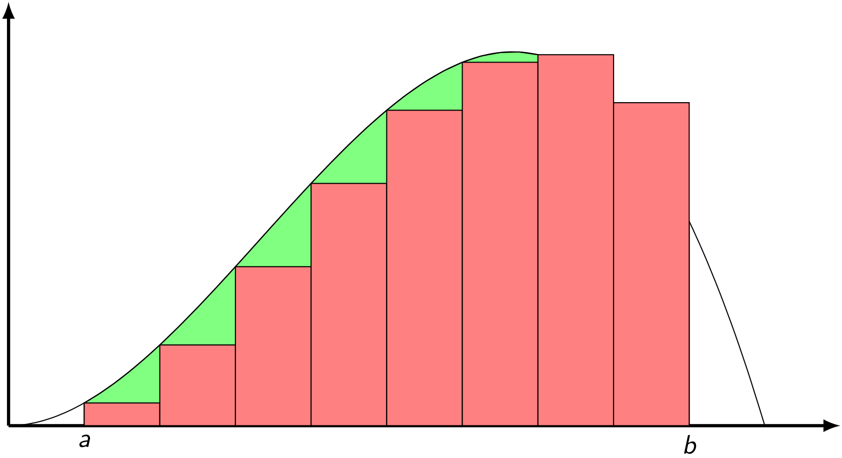
- $\phi(x)$ can't be obtained in terms of known functions or has a complex form computing which is expensive
- $f(x)$ is not known in its analytical form but is represented by a table of values

Integral as area :



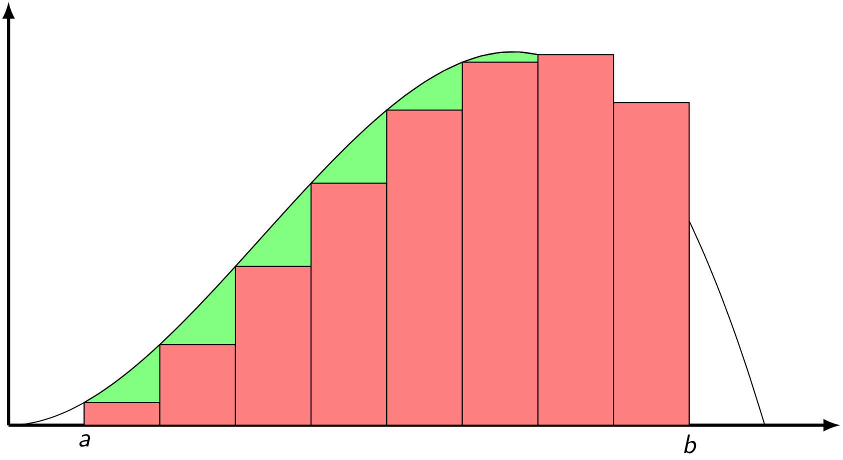
$$\int_a^b f(x)dx = \lim_{N\to\infty} h \sum_{i=0}^{N-1} f(a+ih), \qquad h = \frac{b-a}{N}$$

Integral as area : The Riemann sum



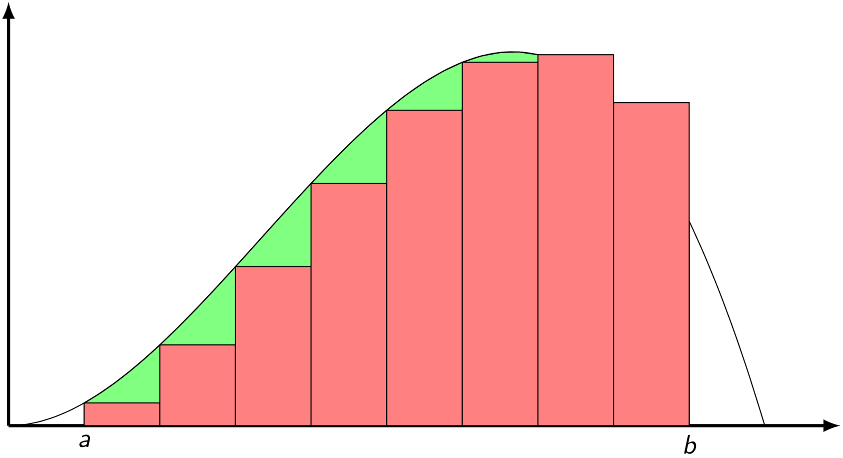
$$\int_a^b f(x)dx = \lim_{N\to\infty} h\left[f(a) + f(a+h) + \ldots + f(a+\overline{N-1}h)\right]$$

Integral as area : Rectangular approximation



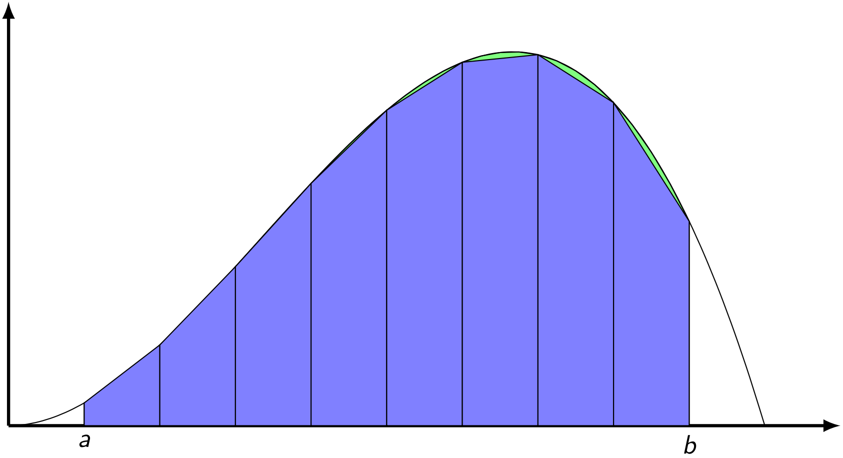
$$\int_a^b f(x)dx \approx h\left[f(a) + f(a+h) + \ldots + f(a+\overline{N-1}h)\right]$$

Integral as area : Rectangular approximation



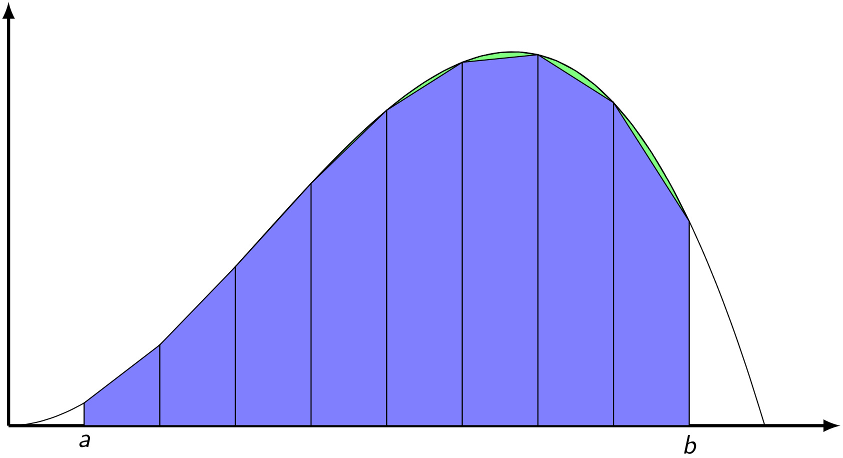
$$\int_a^b f(x)dx \approx h\left[f_0 + f_1 + \ldots + f_{N-1}\right], \qquad f_i \equiv f\left(a + ih\right)$$

Integral as area : The (composite) Trapezoidal rule



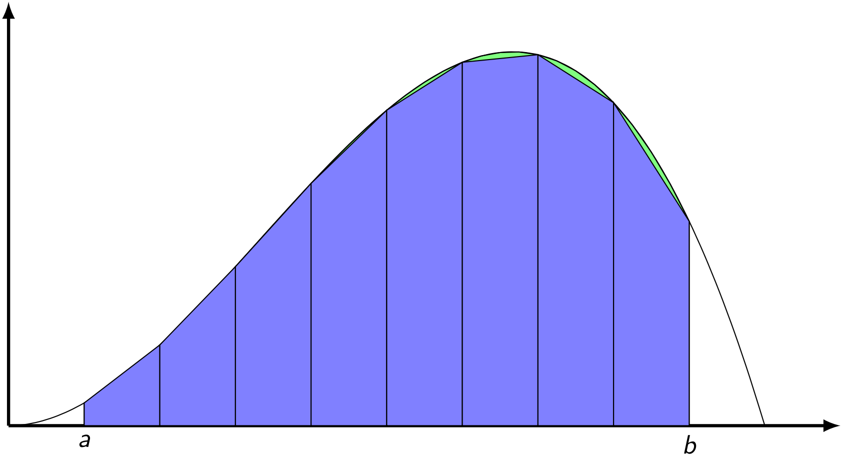
$$\int_a^b f(x)dx \approx h\left[\frac{f_0+f_1}{2}+\frac{f_1+f_2}{2}+\ldots+\frac{f_{N-1}+f_N}{2}\right]$$

Integral as area : The (composite) Trapezoidal rule



$$\int_a^b f(x)dx \approx h\left[\frac{f(a)+f(b)}{2} + (f_1 + f_2 + \ldots + f_{N-1})\right]$$

Integral as area : The (composite) Trapezoidal rule



SciPy Introduction

- SciPy is a scientific computation library that uses NumPy underneath.
- SciPy stands for Scientific Python.
- It provides utility functions for optimization, integration, interpolation etc.

Trapz function

Format

scipy.integrate.trapz(y, x=None, dx=1.0,...)

Parameters

- y : Input array to integrate
- x : (optional) If x is None, then spacing between all y elements is dx.
- dx : (optional) If x is None, spacing given by dx is assumed. Default is 1.

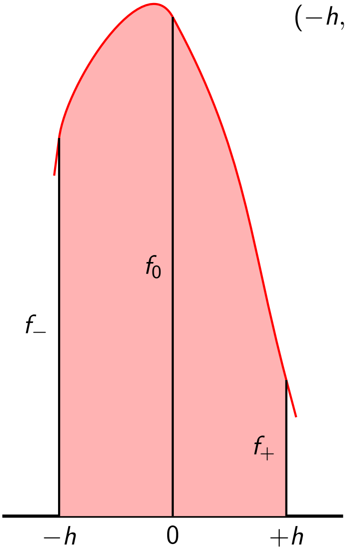
Output

Returns the definite integral of y along x-axis using the trapezoidal rule

Numpy alternative

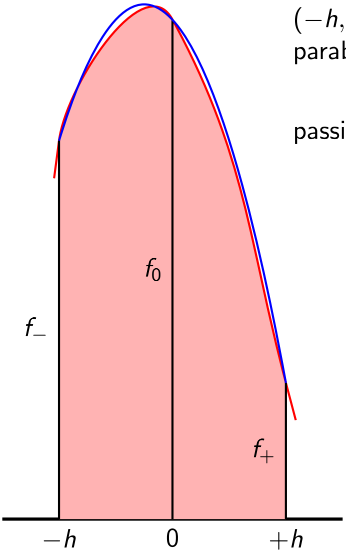
numpy.trapz(y, x=None, dx=1.0,...)

Simpson's one-third rule



To estimate the are under the curve passing through $(-h, f_-)$, $(0, f_0)$ and $(+h, f_+)$

Simpson's one-third rule

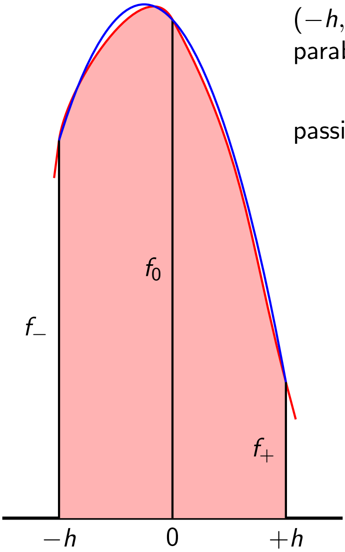


To estimate the are under the curve passing through $(-h, f_-)$, $(0, f_0)$ and $(+h, f_+)$ we replace the curve by a parabola

$$y = a_0 + a_1 x + a_2 x^2$$

passing through these points.

Simpson's one-third rule



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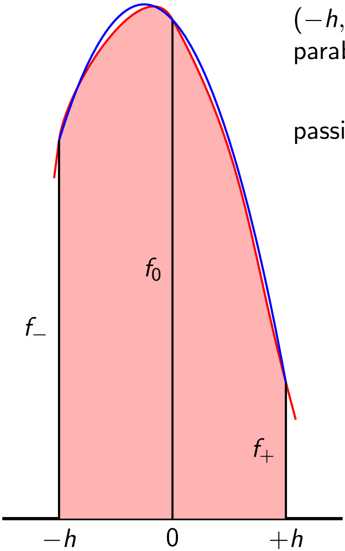
$$f_0 = a_0$$

Simpson's one-third rule



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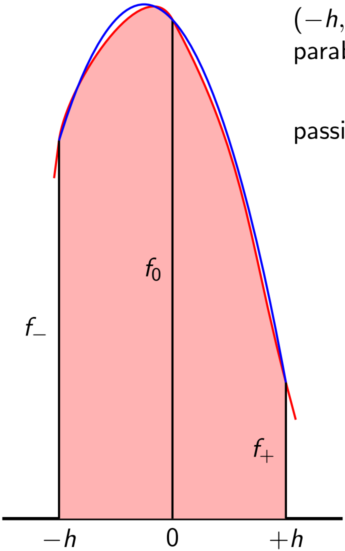
passing through these points.

$$\begin{aligned} f_0 &= a_0 \\ f_- &= a_0 - a_1 h + a_2 h^2 \end{aligned}$$

Simpson's one-third rule



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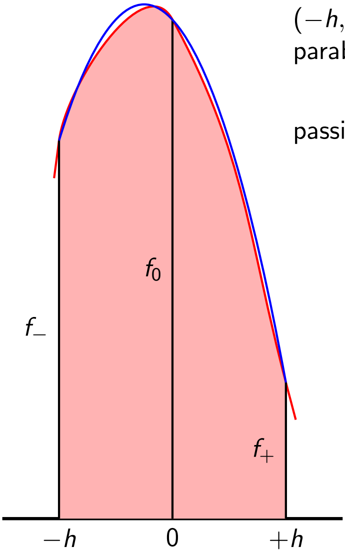

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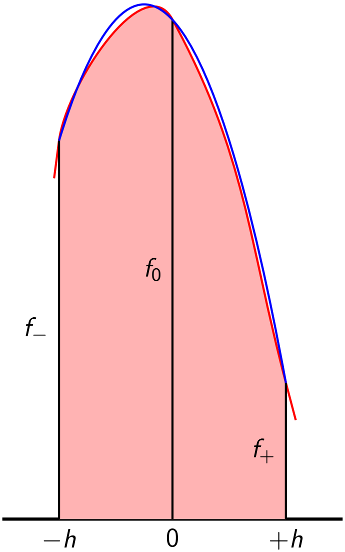
$$y = a_0 + a_1 x + a_2 x^2$$

passing through these points.

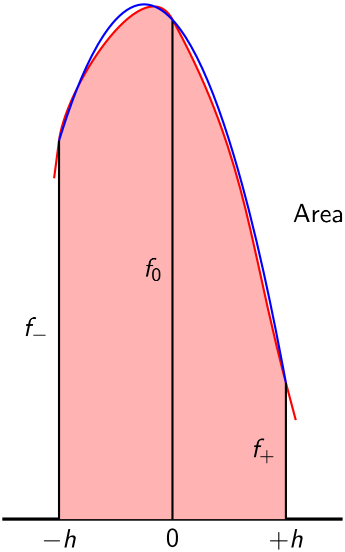
$$\begin{aligned} f_0 &= a_0 \\ f_- &= a_0 - a_1 h + a_2 h^2 \\ f_+ &= a_0 + a_1 h + a_2 h^2 \\ a_0 &= f_0 \\ a_1 &= \frac{f_+ - f_-}{2h} \\ a_2 &= \frac{f_+ + f_- - 2f_0}{2h^2} \end{aligned}$$

Simpson's one-third rule



$$
\begin{aligned}
a_0 &= f_0 \\
a_1 &= \frac{f_+ - f_-}{2h} \\
a_2 &= \frac{f_+ + f_- - 2f_0}{2h^2}
\end{aligned}
$$

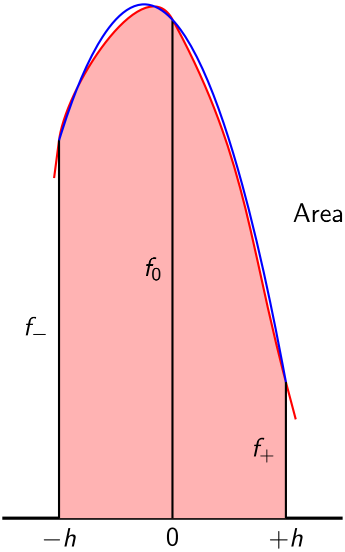
Simpson's one-third rule



$$\begin{aligned} a_0 &= f_0 \\ a_1 &= \frac{f_+ - f_-}{2h} \\ a_2 &= \frac{f_+ + f_- - 2f_0}{2h^2} \end{aligned}$$

Area : $\int_{-h}^{h} \left(a_0 + a_1 x + a_2 x^2\right) dx$

Simpson's one-third rule



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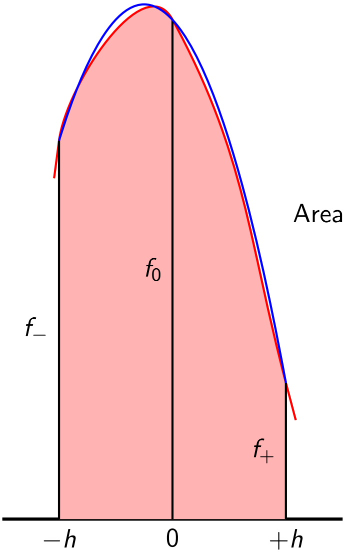
\begin{aligned}
a_0 &= f_0 \\
a_1 &= \frac{f_+ - f_-}{2h} \\
a_2 &= \frac{f_+ + f_- - 2f_0}{2h^2}
\end{aligned}
$$

Area : $\int_{-h}^{h} \left(a_0 + a_1 x + a_2 x^2\right) dx$

$$= \quad 2a_0 h + \frac{2}{3} a_2 h^3$$

Simpson's one-third rule



$$a_0 = f_0$$

$$a_1 = \frac{f_+ - f_-}{2h}$$

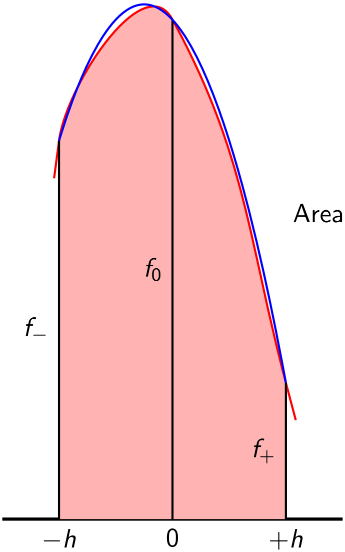
$$a_2 = \frac{f_+ + f_- - 2f_0}{2h^2}$$

Area : $\int_{-h}^{h} \left(a_0 + a_1 x + a_2 x^2\right) dx$

$$= 2a_0 h + \frac{2}{3} a_2 h^3$$

$$= h\left(2f_0 + \frac{f_+ + f_- - 2f_0}{3}\right)$$

Simpson's one-third rule

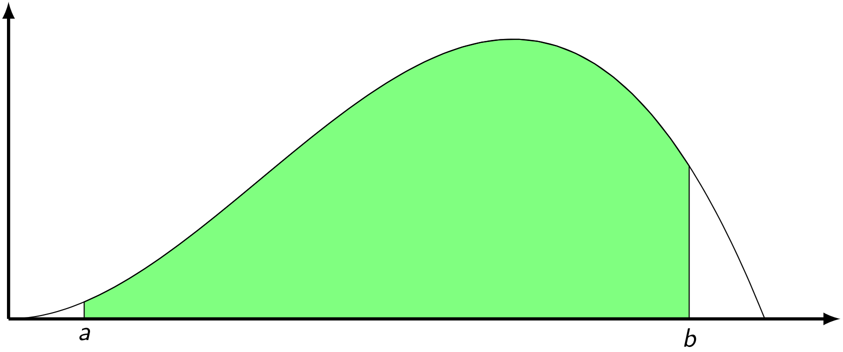


$$
\begin{aligned}
a_0 &= f_0 \\
a_1 &= \frac{f_+ - f_-}{2h} \\
a_2 &= \frac{f_+ + f_- - 2f_0}{2h^2}
\end{aligned}
$$

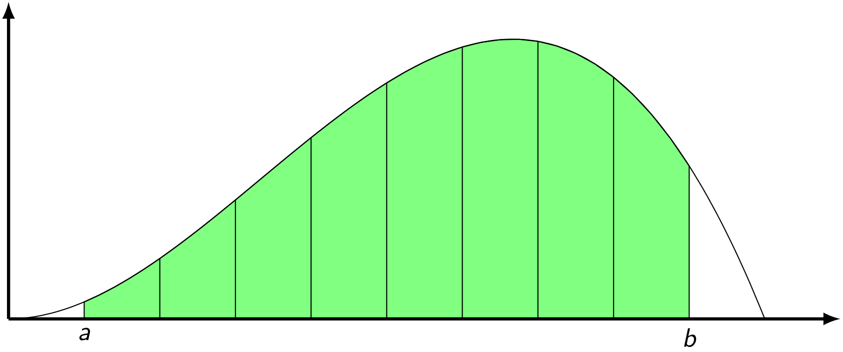
Area : $\int_{-h}^{h} \left(a_0 + a_1 x + a_2 x^2\right) dx$

$$
\begin{aligned}
&= 2a_0 h + \frac{2}{3} a_2 h^3 \\
&= h\left(2f_0 + \frac{f_+ + f_- - 2f_0}{3}\right) \\
&= \frac{h}{3}\left(f_+ + 4f_0 + f_-\right)
\end{aligned}
$$

The composite Simpson one-third rule



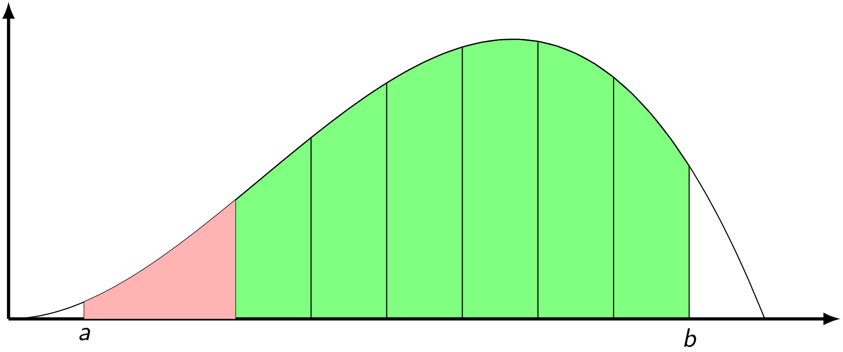
The composite Simpson one-third rule



Divide interval from a to b into **even** number of pieces:

$$h = \frac{b-a}{2N}$$

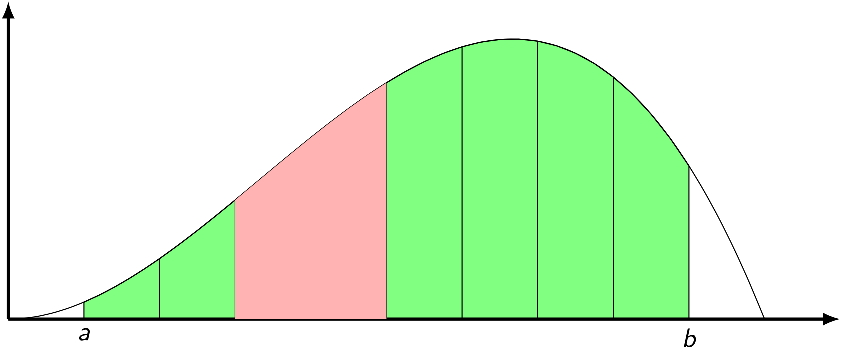
The composite Simpson one-third rule



Area

$$\frac{h}{3}\left[(f_0 + 4f_1 + f_2) + \qquad \cdots \qquad \right]$$

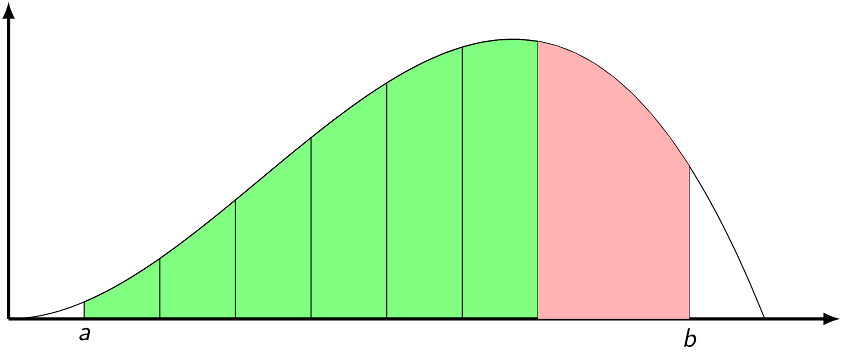
The composite Simpson one-third rule



Area

$$\frac{h}{3}\left[(f_0 + 4f_1 + f_2) + \ (f_2 + 4f_3 + f_4) + \ \ldots \qquad\qquad\qquad\qquad \right]$$

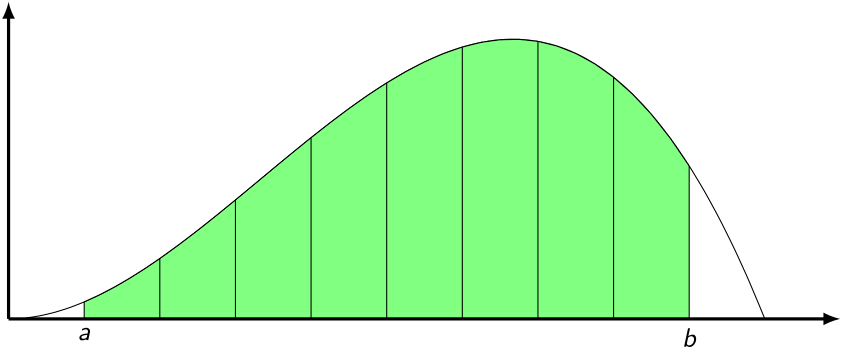
The composite Simpson one-third rule



Area

$$\frac{h}{3}\left[(f_0 + 4f_1 + f_2) + \ (f_2 + 4f_3 + f_4) + \ \dots + (f_{2N} + 4f_{2N-1} + f_{2N})\right]$$

The composite Simpson one-third rule



$\int_a^b f(x)dx$

$$- - - - \approx \frac{h}{3}[(f(a) + f(b)) + 4(f_1 + f_3 + ... + f_{2N-1}) + 2(f_2 + f_4 + ... + f_{2N-2})]$$

Simpson's function

Format

scipy.integrate.simpson(y, x=None, dx=1.0, ...even='avg')

Parameters

- y : Input array to integrate
- x : If given, the points at which y is sampled.
- dx : (optional) If x is None, spacing given by dx is assumed. Default is 1.

Output

Returns the definite integral of y along x-axis using the Simpson's rule

Notes

If there are an even number of samples, N, then there are an odd number of intervals (N-1), but Simpson's rule requires an even number of intervals. The parameter 'even' controls how this is handled.

Simpson's function: Parameter 'even'

- **avg**: Average two results:1) use the first N-2 intervals with a trapezoidal rule on the last interval and 2) use the last N-2 intervals with a trapezoidal rule on the first interval.
- **first**: Use Simpson's rule for the first N-2 intervals with a trapezoidal rule on the last interval.
- **last**: Use Simpson's rule for the last N-2 intervals with a trapezoidal rule on the first interval.

Acknowledgement

Slides of Prof. Ananda Dasgupta reused

THANK YOU !!!