ASSIGNMENT #1: due before TUESDAY 3/2

ASSIGNMENT #2: due before THURSDAY 3/4

Numerical Methods III: quadratures

Quadratures = integration of functions

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All the methods we will discuss are for equally spaced abscissas: $f(x_i)$ so that $x_{i+1}-x_i=h$ for every i:
$x_i=x_0+ih$, for $i=0,\dots,N-1$ $\quad$ $f_i=f(x=x_i)$

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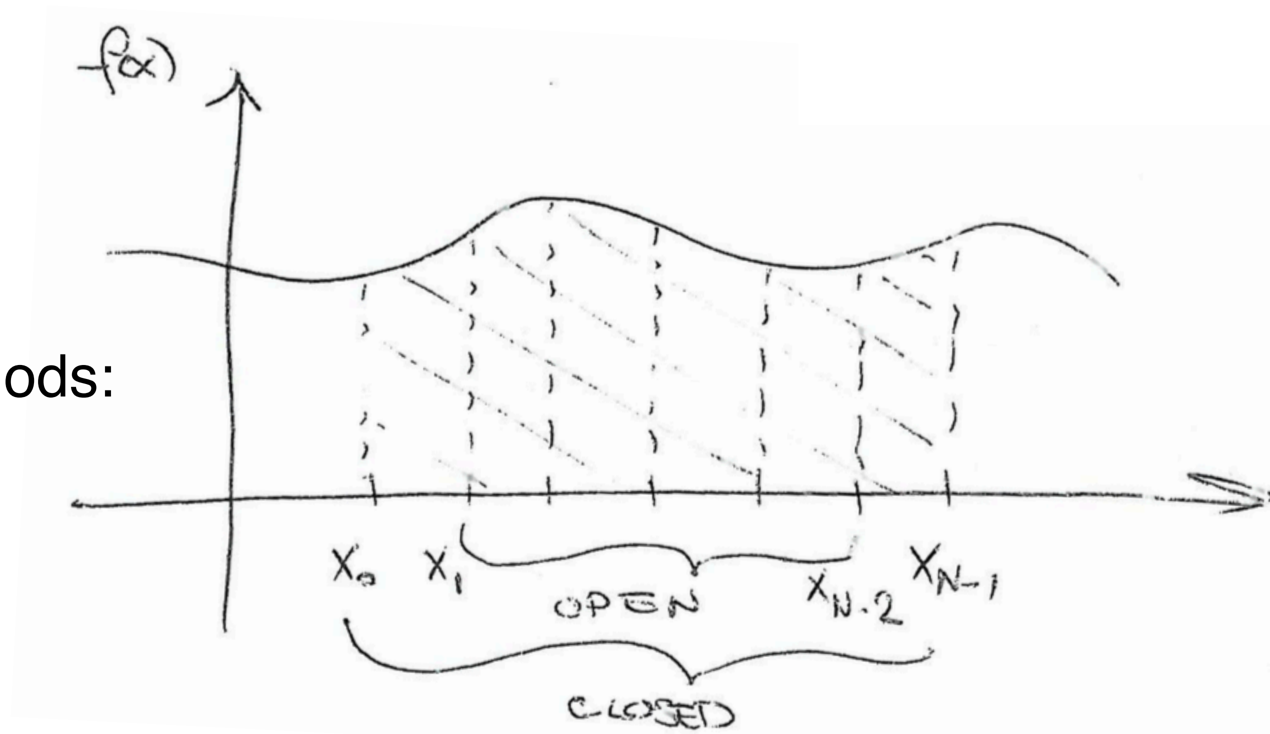

Within this approach, there are two families of methods:
1) **CLOSED** formulas make use of f_0 and f_{N-1}
2) **OPEN** formulas do not make use of f_0 and f_{N-1},
i.e., they use $f_1,\dots f_{N-2}$.

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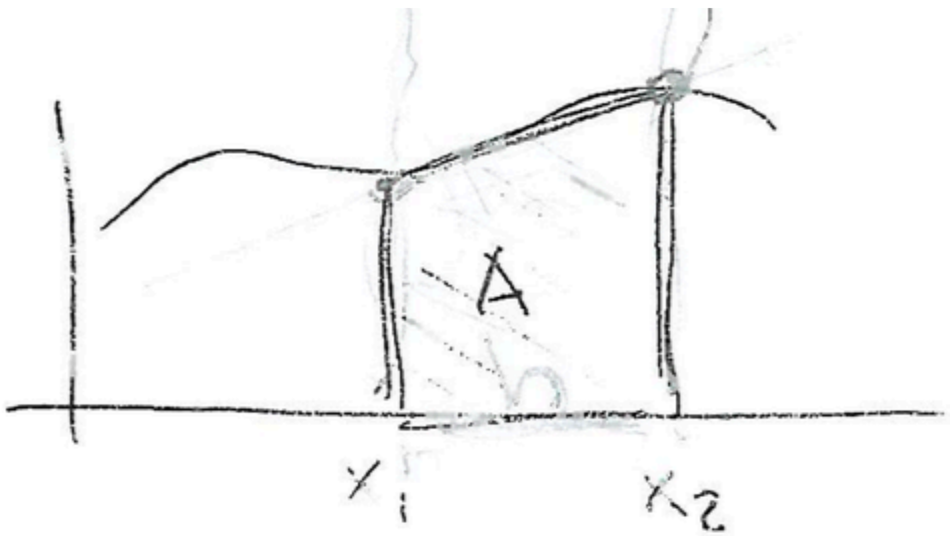

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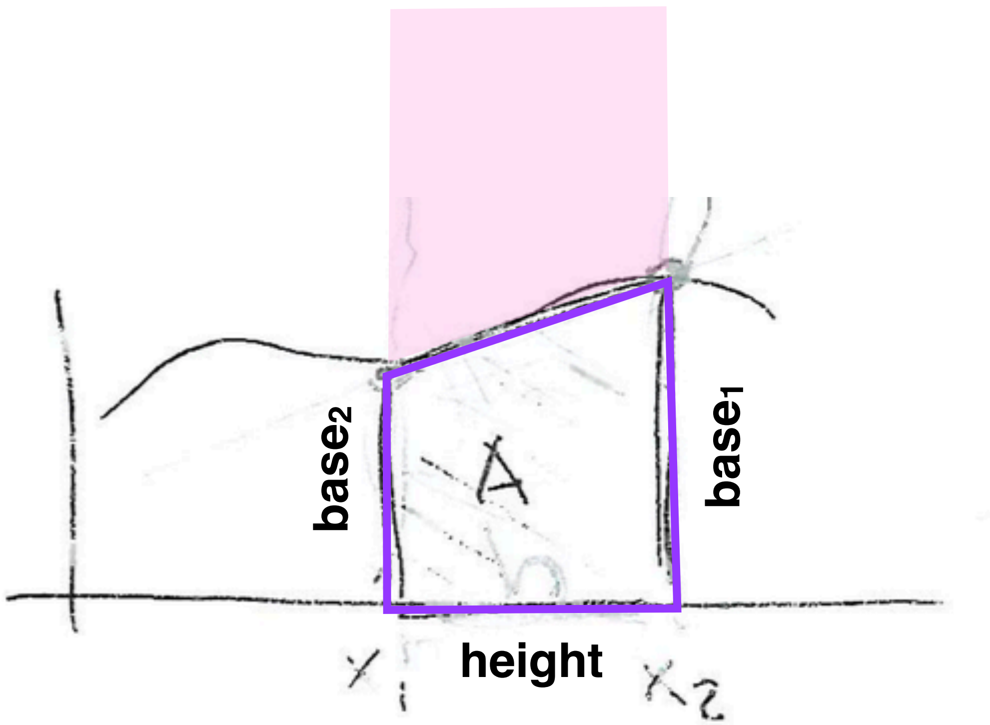

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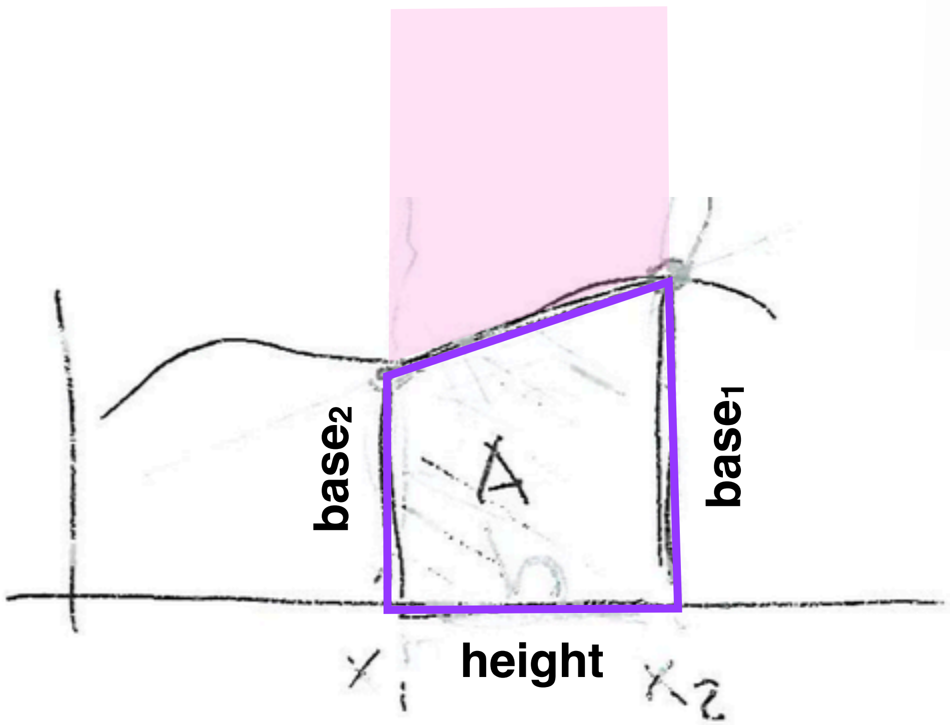

$$I = \int_{x_1}^{x_2} f(x)\,dx = (f_1 + f_2)\,\frac{h}{2} + \mathcal{O}\left(h^3 f''\right) \qquad (2)$$

error of order of f''h^3

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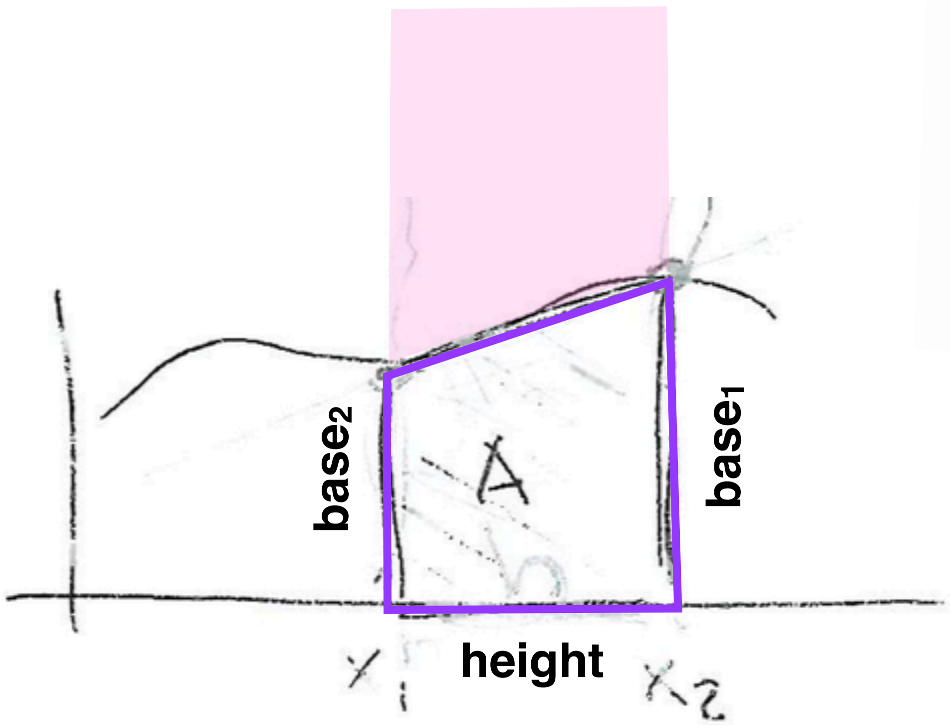

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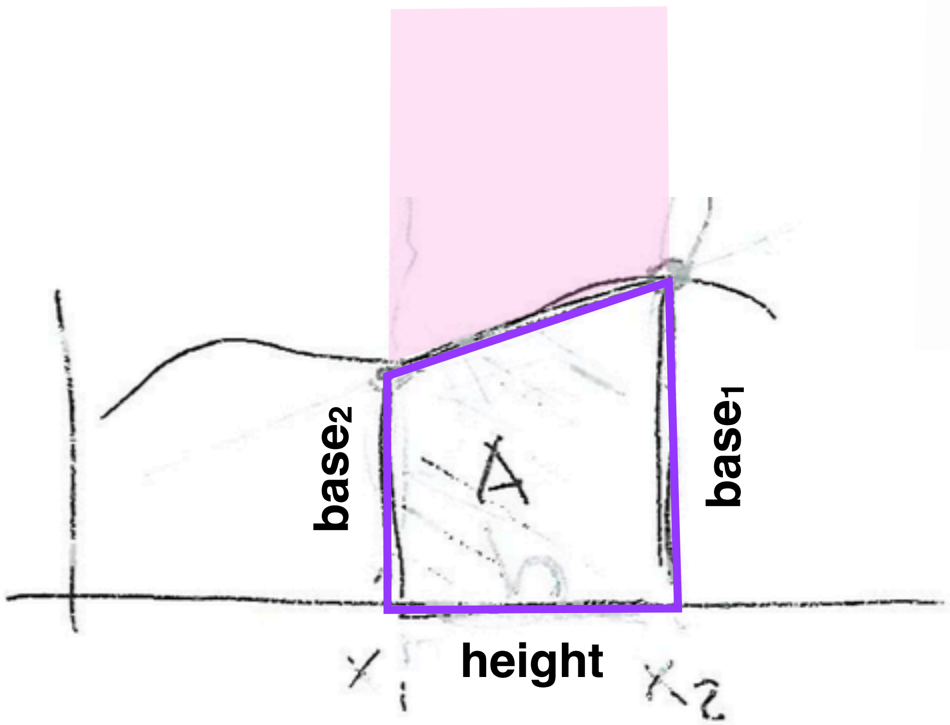

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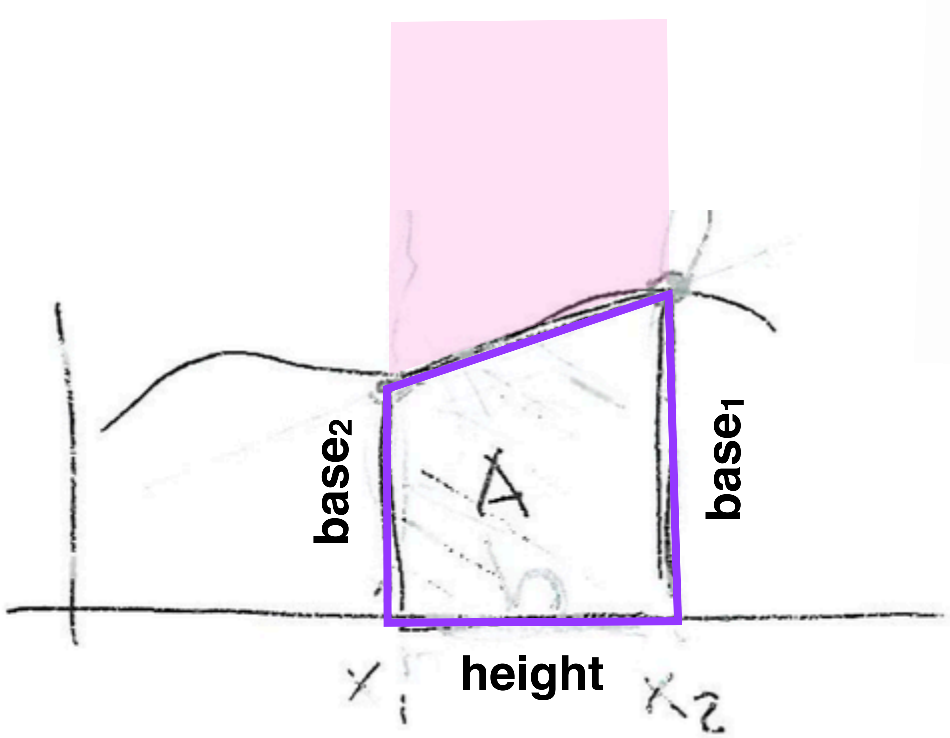

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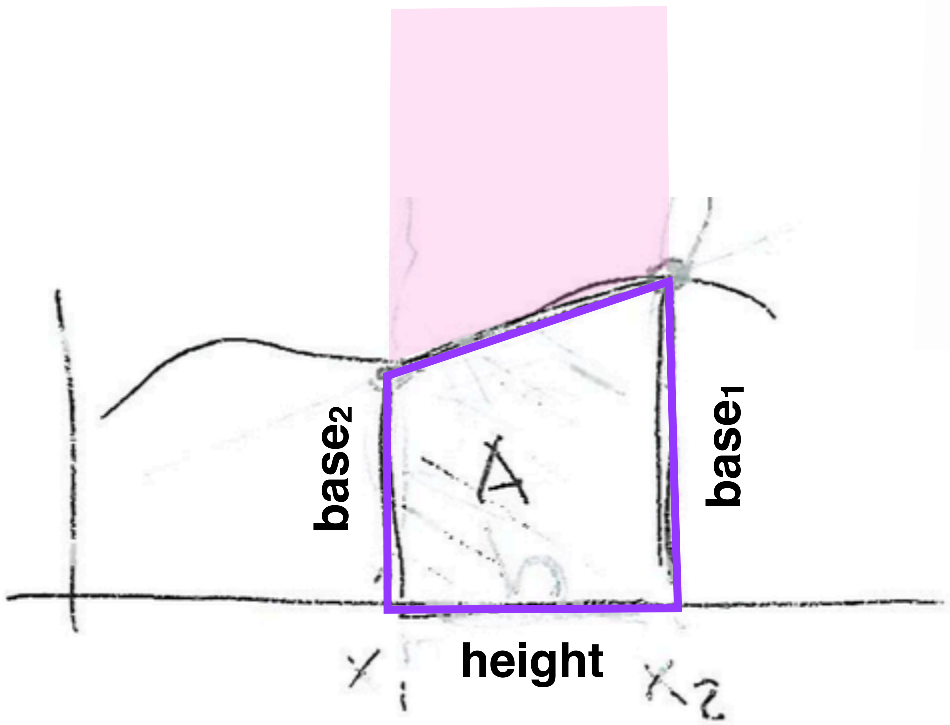

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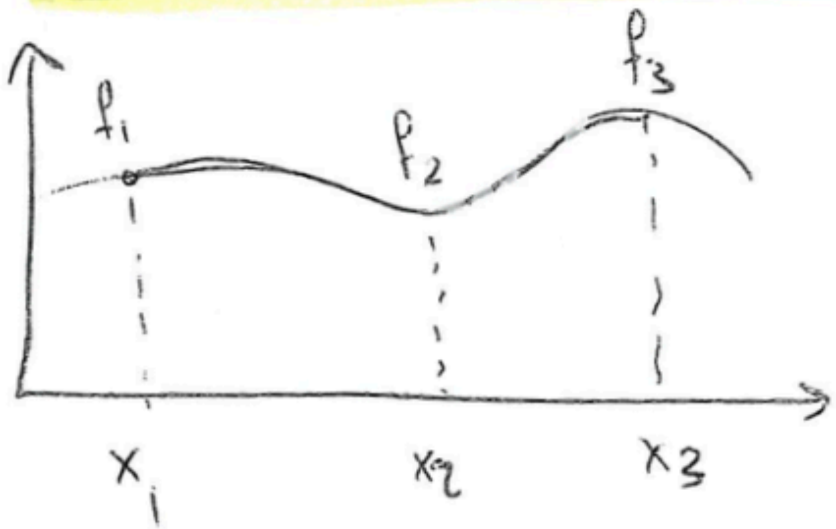
A: YES, and even better!

2) Simpson formula

$$I = \int_{x_1}^{x_3} f(x)dx = h\left[\frac{1}{3}f_1 + \frac{4}{3}f_2 + \frac{1}{3}f_3\right] + O(h^5 f'') \quad (3)$$



Taylor expand f(x) around x_1, x_2, and x_3, trying to get rid of all the error that you can and you end up with this formula.

This is exact for a polynomial of order 3 included, because there is cancellation of error, i.e., we have chosen our coefficients so as to remove the $O(h^4)$ error term.

Q: How about a 4 point formula?
A: in this case, there is no cancellation of terms and I get **Simpson's 3/8 formula**:

$$\int_{x_0}^{x_3} f(x)dx = h\left[\frac{3}{8}f_0 + \frac{9}{8}f_1 + \frac{9}{8}f_2 + \frac{3}{8}f_3\right] + O(h^5 f^{(4)}) \qquad \textbf{(4)}$$

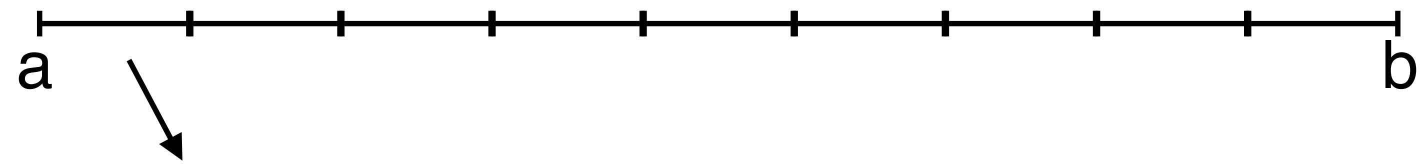
NOTE 1: in general, (4) is more accurate than (3) because usually $f^{(4)}$ is smaller than f", unless for some pathological function (at fixed h).

NOTE 2: because both (3) and (4) have errors ~$O(h^5)$, Simpson's formula with 3 points is generally more efficient.

5) Bode's formula: with 5 points

$$\int_{x_0}^{x_4} f(x)dx = h\left[\frac{14}{45}f_0 + \frac{64}{45}f_1 + \frac{24}{45}f_2 + \frac{64}{45}f_3 + \frac{14}{45}f_4\right] + O(h^7 f^{(6)})$$

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



$$I = \sum_j I_j$$

L: over L I use one of the above formulas, i.e., the number of points for each sub interval depends on the formula that I want to use.

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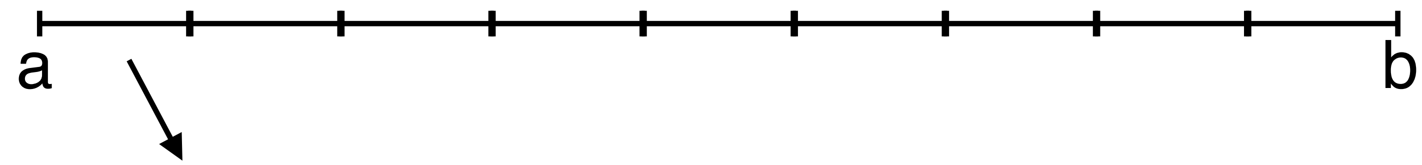

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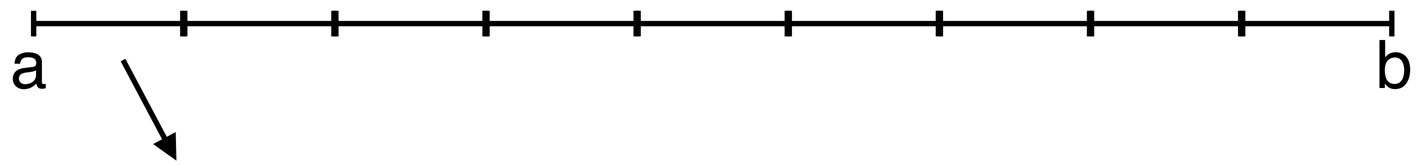

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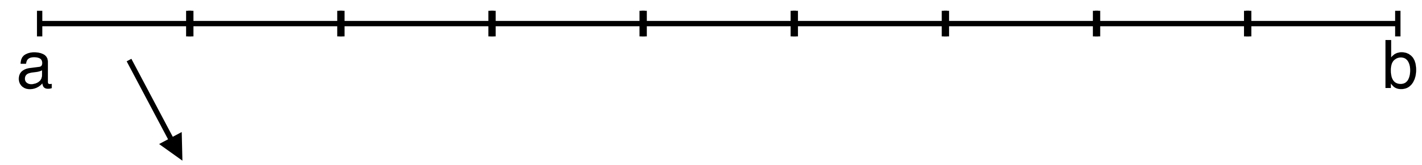

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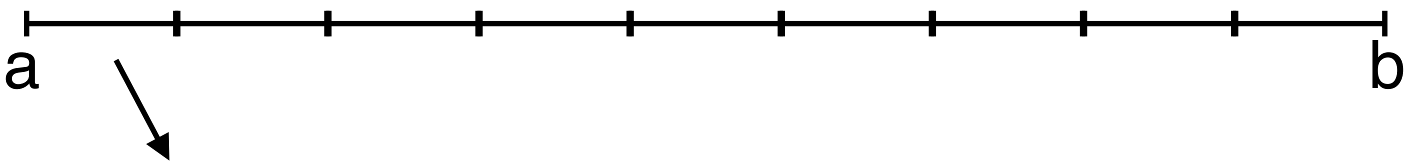

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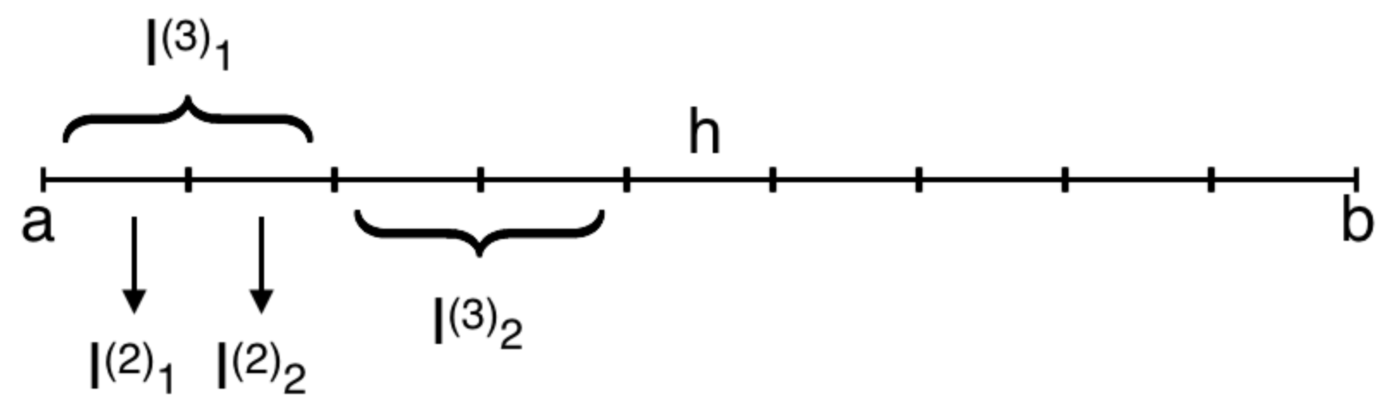

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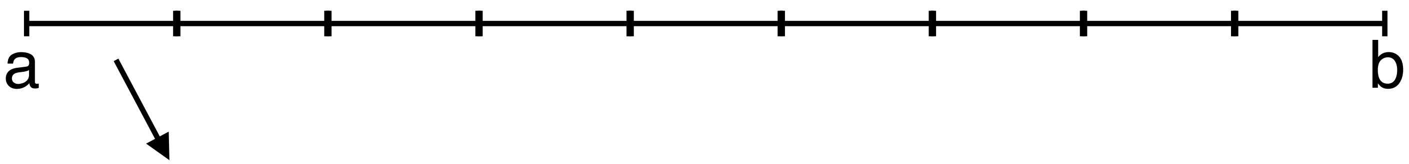

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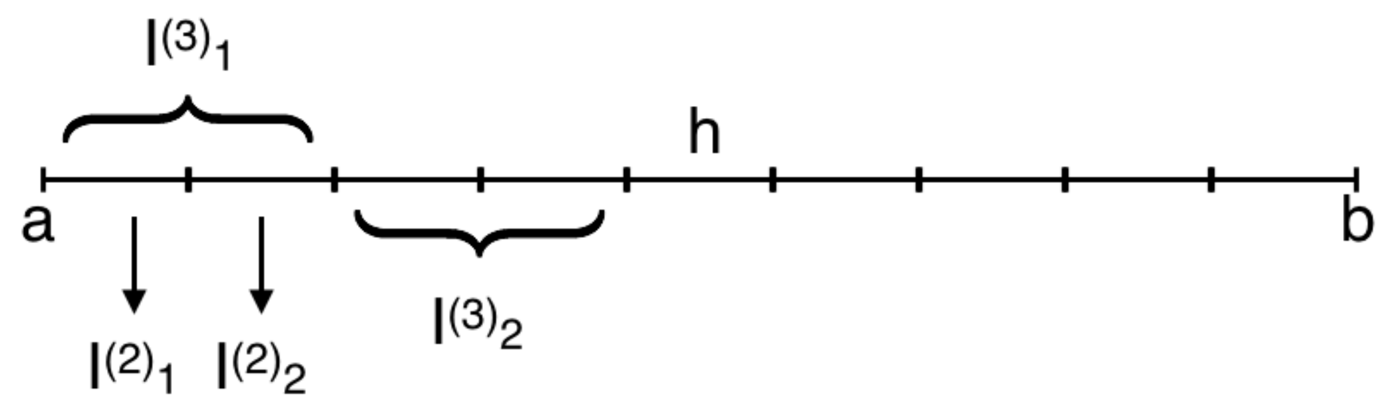

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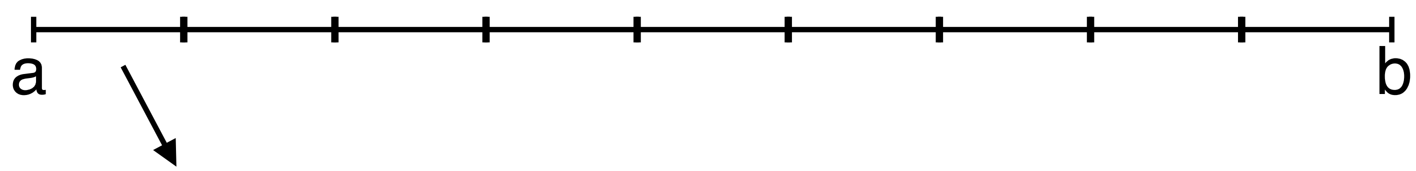

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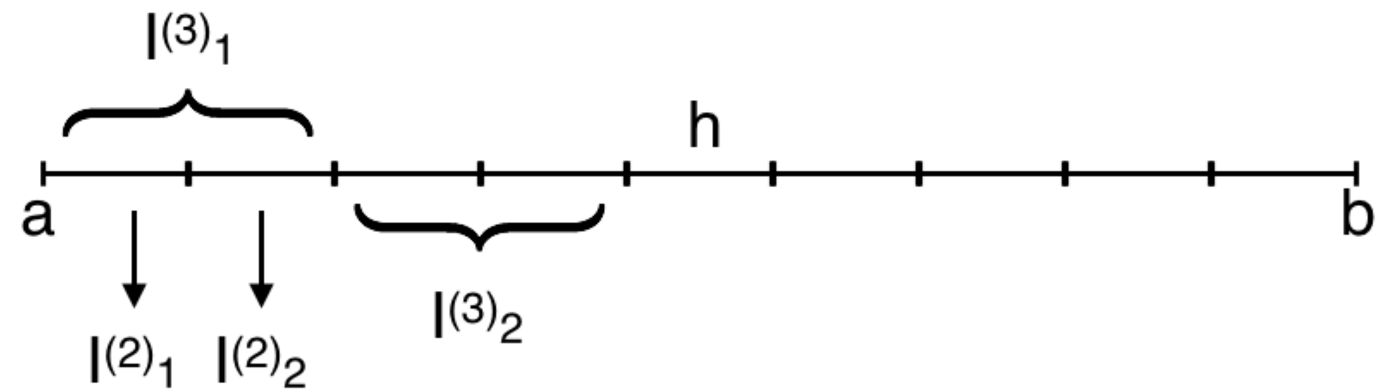


I can then write:

$$I = \sum_j I_j^{(2)} + O(h^3 f'')$$

$$I = \sum_j I_j^{(3)} + O(h^5 f'')$$

$$I = \sum_j I_j^{(4)} + O(h^5 f^{(4)})$$

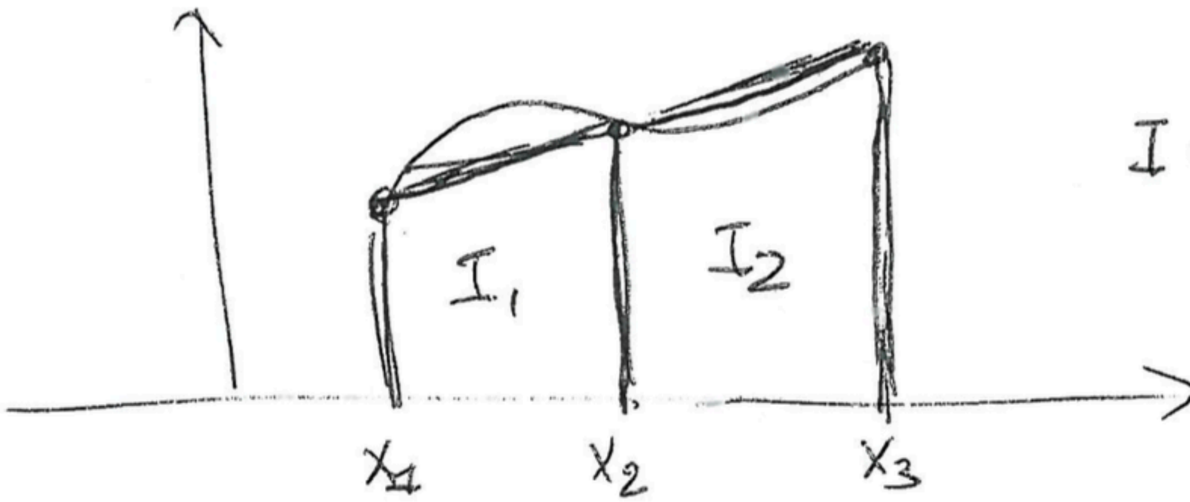
and so on…

Following this logic, we can write **extended formulas**

Q: Why are these extended formulas useful?

A: They allow us to forget about the number of points and minimize computational cost.

Example:



$$I = I_1 + I_2 = \frac{f_1 + f_2}{2} h + \frac{f_2 + f_3}{2} h$$

I need to calculate f_2 twice, whereas with the extended formulas only once.

6) Extended trapezoidal rule (*)

$$\int_{x_1}^{x_N} f(x)\,dx = h\left[\frac{1}{2} f_1 + f_2 + \ldots + f_{N-1} + \frac{1}{2} f_N\right] + O\left(\frac{\mathcal{L}^3}{N^2} f''\right)$$

7) Simpson's extended formula (*)

$$I = \int_{x_1}^{x_N} f(x)\,dx = h\left[\frac{1}{3} f_1 + \frac{4}{3} f_2 + \frac{2}{3} f_3 + \frac{4}{3} f_4 + \frac{2}{3} f_5 + \ldots + \frac{2}{3} f_{N-2} + \frac{4}{3} f_{N-1} + \frac{1}{3} f_N\right] + O\left(N^{-4}\right)$$

The 2/3, 4/3 alternation continues throughout the interior of the evaluation

There is a beauty about the numerical implementation of the trapezoidal rule

$$\int_{x_1}^{x_2} f(x)dx = h[\frac{1}{2}f_1 + f_2 + ... + f_{N-1} + \frac{1}{2}f_N]$$

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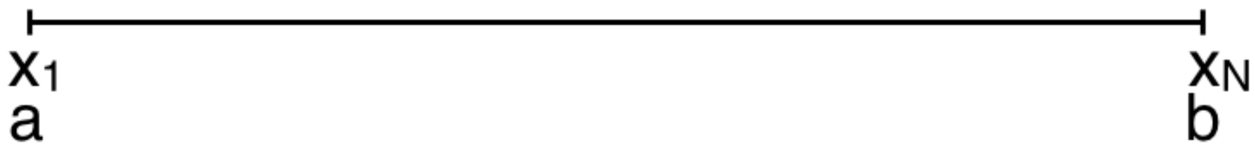

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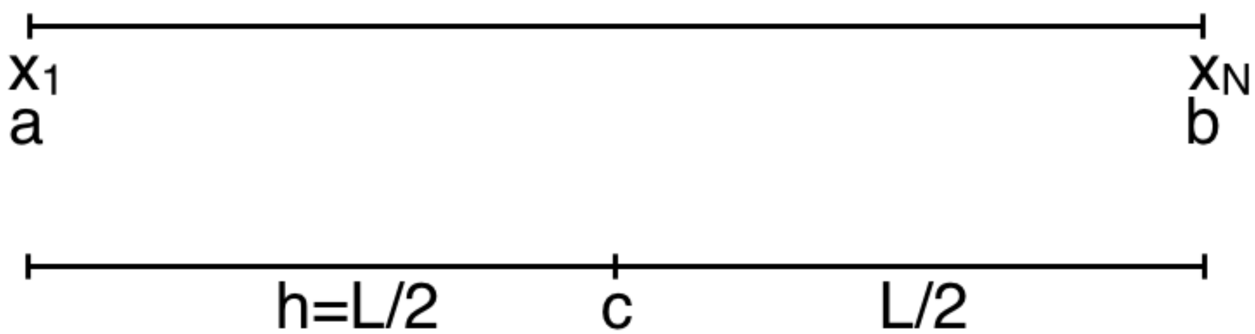

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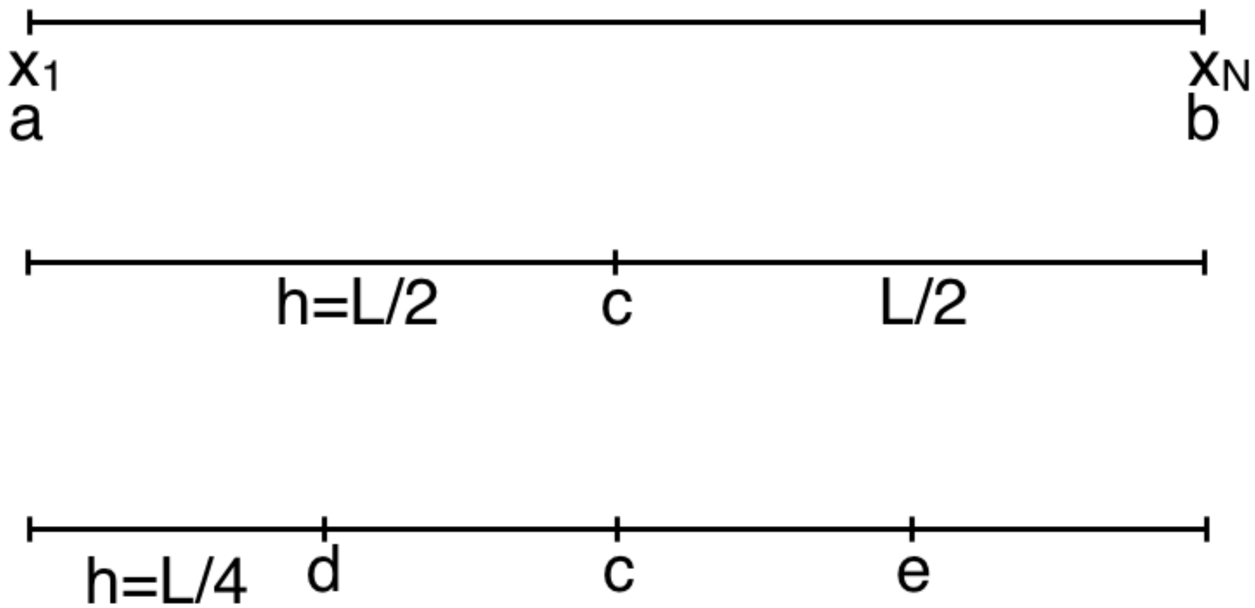

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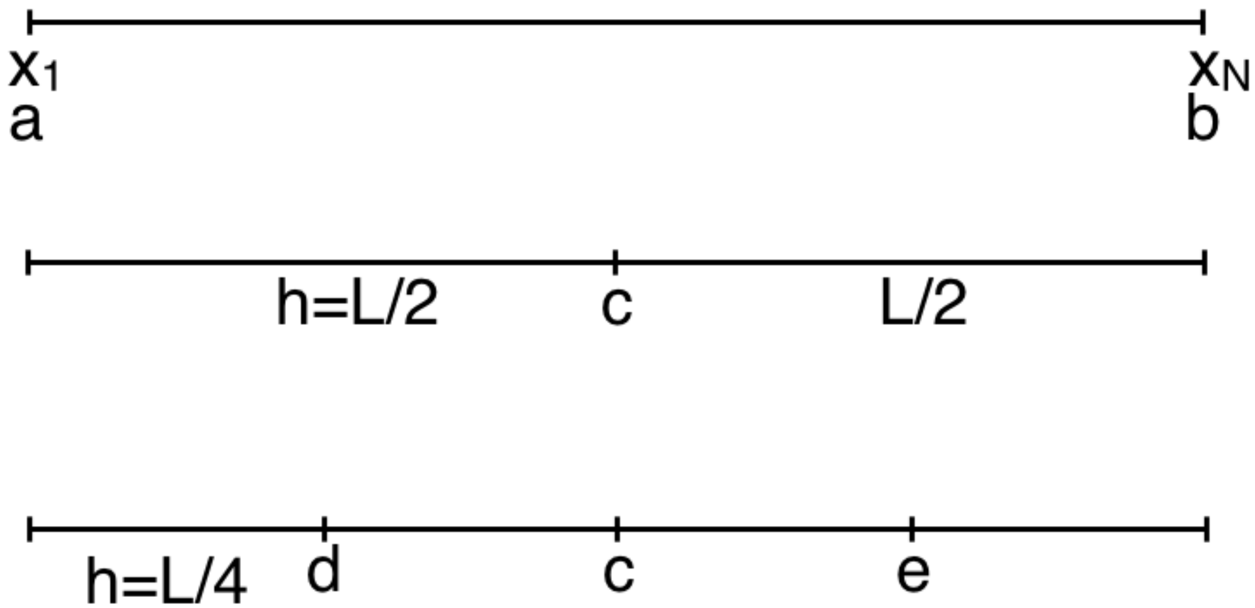

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$$= \frac{1}{2}(\frac{I_1}{2} + \frac{L}{2}f_c) + \frac{L}{4}(f_d + f_e) =$$

$$= \frac{1}{2}[\frac{L}{4}(f_a + f_b)] + \frac{L}{4}f_c + \frac{L}{4}(f_d + f_e)$$

$$= \frac{h}{2}(f_a + f_b) + hf_c + h(f_d + f_e)$$

i.e., the trapezoidal rule!

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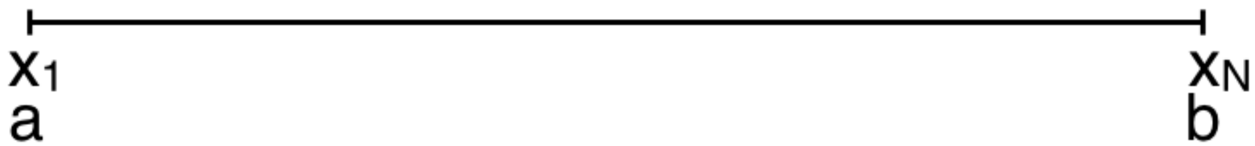

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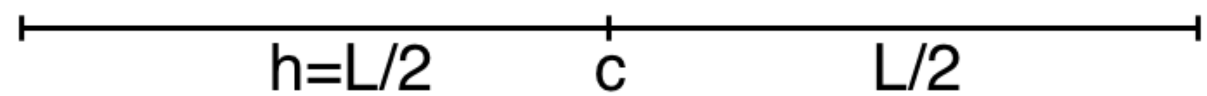
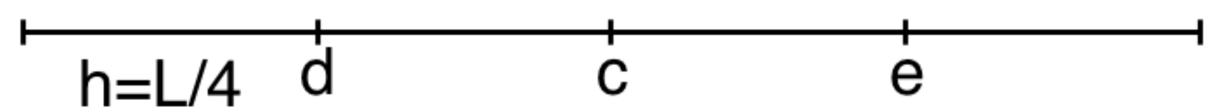


$$I_2 = \frac{1}{2}(I_1 + Lf_c)$$



$$I_3 = \frac{I_2}{2} + \frac{Lf_d}{4} + \frac{Lf_e}{4} =$$

$$= \frac{1}{2}(\frac{I_1}{2} + \frac{L}{2}f_c) + \frac{L}{4}(f_d + f_e) =$$

$$= \frac{1}{2}[\frac{L}{4}(f_a + f_b)] + \frac{L}{4}f_c + \frac{L}{4}(f_d + f_e)$$

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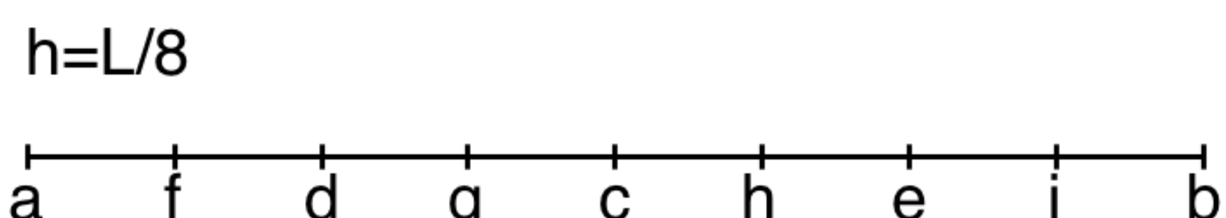

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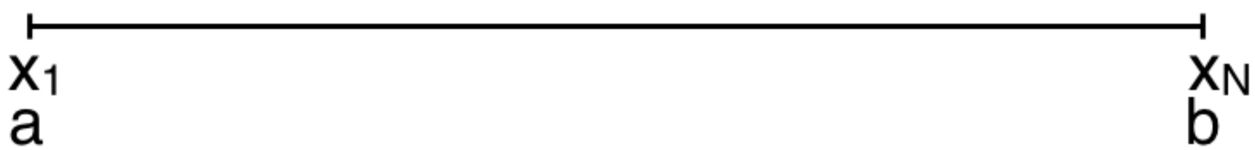
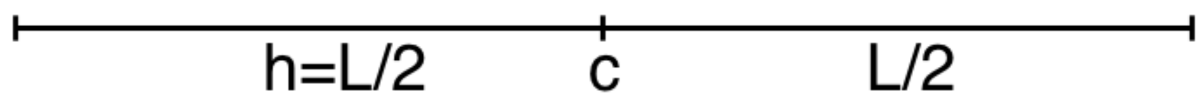
$$I_4 = \frac{I_3}{2} + \frac{1}{8}L[f_f + f_g + f_h + f_i] = ... = \frac{h}{2}(f_a + f_b) + h(f_c + f_d + f_e + f_f + f_g + f_h + f_i)$$

There is a beauty about the numerical implementation of the trapezoidal rule

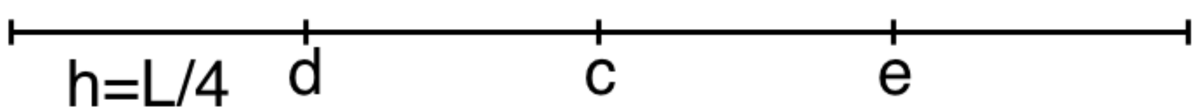
$$\int_{x_1}^{x_2} f(x)dx = h[\frac{1}{2}f_1 + f_2 + ... + f_{N-1} + \frac{1}{2}f_N]$$



$$I_1 = \frac{L}{2}(f_a + f_b)$$



$$I_2 = \frac{1}{2}(I_1 + Lf_c)$$



$$I_3 = \frac{I_2}{2} + \frac{Lf_d}{4} + \frac{Lf_e}{4} =$$

$$= \frac{1}{2}(\frac{I_1}{2} + \frac{L}{2}f_c) + \frac{L}{4}(f_d + f_e) =$$

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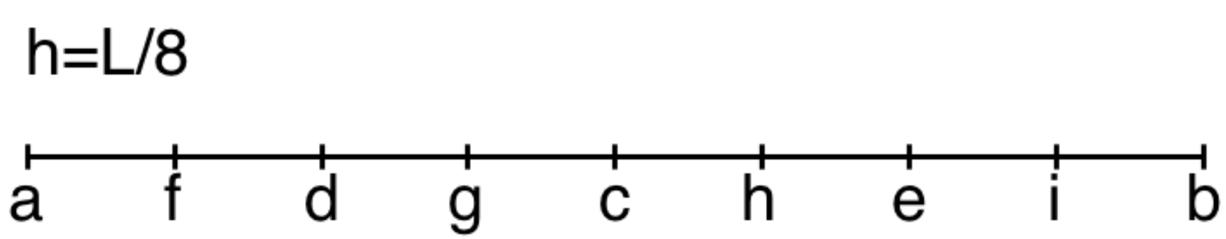

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Try this algorithm in the assignment

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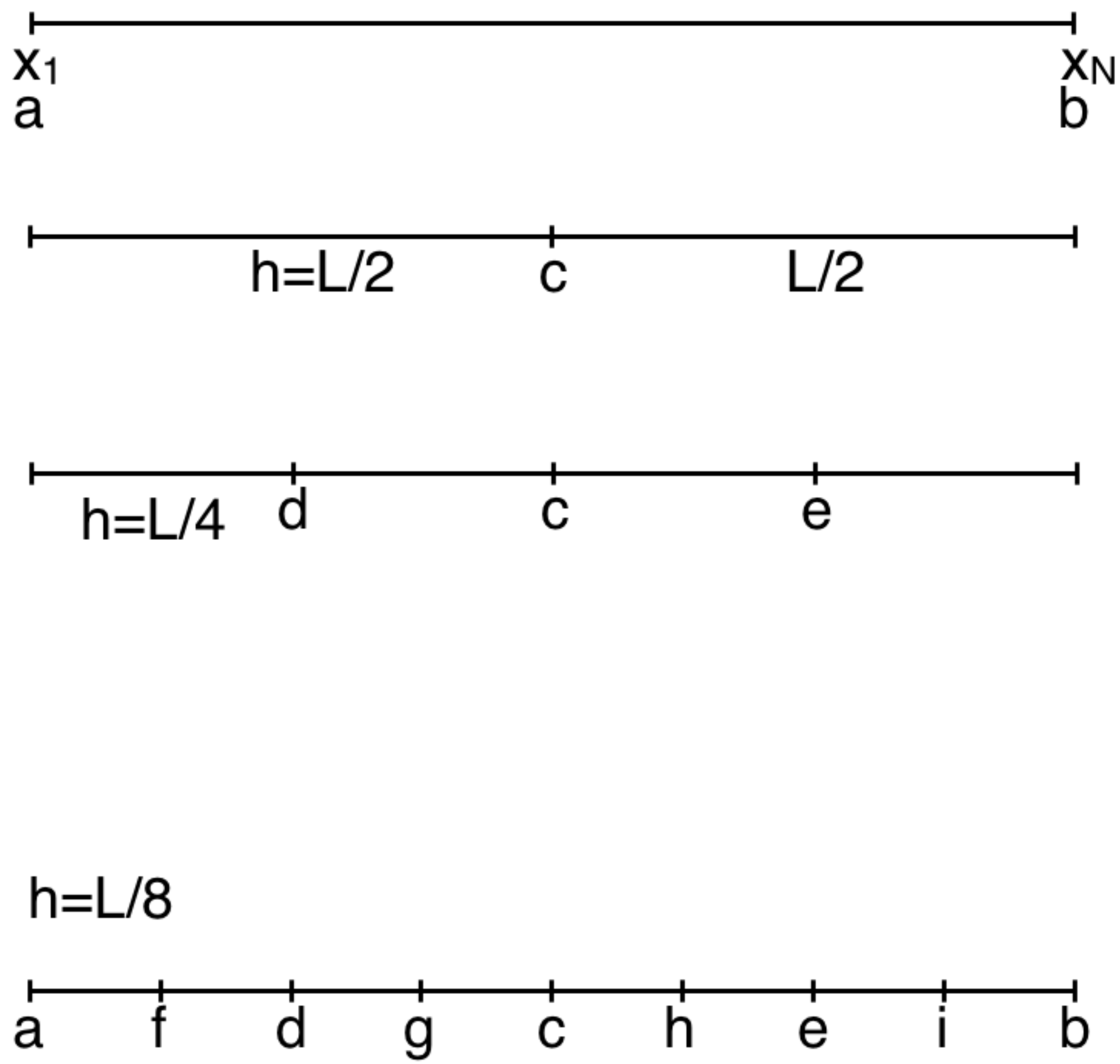

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Try this algorithm in the assignment

In Num. Rec. this is TRAPZD

In Num. Rec., there is QTRAP: this is the TRAPZD implementation until some specific degree of accuracy is achieved.

In Num. Rec., QSIMP is the integration routine to be preferred.

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Examples:

a) the integrand is finite at one extreme but cannot be evaluated, e.g., $\frac{\sin x}{x}$ for $x \approx 0$

$$\int_0^1 \frac{\sin x}{x} dx$$

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NOTE: if an integral is infinite ($\int_1^\infty x^{-1} dx$) or does not exist in a limiting sense ($\int_{-\infty}^{\infty} \cos x dx$), we do not call it improper, we call it IMPOSSIBLE! No amount of clever algorithms will return a meaningful answer to an ill-posed problem!!

Midpoint formula:

$$\int_{x_1}^{x_N} f(x)\,dx = h\left[f_{1/2} + f_{3/2} + f_{5/2} + \ldots + f_{N-3/2} + f_{N-1/2}\right] + O\left(\frac{1}{N^2}\right)$$

Open extended formula:

$$\int_{x_1}^{x_N} f(x)dx = h\left[\frac{55}{24}f_2 - \frac{1}{6}f_3 + \frac{11}{8}f_4 + f_5 + f_6 + \ldots + f_{N-5} + f_{N-4} + \frac{11}{8}f_{N-3} - \frac{1}{6}f_{N-2} + \frac{55}{24}f_{N-1}\right] + O(1/N^4)$$