Numerical Differentiation
and
Integration

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Numerical Differentiation

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or even the **central difference** formula:

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We expect these approximations to improve as h becomes smaller!

Numerical Differentiation : an example

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For $h = 0.1$

	calculated	**error**
foward	1.0517	0.0517
backward	0.9516	0.0484
central	1.0017	0.0017

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central	1.0017	0.0017

For $h = 0.01$

	calculated	**error**
foward	1.00501667	0.00501667
backward	0.9950166	0.00498337
central	1.00001667	0.00001667

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For $h = 0.01$

	calculated	**error**
foward	1.00501667	0.00501667
backward	0.9950166	0.00498337
central	1.00001667	0.00001667

- Central difference does much better than the other two!

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backward	0.9950166	0.00498337
central	1.00001667	0.00001667

- Central difference does much better than the other two!
- It improves at a better rate with smaller h as well!

Numerical Differentiation : the math behind it!

A smooth function can be expanded in a **Taylor series** :

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f^{(\mathrm{iv})}(x) + \dots$$

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Cutting down h by a factor of 10, reduces the error by the same factor!

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The error in the forward difference formula is $\mathcal{O}(h)$
Cutting down h by a factor of 10, reduces the error by the same factor!
Backward difference exhibits similar behavior!

Numerical Differentiation : the math behind it!

Why is central difference better?

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f^{(\mathrm{iv})}(x) + \dots$$

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$$f(x+h) - f(x-h) = 2hf'(x) + \frac{h^3}{3}f'''(x) + \mathcal{O}\left(h^5\right)$$

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- cutting down h by a factor of 10, reduces the error by a factor of 100!

Numerical Differentiation : the math behind it!

Can we do better?

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Eliminate $f'''(x)$!

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$$8\left(f(x+h) - f(x-h)\right) - \left(f(x+2h) - f(x-2h)\right) = 12hf'(x) + \mathcal{O}\left(h^5\right)$$

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$$f'(x) = \frac{8\left(f(x+h) - f(x-h)\right) - \left(f(x+2h) - f(x-2h)\right)}{12h} + \mathcal{O}\left(h^4\right)$$

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This is the so called **5-point stencil formula** for the first derivative.

Smaller h makes for better accuracy

```
>>> from math import exp
>>> h = 1.0
>>> for i in range(20):
...     print h,abs((exp(h)-1)/h-1.)
...     h /= 10.
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```

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1.0	0.718281828459
0.1	0.051709180756
0.01	0.00501670841679
0.001	0.000500166708385
0.0001	5.0001667141e-05
1e-05	5.00000696491e-06
1e-06	4.99962183431e-07
1e-07	4.94336800383e-08
1e-08	6.07747119297e-09

Smaller *h* makes for better accuracy

Or does it?

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1e-09	8.2740370777e-08
1e-10	8.2740370777e-08
1e-11	8.2740370777e-08
1e-12	8.89005823408e-05
1e-13	0.000799277837359
1e-14	0.000799277837359
1e-15	0.110223024625
1e-16	1.0
1e-17	1.0

Higher order derivatives

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Adding:

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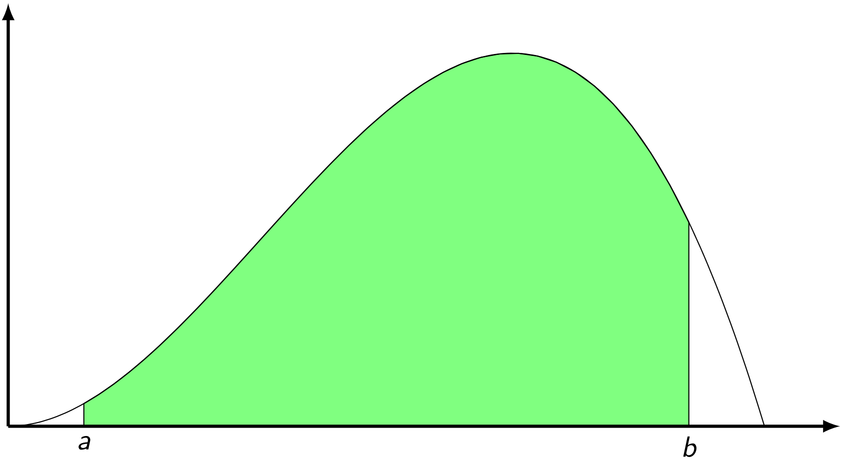
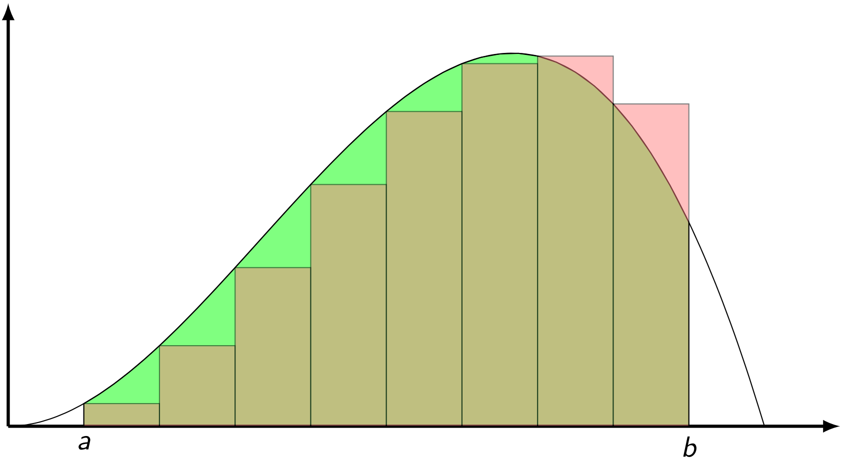
$$f''(x) = \frac{f(x+h) + f(x-h) - 2f(x)}{h^2} + \mathcal{O}\left(h^2\right)$$

Integral as area :



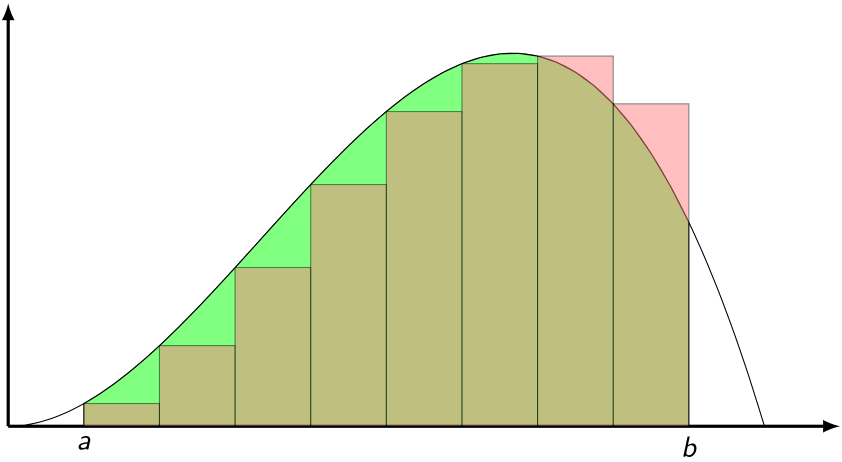
$$\int_a^b f(x)dx = \lim_{N\to\infty} h \sum_{i=0}^{N-1} f(a+ih), \qquad h = \frac{b-a}{N}$$

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



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

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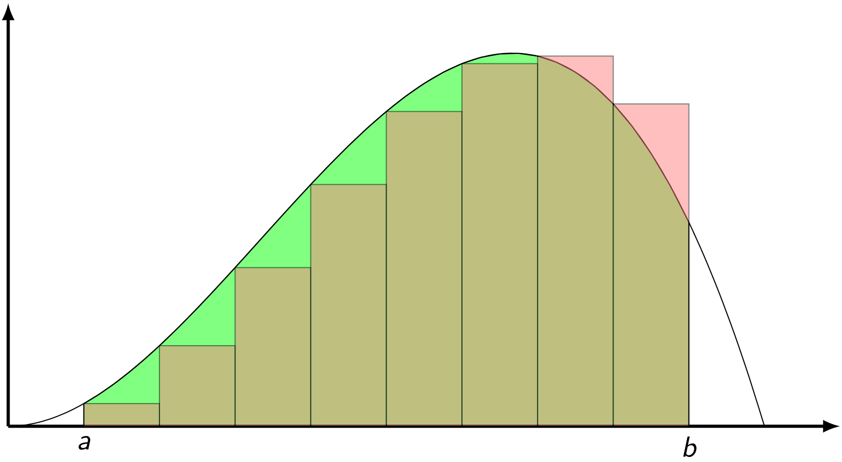
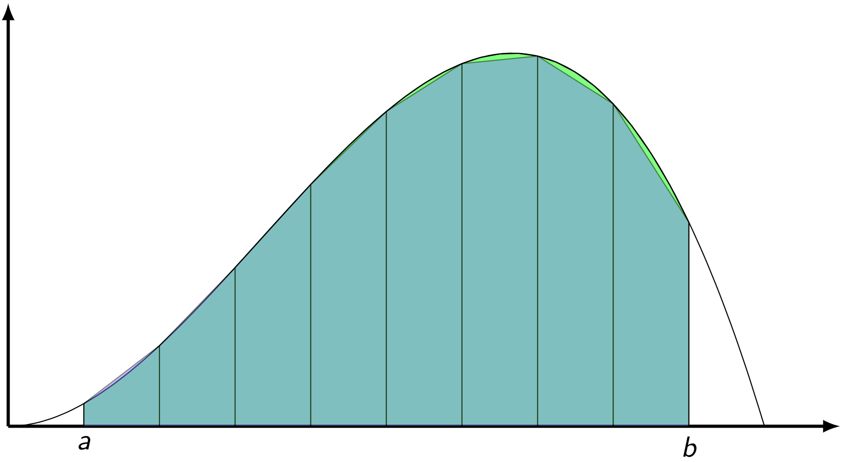


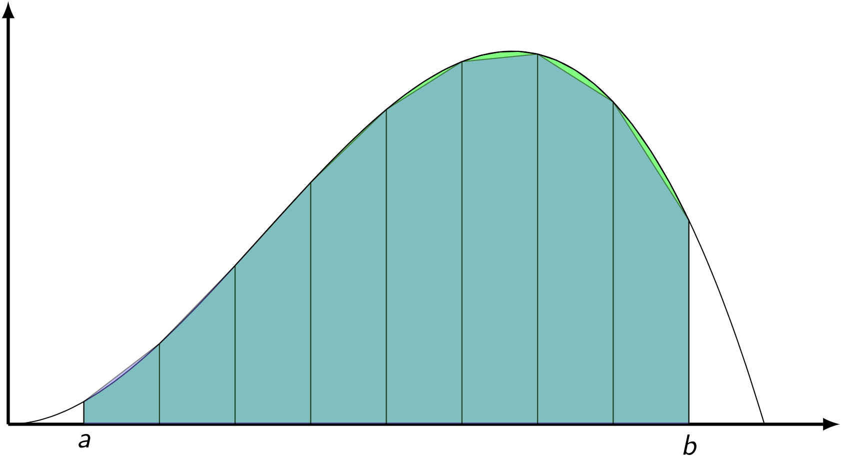
$$\int_a^b f(x)dx \approx h\left[f_0 + f_1 + \ldots + f_{N-1}\right], \qquad f_i \equiv f\left(a + \overline{i-1}h\right)$$

Integral as area : The (composite) Trapezoidal rule



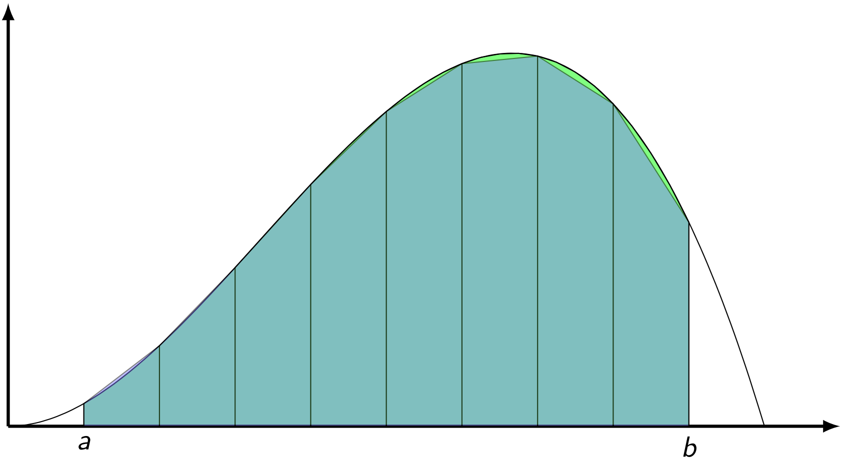
$$\int_a^b f(x)dx \approx h\left[\frac{f_0+f_1}{2}+\frac{f_1+f_2}{2}+\ldots+\frac{f_{N-1}+f_N}{2}\right]$$

Integral as area : The (composite) Trapezoidal rule



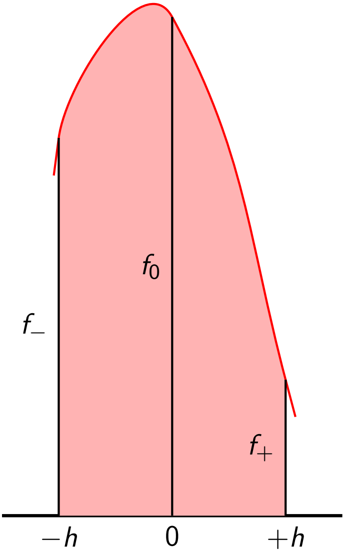
$$\int_a^b f(x)dx \approx h\left[\frac{f(a)+f(b)}{2} + (f_1 + f_2 + \ldots + f_{N-1})\right]$$

Integral as area : The (composite) Trapezoidal rule



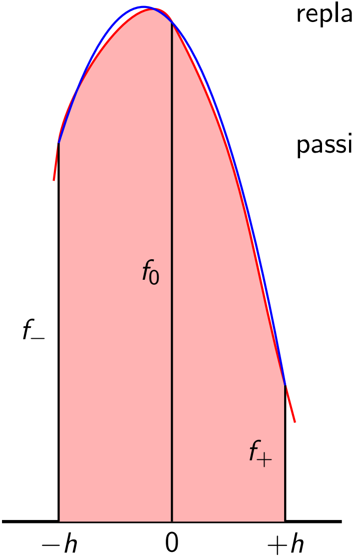
How can we do better?

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

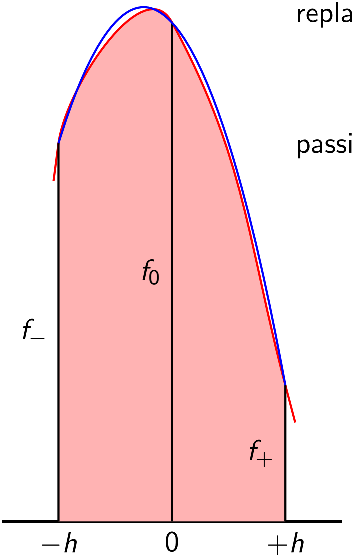


To estimate the are under the curve passing through $(-h, f_-)$, $(0, f_0)$ and $(+h, f_+)$ we replace the curve by a parabola

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

passing through these points.

Simpson's one-third rule



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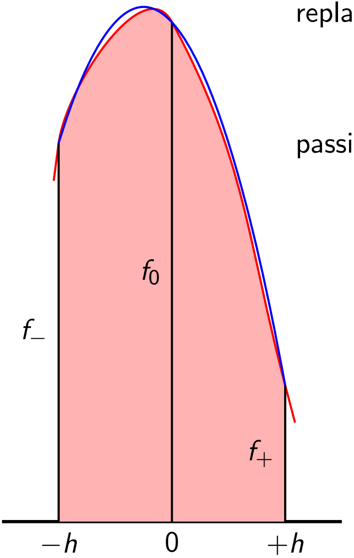

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$$\begin{aligned} f_0 &= a_0 \\ f_- &= a_0 - a_1 h + a_2 h^2 \end{aligned}$$

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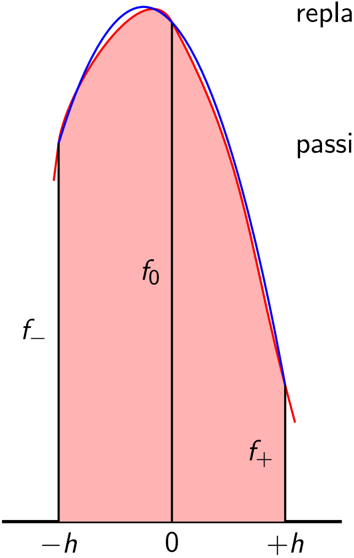

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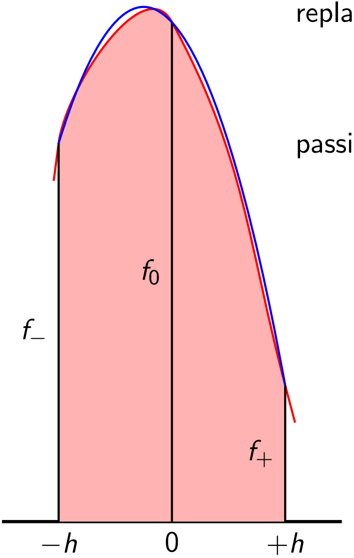

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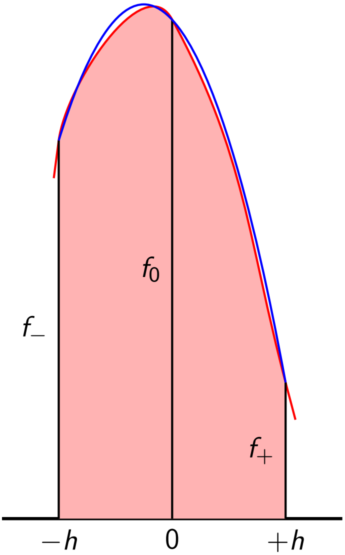
$$\begin{aligned}
f_0 &= a_0 \\
f_- &= a_0 - a_1 h + a_2 h^2 \\
f_+ &= a_0 + a_1 h + a_2 h^2 \\
a_0 &= f_0 \\
a_1 &= \frac{f_+ - f_-}{2h} \\
a_2 &= \frac{f_+ + f_- - 2f_0}{2h^2}
\end{aligned}$$

Simpson's one-third rule



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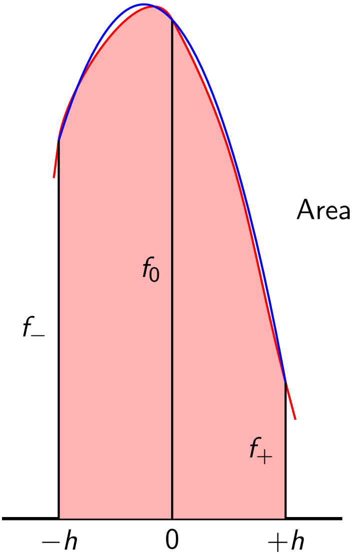

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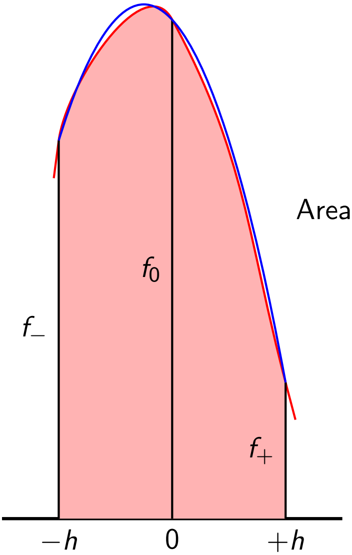

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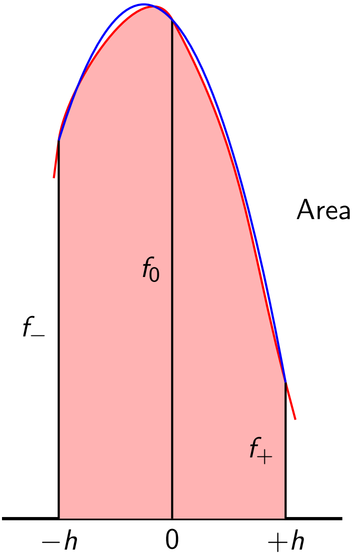

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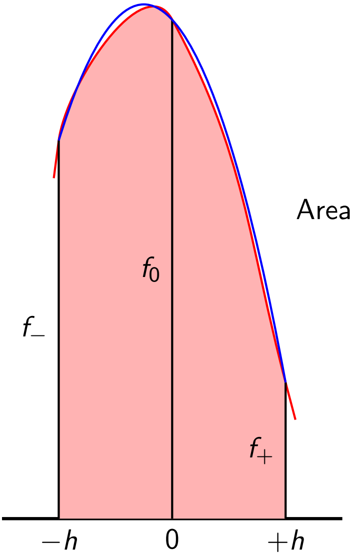

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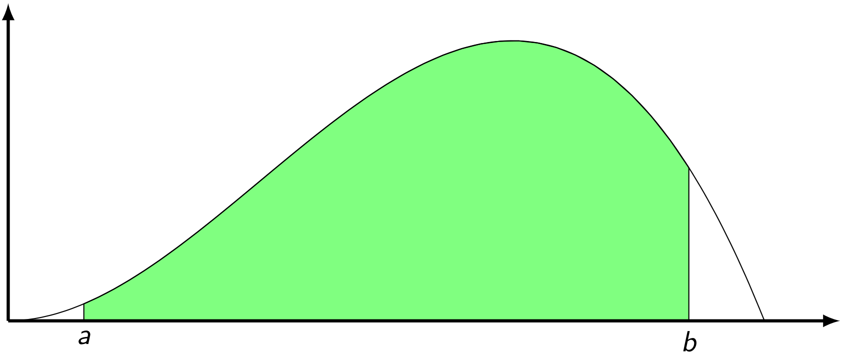
$$= \frac{h}{3}\left(f_+ + 4f_0 + f_-\right)$$

The composite Simpson one-third rule



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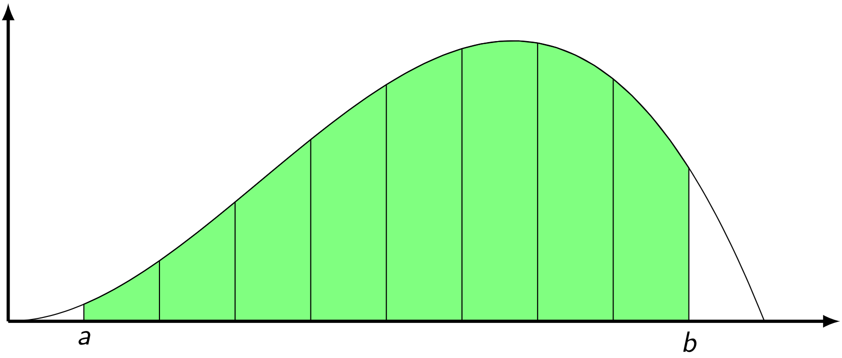
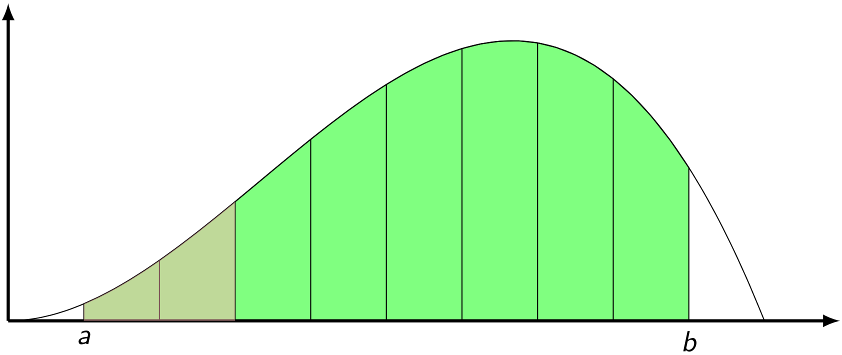


Divide interval from a to b into **even** number of pieces:

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

The composite Simpson one-third rule



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

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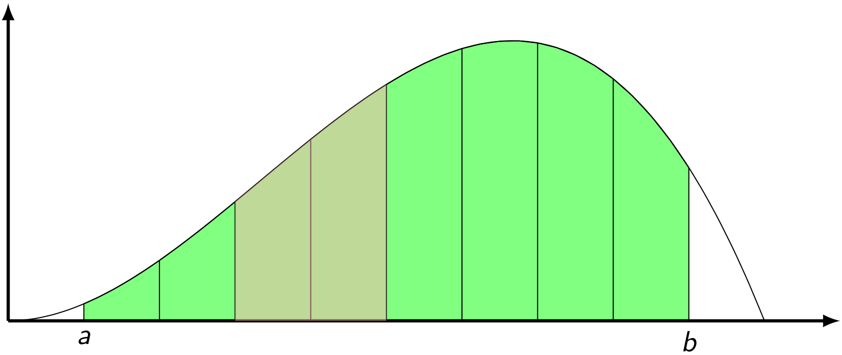

Area

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

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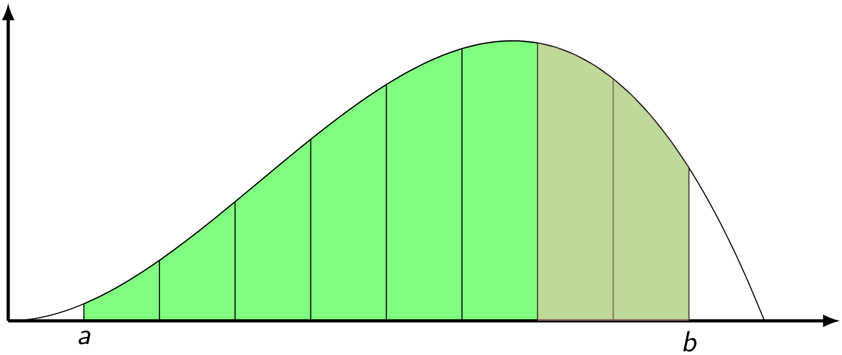

Area

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

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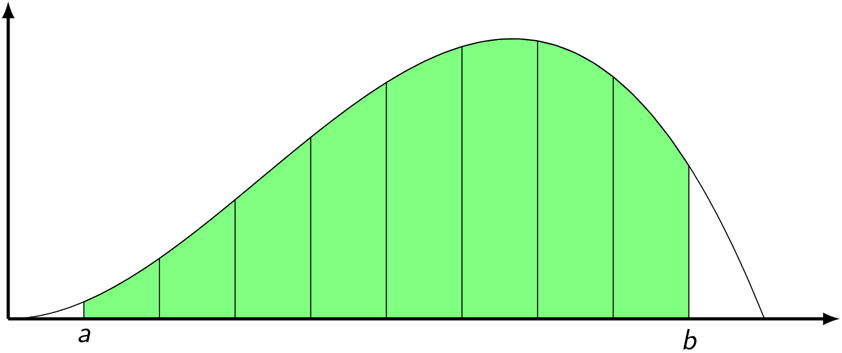

$$\int_a^b f(x)dx$$

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

Newton-Cotes Quadrature Formulae

Trapezoidal rule	$\frac{b-a}{2}(f_0 + f_1)$	$-\frac{(b-a)^3}{12} f^{(2)}(\xi)$
Simpson's $\frac{1}{3}$ rule	$\frac{b-a}{6}(f_0 + 4f_1 + f_2)$	$-\frac{(b-a)^5}{2880} f^{(4)}(\xi)$
Simpson's $\frac{3}{8}$ rule	$\frac{b-a}{8}(f_0 + 3f_1 + 3f_2 + f_3)$	$-\frac{(b-a)^5}{6480} f^{(4)}(\xi)$

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Two point Gauss Quadrature

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$$\approx \frac{b-a}{2}\left[f\left(\frac{b+a}{2} - \frac{\sqrt{3}(b-a)}{6}\right) + f\left(\frac{b+a}{2} + \frac{\sqrt{3}(b-a)}{6}\right)\right]$$