Numerical Integration of Non-Analytical Functions Using Area Estimates

$$\int_0^3 2\exp(-x)\,dx = 2\left[1-\frac{1}{e^3}\right]$$

analytic: has an "anti-derivative"

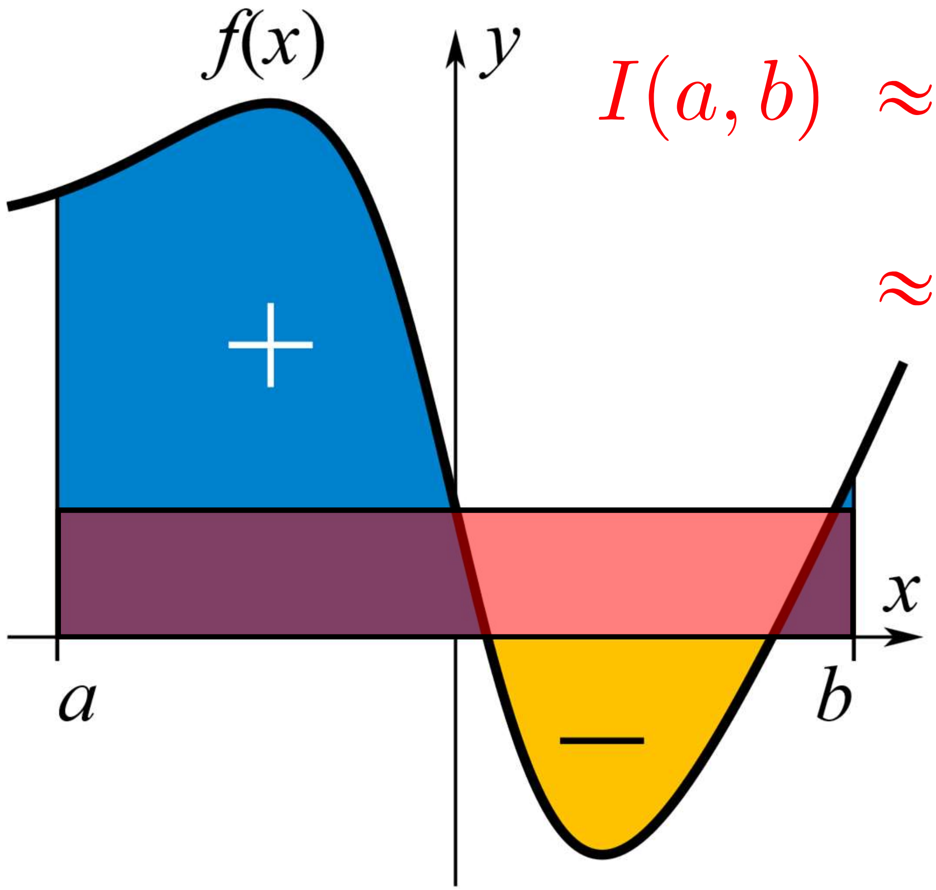
$$\int_0^3 2\exp(-x^2)\,dx \;=\; \mathrm{erf}(3)\sqrt{\pi}$$

$$\mathrm{erf}(z) \;=\; \frac{2}{\sqrt{\pi}}\int_0^z \exp(-t^2)\,dt$$

non-analytic:
error function comes up so often,
it is given a special name,
but must be calculated numerically!

$$\begin{aligned} I(a,b) &\equiv \int_a^b f(x)\,dx \\ &= \text{integral of } f(x) \text{ over the interval } a \leqslant x \leqslant b \\ &= \text{area between the curve and the } x\text{-axis over the interval } a \leqslant x \leqslant b \\ &\approx \textbf{estimate} \text{ of area "under the curve"} \end{aligned}$$

Attempt 0 – "Order of Magnitude" Rule: Single Rectangle



$$I(a,b) \approx (\text{width}) \times (\text{height})$$
$$\approx (b-a) \times f\left(\frac{b+a}{2}\right)$$

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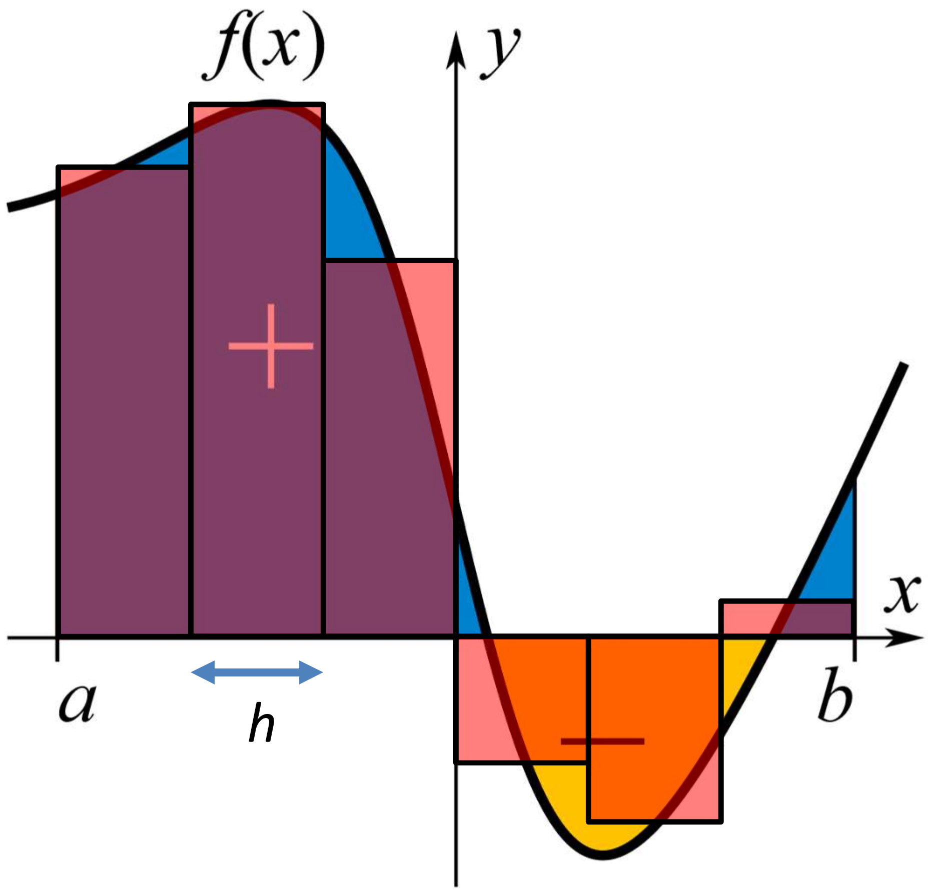
Attempt 1 - Rectangle Rule: Many Rectangles ("Horizontal Tops")



$$I(a,b) \approx \sum_{k=0}^{N-1} h f(x_k)$$

$$N = \text{Number of rectangles}$$

$$h \equiv \frac{b-a}{N}$$

$$x_k = a + \frac{h}{2} + kh$$

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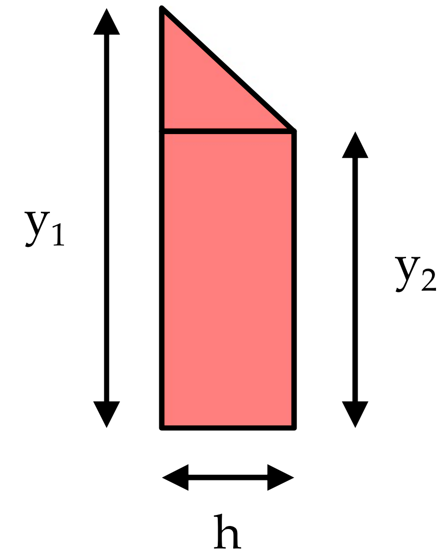
Clicker: (30 s)

What is the area of the trapezoid to the right?



A: area of triangle + area of rectangle = $(y_1\text{-}y_2)*h/2 + y_2*h$

B: (average height of trapezoid)*(width of trapezoid) = $(y_1+y_2)*h/2$

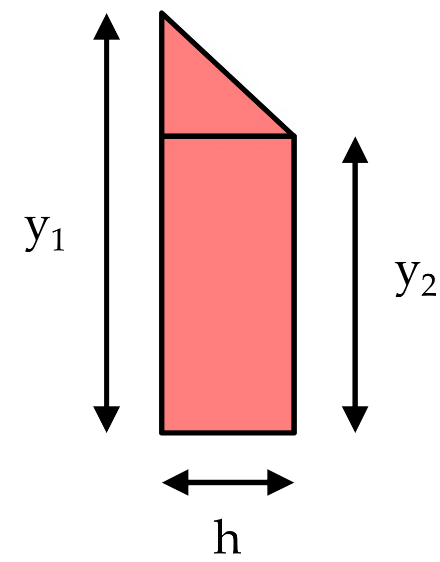
C: A and B

D: not enough information if given

E: none of the above

Clicker:

What is the area of the trapezoid to the right?



A: area of triangle + area of rectangle = $(y_1-y_2)*h/2 + y_2*h$

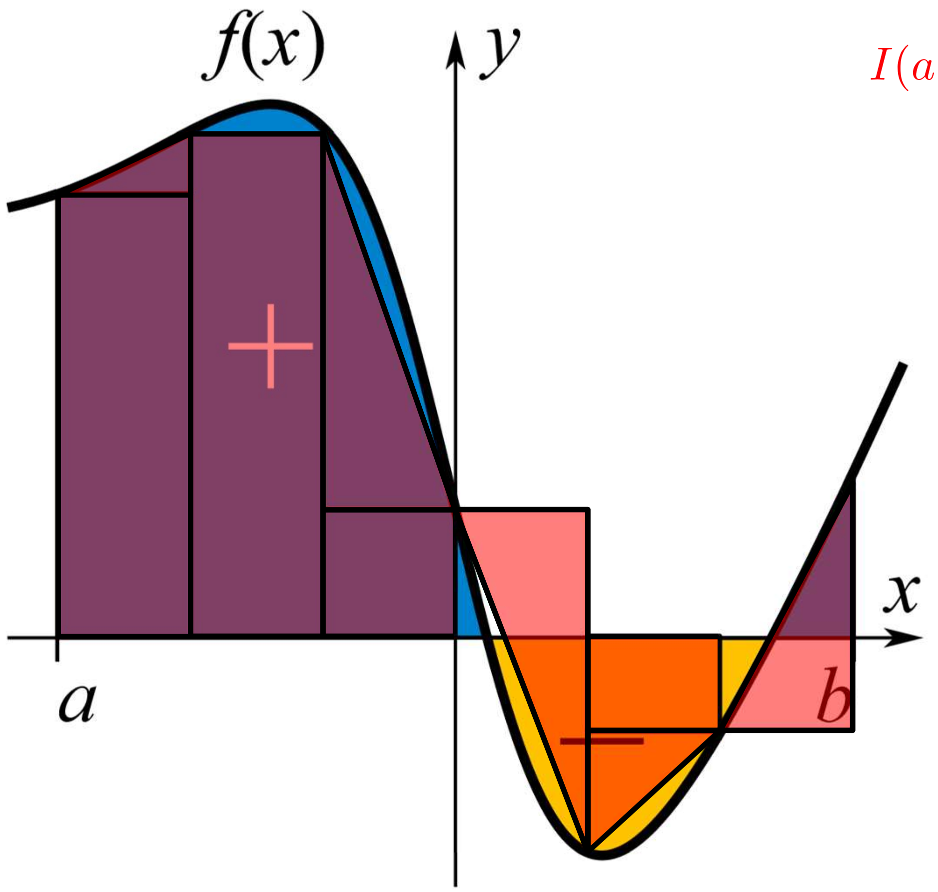
B: (average height of trapezoid)*(width of trapezoid) = $(y_1+y_2)*h/2$

C: A and B

D: not enough information if given

E: none of the above

Attempt 2 - Trapezoid Rule: Many Trapezoids ("Sloped Linear Tops")



$$
\begin{aligned}
I(a,b) &\approx \frac{h}{2}\left[f(a) + f(b) + 2\sum_{k=1}^{N-1} f(x_k) \right] \\
N &= \text{Number of trapezoids} \\
h &\equiv \frac{b-a}{N} \\
x_k &= a + kh
\end{aligned}
$$

https://commons.wikimedia.org/w/index.php?title=File:Integral_example.svg &oldid=463022361

Python Code Example: Trapezoid Rule

```python
# definition of the function
# that needs to be integrated
def f(x):
    return 3*x**2 + 2*x - 100

# Number of trapezoids
N = 10
# value of x at the left
# boundary of integral
a = 0.0
# value of x at the right
# boundary of integral
b = 10.0
# x-interval of integration
# or equivalently width of trapezoid
h = (b-a)/N
# running total of the SUM,
# initialize with the sum of the first and last x-points
s = 0.5*(f(a) + f(b))

# recall that range goes
# from 1 to N-1 in this case
for k in range (1,N):
    s += f(a+k*h)

# the integral is sum of the individual trapezoid areas,
# don't forget to mulitply by h!
area = h*s
print ("area estimate = ",area)
```

```
area estimate =  105.0
```

$$I(a,b) \approx \frac{h}{2}\left[f(a) + f(b) + 2\sum_{k=1}^{N-1} f(x_k) \right]$$

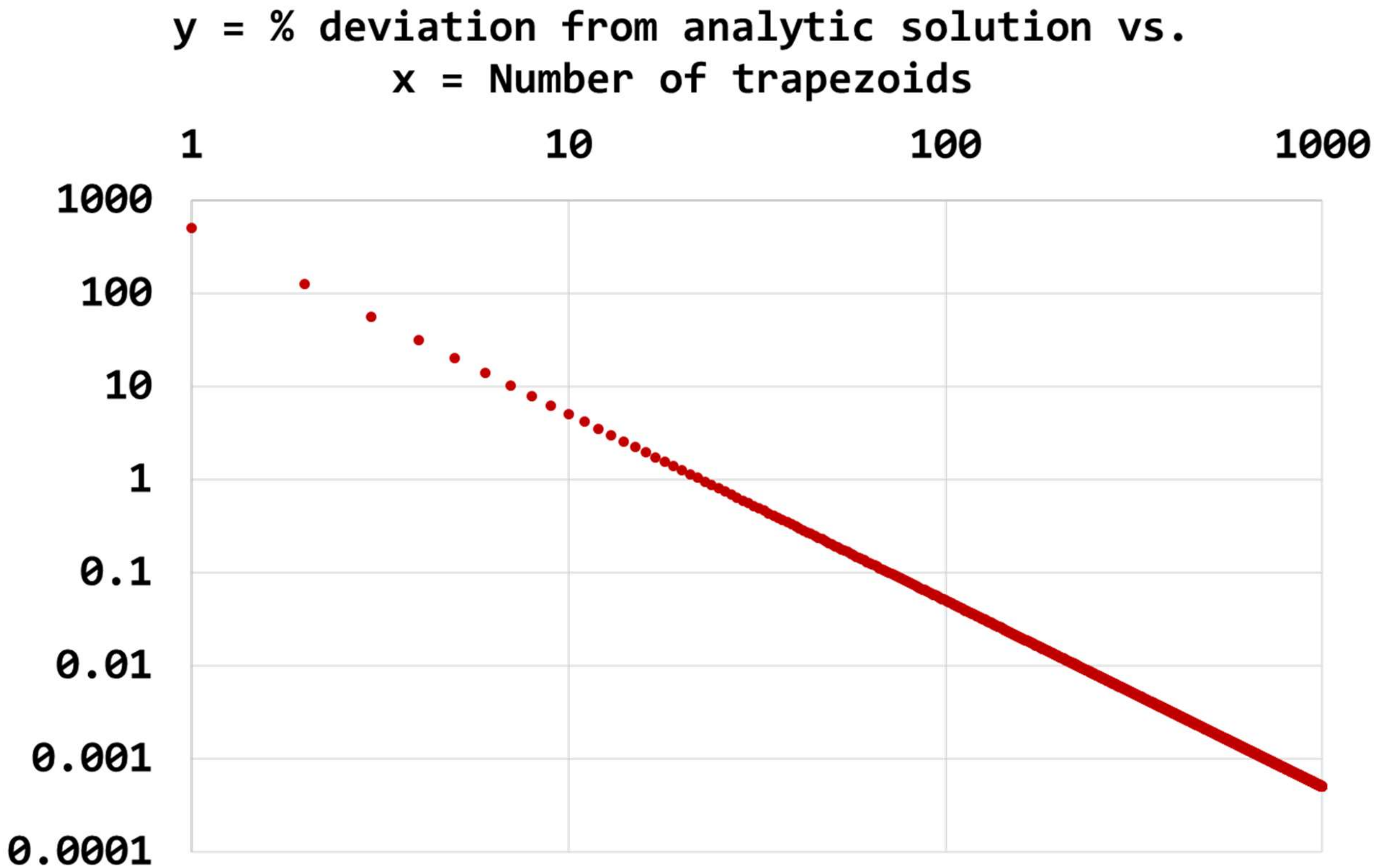
$$N = \text{Number of trapezoids}$$

$$h \equiv \frac{b-a}{N}$$

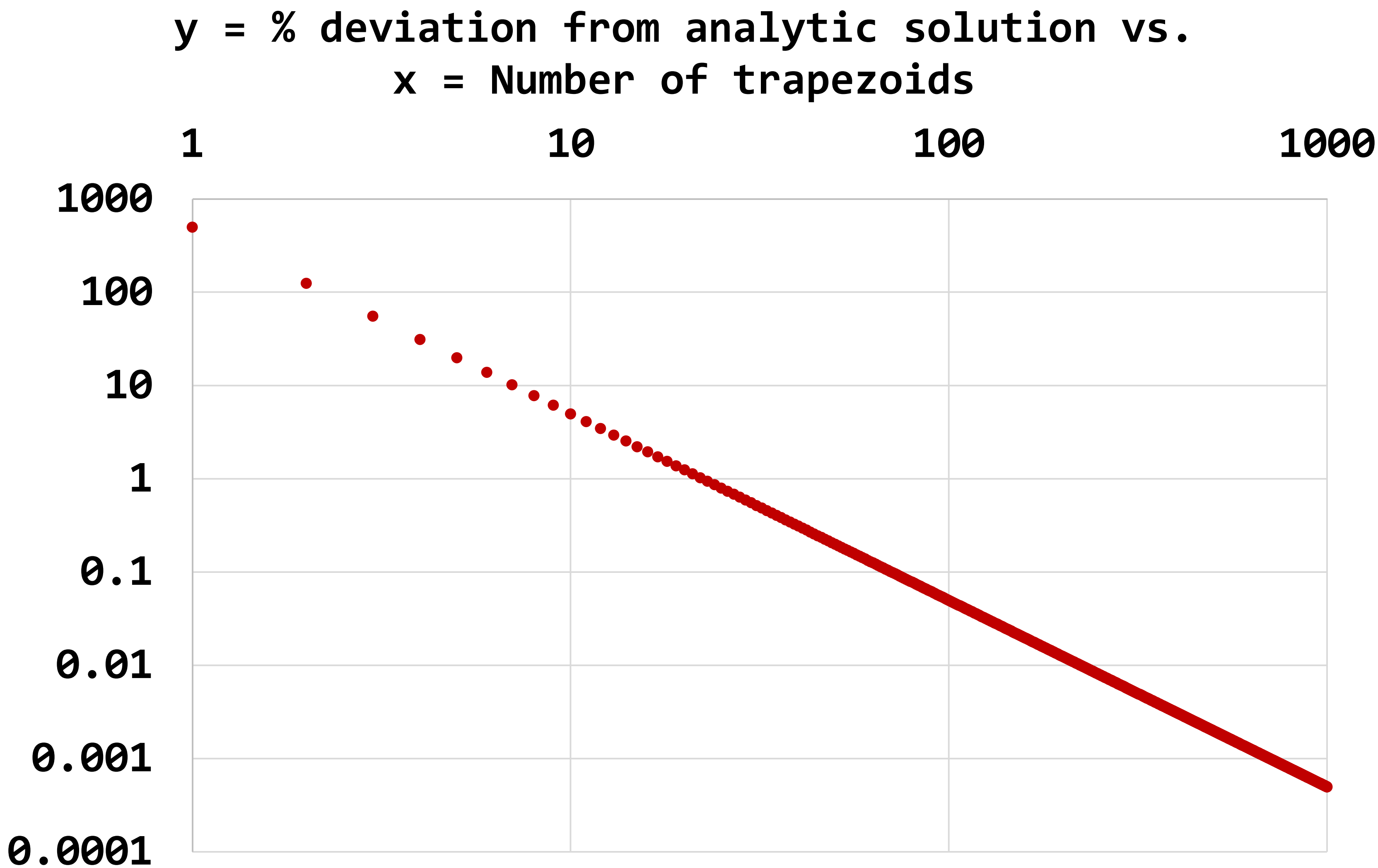
$$x_k = a + kh$$

$$I(0,10) = \int_0^{10} \left(3x^2 + 2x - 100\right)\, dx = 100$$

Python Code Example: “Convergence”



Python Code Example: “Convergence”



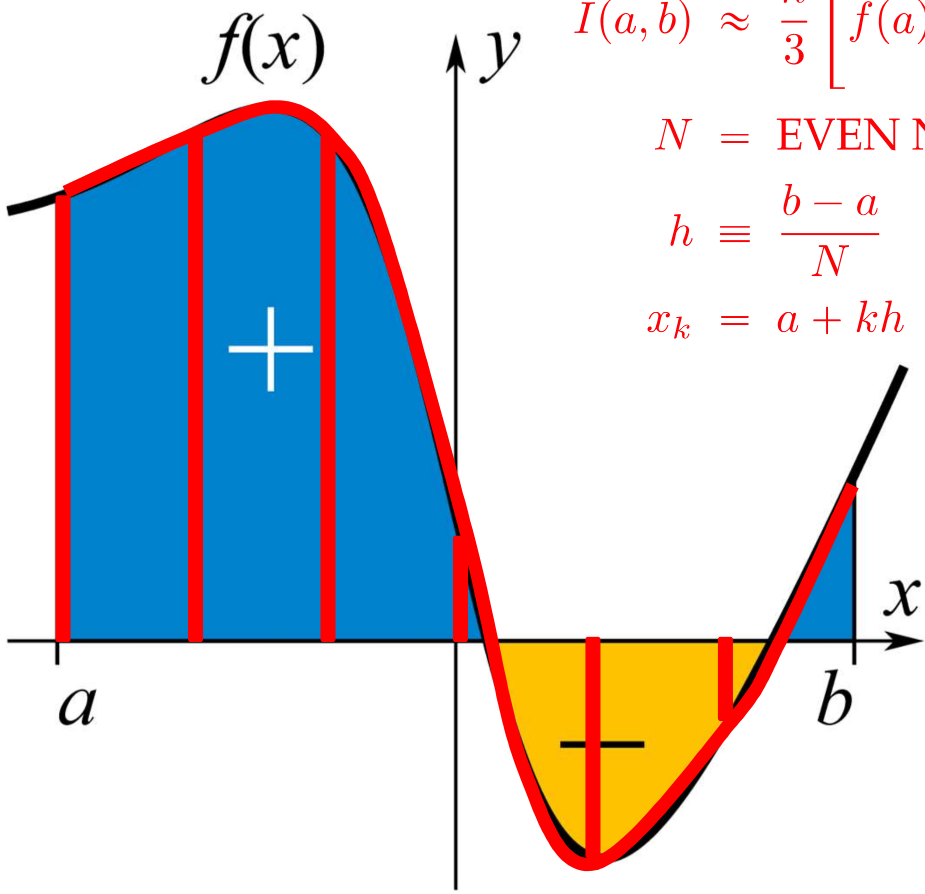
Attempt 3 - Simpson's Rule: Many "Curved Parabolic Tops"

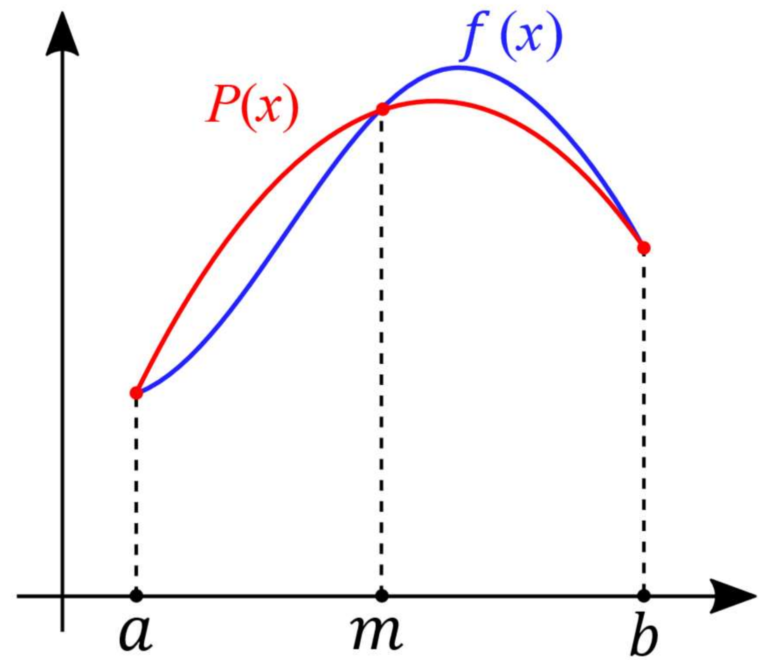
$$I(a,b) \approx \frac{h}{3}\left[f(a) + f(b) + 4\sum_{k_{\mathrm{odd}}=1}^{N-1} f(x_k) + 2\sum_{k_{\mathrm{even}}=2}^{N-2} f(x_k)\right]$$

$$N = \text{EVEN Number of parabolic segments}$$

$$h \equiv \frac{b-a}{N}$$

$$x_k = a + kh$$





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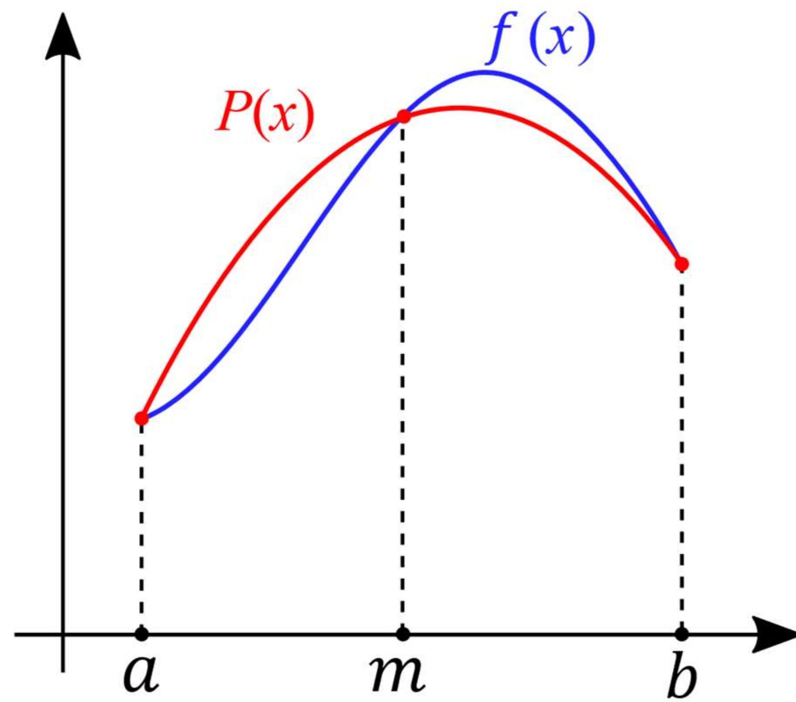
https://commons.wikimedia.org/w/index.php?title=File:Simpsons_method_illustration.svg&oldid=505418410

Simpson's Rule:
Derivation for One Parabolic Segment

Goal: Approximate integral of f(x) for x=a…b with the integral of a parabola P(x) from x=a…b.

1. Approximate function f(x) with parabola $P(x) = A*x^2 + B*x + C$
2. How? **Choose** the coefficients A, B, and C such that :
   - P(a) = f(a)
   - P(m) = f(m=(b+a)/2)
   - P(b) = f(b)
3. Lots of algebra (3 equations and 3 unknowns)!
   - note that h = (b-a)/2
   - $A = [\ f(b) - 2*f(m) + f(a)\ ]/(2*h^2)$
   - $B = [\ f(b) - f(a)\ ]/(2*h)$
   - C = f(m)
4. **Analytically** integrate P(x) from x=a…b to get:
   - $I(a,b) = (2/3)*A*h^3 + 2*C*h$
   - **I(a,b) = (h/3)*[f(a) + 4*f(m) + f(b)]**



https://commons.wikimedia.org/w/index.php?title=File:Simpsons_method_illustration.svg&oldid=505418410

For derivation : https://www.youtube.com/watch?v=7MoRzPObRf0

Clicker:

Simpson's Rule is the approximation of the integral of f(x) for x=a…b with the integral of a parabola $P(x) = A*x^2 + B*x + C$ from x=a…b.

- note that $h = (b-a)/2$
- $A = [\ f(b) - 2*f(m) + f(a)\ ]/(2*h^2)$
- $B = [\ f(b) - f(a)\ ]/(2*h)$
- $C = f(m)$

What are the geometrical interpretation of A, B, and C?

A: A is the **curvature** of f(x) and related to the second derivative of f(x)

B: B is the **average slope** of f(x) and related to the first derivative of f(x)

C: C is the **central value** of f(x)

D: all of the above

E: none of the above

Clicker:

Simpson's Rule is the approximation of the integral of f(x) for x=a…b with the integral of a parabola $P(x) = A*x^2 + B*x + C$ from x=a…b.

- note that $h = (b-a)/2$
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Simpson's Rule:
Just Sum Up N (must be EVEN!) Parabolic Segments

$$
\begin{aligned}
I(a,b) &\approx \frac{h}{3}\left[f(a)+f(b)+4\sum_{k_{\mathrm{odd}}=1}^{N-1} f(x_k)+2\sum_{k_{\mathrm{even}}=2}^{N-2} f(x_k)\right] \\
N &= \text{EVEN Number of parabolic segments} \\
h &\equiv \frac{b-a}{N} \\
x_k &= a+kh
\end{aligned}
$$

`Python` hint for generating even and odd integers:

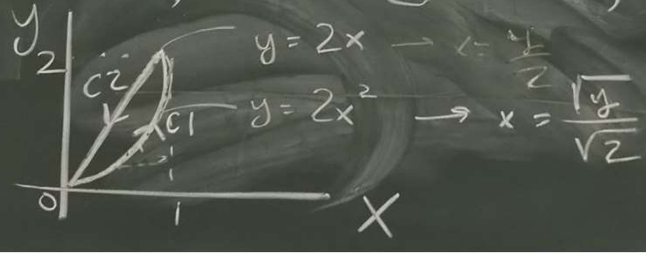
`range(1,10,2)` will output = 1,3,5,7,9
`range(2,10,2)` will output = 2,4,6,8

Rectangle vs. Trapezoid vs. Simpson

property	Rectangle Rule (aka Midpoint Rule)	Trapezoid Rule	Simpson's Rule
shape	rectangle	trapezoid	parabolic segment
top	horizontal line	sloped line	curved line
takes into account	value	value slope	value slope curvature
related to	function	function first derivative	function first derivative second derivative
accuracy $h = (b-a)/N$	weirdly as good as trapezoid rule	okay, error scales like $O(h^3/N^2)$	surprisingly good, error scales as $O(h^5/N^4)$

An example on integral calculus

$\vec{E} = (x^2 - y^2)\,\hat{x} + 2xy\,\hat{y}$. Evaluate $\oint \vec{E}\cdot d\vec{l}$ on the curve bounded by $\{(x,y)\,;\ 0 \le x \le 1\,,\ 2x^2 \le y \le 2x\}$ in CCW-dir.



Do the line integral:

$$d\vec{l} = dx\,\hat{x} + dy\,\hat{y}$$

$$\oint \vec{E}\cdot d\vec{l} = \oint (x^2 - y^2)\,dx + 2xy\,dy = \int_0^1 (x^2 - 4x^4)\,dx + \int_0^2 2\frac{\sqrt{y}}{\sqrt{2}}\,y\,dy + \int_1^0 (x^2 - 4x^2)\,dx$$

$$+ \int_2^0 2\,\frac{y}{2}\,y\,dy$$

Or use the Stoke's theorem:

$$\oint \vec{E}\cdot d\vec{l} = \int_S (\vec{\nabla}\times\vec{E})\cdot d\vec{a}$$

$$d\vec{a} = dx\,dy\,\hat{z}$$

$$(\vec{\nabla}\times\vec{E})\cdot d\vec{a} = 4y$$

$$|\vec{\nabla}\times\vec{E}| = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ \partial/\partial x & \partial/\partial y & \partial/\partial z \\ x^2 - y^2 & 2xy & 0 \end{vmatrix} = 0\,\hat{x} - 0\,\hat{y} + 4y\,\hat{z}$$

$$\int\int_{y=2x^2}^{y=2x} 4y\,dy\,dx = \int_{x=0}^{x=1} \Big[2y^2\Big]_{2x^2}^{2x} dx$$

$$= 16/15$$