CS 3200
Introduction to Scientific Computing

Instructor: Martin Berzins

Topic: Numerical Integration

Application of polynomial theory already covered

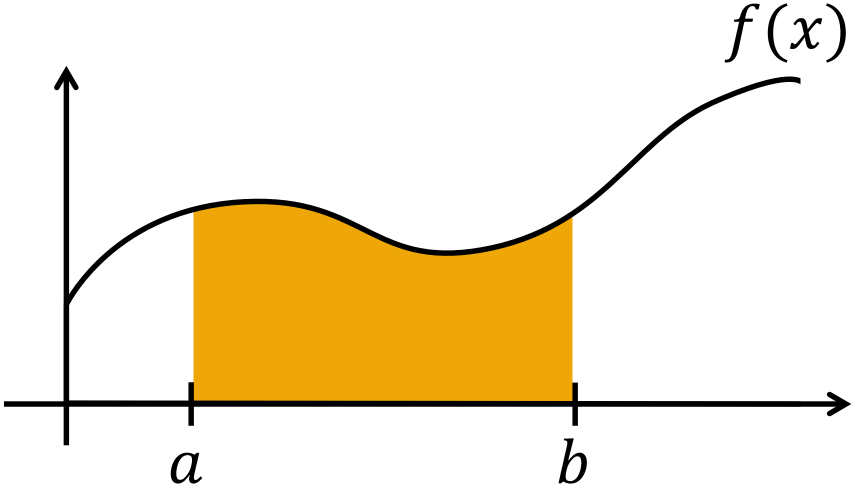
Numerical Integration

- Goal: find the area under the curve

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

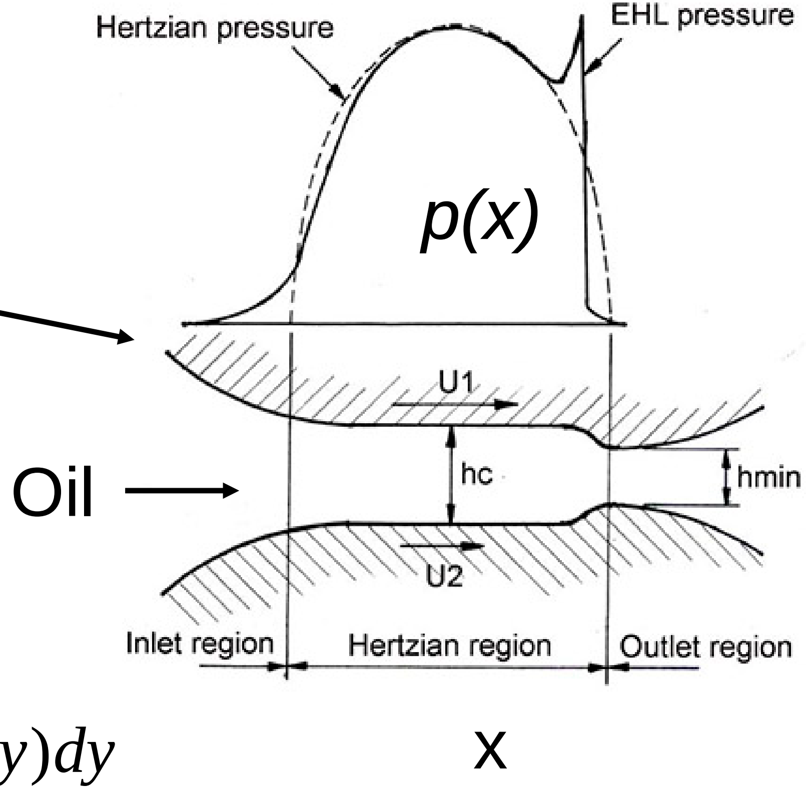
This application occurs with great frequency e.g. in the clean coal boiler or in finance

We often model f(x) by using a polynomial, as we have already covered



Example from Engineering

- When oil is used in lubricating a car engine the pressures are sufficiently high that the steel deforms from the original semi-circular shape to
- The relationship between the pressure *p(x)* and the thickness of the oil film *h(x)* is given by the integral. Note this is part of a much larger problem.

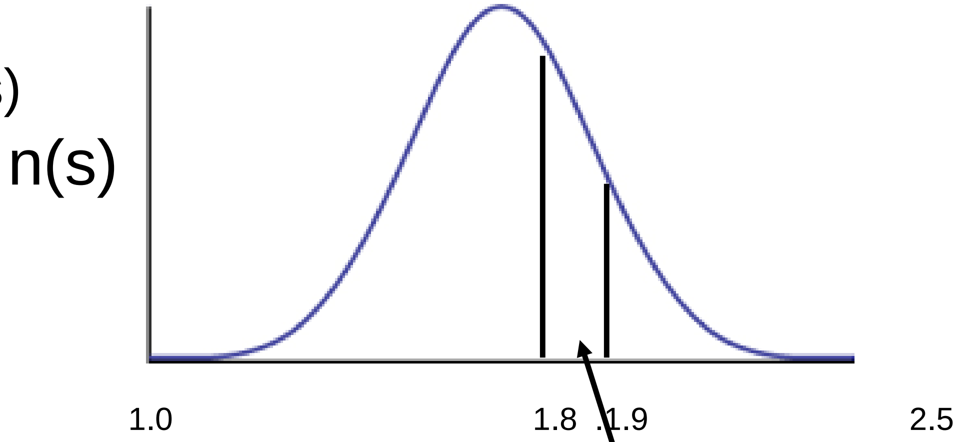


$$h(x) = h_{00} + \frac{x^2}{2R_x} - \frac{4}{\pi E}\int_{-\infty}^{\infty} \ln\left|\frac{x-y}{x_0}\right| p(y)\,dy$$

Quadrature Example – Normal Distribution

Consider population of large number (M) of individuals. Distribution of their heights, n(s) given by

$$n(s) = \frac{M}{\sigma\sqrt{2\pi}} e^{-(s-mean)^2/(2\sigma^2)}$$



$$N_{[h_1,h_2]} = \int_{h_1}^{h_2} n(s)ds, \quad \text{where } h_1 = 1.8, h_2 = 1.9, mean = 1.7m, \sigma = 0.1,$$

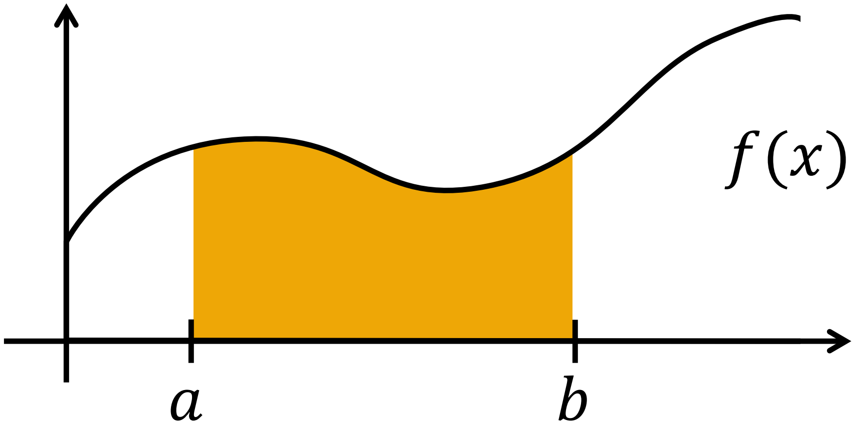
$$M = 200$$

We need to calculate this area to estimate how many of the 200 are between 1.8m and 1.9m tall

Numerical Integration

- How: the weighted sum of the function sampled N-times

$$\int_a^b f(x)dx \approx \sum_{i=1}^{N} w_i f(x_i)$$



- With each –
  - w_i: sampling weight
  - x_i: sampling location

Calculation of $\{w_i, x_i\}$ pairs known as:

QUADRATURE SCHEMES

Newton-Cotes Formula

- Newton-Cotes formulae are formed using interpolating polynomials over equally spaced sample points
- We will discuss:
    - Constant interpolant (over a closed interval): *midpoint rule*
    - Linear interpolant (over a closed interval): *trapezoidal rule*
    - Quadratic interpolant (over a closed interval): *simpson's rule*
- Formulae exist for higher-order interpolants over both closed (includes end points) and open (does not include end points) intervals

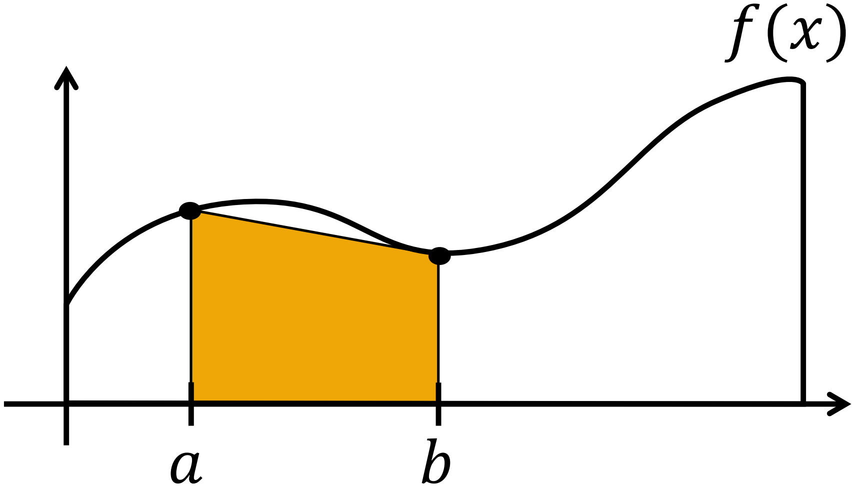
Trapezoidal Rule

- Approximate the integral by the area of a trapezoid with endpoints a and b:

$$\int_a^b f(x)dx \approx \frac{1}{2}(b-a)(f(a)+f(b))$$

- The rule's error on one interval is given by:

$$\epsilon \leq \frac{(b-a)^3}{12} f''(\zeta) = \mathcal{O}((b-a)^3)$$



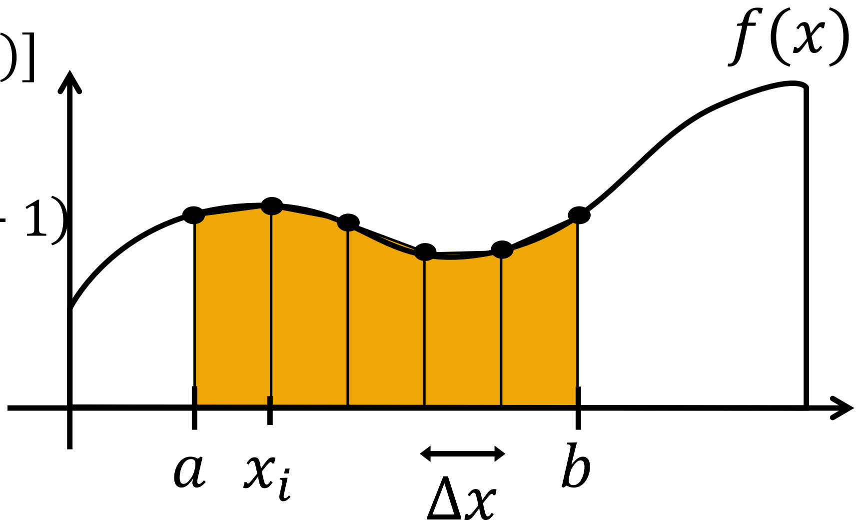
Composite Trapezoidal Rule

- Approximate the integral by $N-1$ applications of the trapezoidal rule

$$\int_a^b f(x)dx \approx \sum_{i=1}^{N-1} \frac{1}{2}\frac{b-a}{N}[f(x_\mathrm{i}) + f(x_{i+1})]$$

where $x_i = a + \frac{(\mathrm{b-a})}{\mathrm{N}}(\mathrm{i}-1)$

- Can we simplify this to fit Quadrature Notation?



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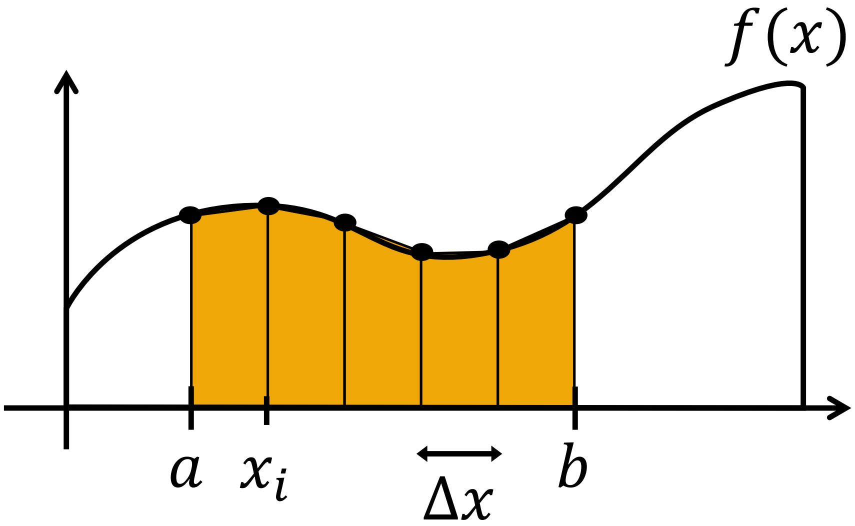
where $x_i = a + \frac{(\mathrm{b-a})}{\mathrm{N}}(\mathrm{i}-1)$

- Can we simplify this to fit Quadrature Notation?
- What if we rewrite as:

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

$$\approx \frac{1}{2}\frac{(\mathrm{b}-\mathrm{a})}{\mathrm{N}}\left[f(x_1) + \left(\sum_{i=2}^{N-1} 2f(x_i)\right) + f(x_N)\right]$$



Composite Trapezoidal Rule

- Quadrature notation

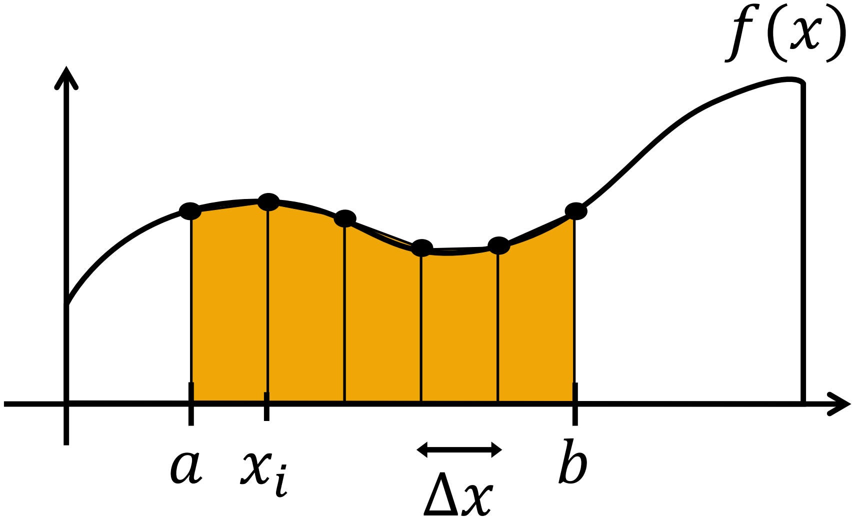
$$\int_a^b f(x)dx \approx \sum_{i=1}^{N} w_i f(x_i)$$

- This can be written as

$$x_i = a + (i-1)\Delta x$$

$$w_i = \begin{cases} \frac{\Delta x}{2}, & i = 1, N \\ \Delta x, & i = 2, \dots, N-1 \end{cases}$$

where $\Delta x = \frac{b-a}{N-1}$



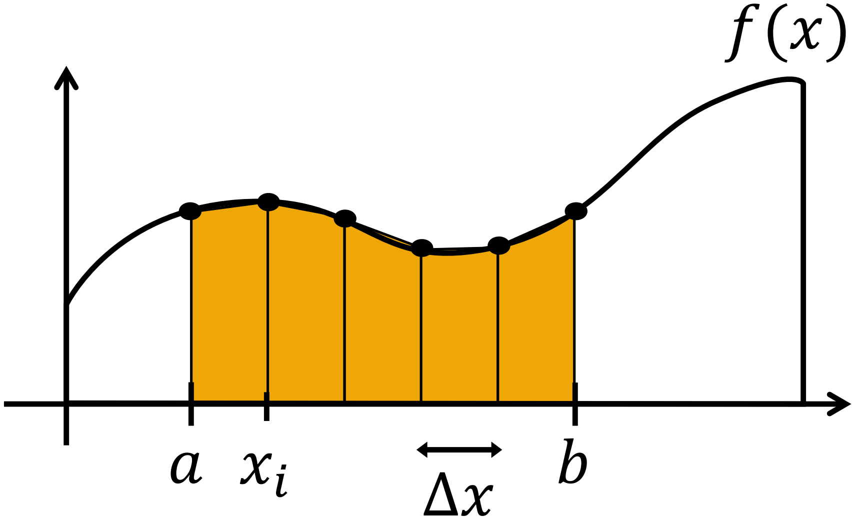
Composite Trapezoidal Rule

- The rule's error on N intervals is governed by:

$$\epsilon \le \frac{N\Delta x^3}{12} f''(\zeta)$$

$$= \frac{(b-a)\Delta x^2}{12} f''(\zeta)$$

$$= \mathcal{O}(\Delta x^2)$$



Estimating the error?

Estimating the error?

- Linear polynomial has error

$$f(x) - p_{lin,i}(x) = \frac{(x - x_i)(x - x_{i-1})}{2} f''(\xi_i), \xi \in (x_{i-1}, x_i)$$

Estimating the error?

- Linear polynomial approx. $f(x), p_{lin,i}(x)$ has error

$$f(x) - p_{lin,i}(x) = \frac{(x - x_i)(x - x_{i-1})}{2} f''(\xi_i), \xi_i \in (x_{i-1}, x_i)$$

- Integrate over interval

$$\int_{x_{i-1}}^{x_i} f(x) - p_{lin,i}(x) dx = \int_{x_{i-1}}^{x_i} \frac{(x - x_i)(x - x_{i-1})}{2} f''(\xi_i) dx, \xi_i \in (x_{i-1}, x_i)$$

Estimating the error?

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- Integrate over interval

$$\int_{x_{i-1}}^{x_i} f(x) - p_{lin,i}(x)dx = \int_{x_{i-1}}^{x_i} \frac{(x-x_i)(x-x_{i-1})}{2} f''(\xi_i)dx, \xi_i \in (x_{i-1}, x_i)$$

- Problem ξ_i depends on x –use **M**ean **V**alue **T**hm for integrals

$$f''(\xi_i^*) \int_{x_{i-1}}^{x_i} \frac{(x-x_i)(x-x_{i-1})}{2} dx = \int_{x_{i-1}}^{x_i} \frac{(x-x_i)(x-x_{i-1})}{2} f''(\xi_i)dx$$

Estimating the error?

- Error on an interval

$$f''(\xi_i^*)\int_{x_{i-1}}^{x_i} \frac{(x-x_i)(x-x_{i-1})}{2}dx = -f''(\xi_i^*)\frac{h^3}{12}$$

Estimating the error

- Error on an interval $$f''(\xi_i^*)\int_{x_{i-1}}^{x_i}\frac{(x-x_i)(x-x_{i-1})}{2}dx=-f''(\xi_i^*)\frac{h^3}{12}$$
- Summing over the intervals
- (note (b-a)=Nh)

$$Error=-\sum_{i=1}^{N} f''(\xi_i^*)\frac{h^3}{12}$$

$$=-\frac{Nh^3}{12}\left(\frac{1}{N}\sum_{i=1}^{N} f''(\xi_i^*)\right)$$

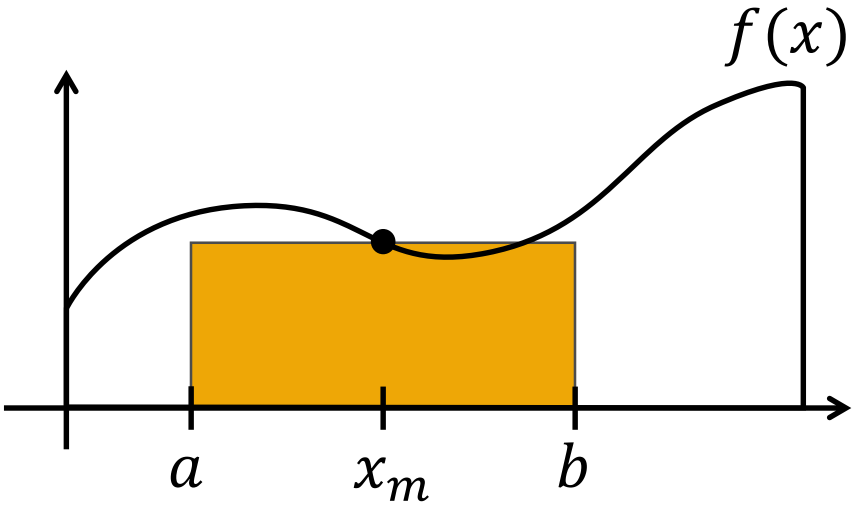
$$=-(b-a)\frac{h^2}{12}f''(\xi)$$

Midpoint Rule

- Approximate the integral by a rectangle defined by the midpoint between a and b:

$$\int_a^b f(x)dx \approx (b-a)f(x_m)$$

$$x_m = \frac{a+b}{2}$$



- The rule's error is given by:

$$\begin{aligned}\epsilon \quad &\leq \frac{(b-a)^3}{24} f''(\zeta)\\ &= \mathcal{O}((b-a)^3)\end{aligned}$$

Composite Midpoint Rule

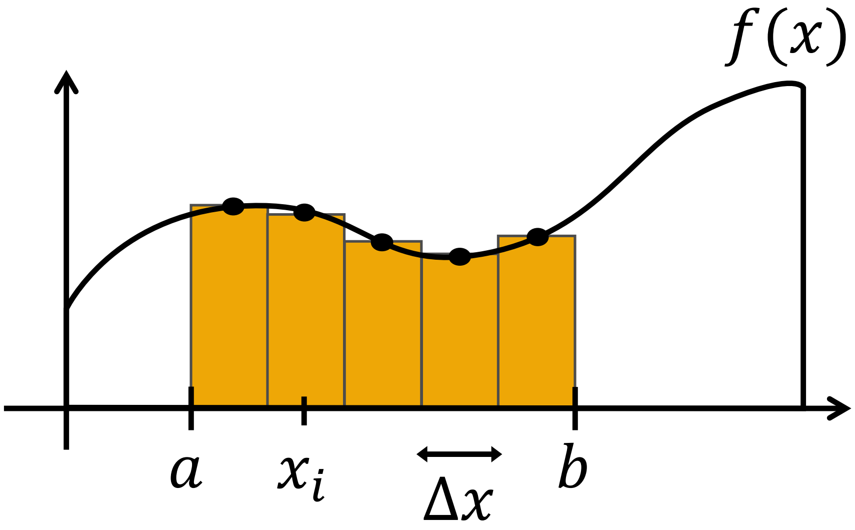
- Approximate the integral by N applications of the midpoint rule between a and b:

$$\int_a^b f(x)dx \approx \sum_{i=1}^{N} w_i f(x_i)$$

  - Given $\Delta x = \frac{b-a}{N}$,

$$x_i = a + (i - .5)\Delta x$$

$$w_i = \Delta x$$



Estimating the error using Taylors Series

Expand the function being integrated about the midpoint

Error =

$$f(x) - f(\frac{x_i + x_{i+1}}{2}) = (x - \frac{x_i + x_{i+1}}{2}) f'(\frac{x_i + x_{i+1}}{2}) + (x - \frac{(x_i + x_{i+1})}{2})^2 f''(\xi_i),$$

where $\xi \in (x_i, x_{i+1})$.

Estimating the error using Taylors Series

Expand the function being integrated about the midpoint

Error =

$$f(x) - f\left(\frac{x_i + x_{i+1}}{2}\right) = \left(x - \frac{x_i + x_{i+1}}{2}\right) f'\left(\frac{x_i + x_{i+1}}{2}\right) + \left(x - \frac{(x_i + x_{i+1})}{2}\right)^2 f''(\xi_i)$$

, where $\xi \in (x_i, x_{i+1})$.

Integrating gives an expression for the error

$$\int_{x_i}^{x_{i+1}} f(x) - f\left(\frac{x_i + x_{i+1}}{2}\right) dx \approx \int_{x_i}^{x_{i+1}} \left(x - \frac{(x_i + x_{i+1})}{2}\right)^2 f''(\xi_i)\, dx$$

Estimating the error using Taylors Series

$$f(x) - f(\frac{x_i + x_{i+1}}{2}) = (x - \frac{x_i + x_{i+1}}{2}) f'(\frac{x_i + x_{i+1}}{2}) + (x - \frac{(x_i + x_{i+1})}{2})^2 f''(\xi_i),$$

where $\xi \in (x_{i-1}, x_i)$. Integrating

$$\int_{x_i}^{x_{i+1}} f(x) - f(\frac{x_i + x_{i+1}}{2}) dx = 0 + \int_{x_i}^{x_{i+1}} (x - \frac{(x_i + x_{i+1})}{2})^2 f''(\xi_i) dx$$

$$= f''(\xi^*) \int_{x_i}^{x_{i+1}} (x - \frac{(x_i + x_{i+1})}{2})^2 dx, \quad \text{MVT for integrals}$$

$$= f''(\xi^*) \frac{\Delta x^3}{24}, \text{ where } \Delta x = x_{i+1} - x_i$$

Composite Midpoint Rule

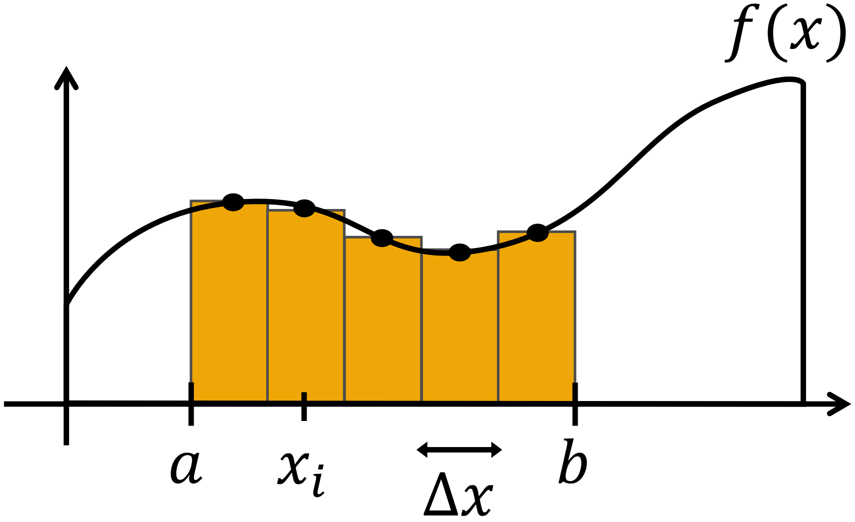
- This rule's error is given by summing over the intervals:

$$\epsilon \leq \frac{N\Delta x^3}{24} f''(\zeta)$$

As $N\Delta x = (b - a)$

$$= \frac{(b-a)\Delta x^2}{24} f''(\zeta)$$

$$= \mathcal{O}(\Delta x^2)$$

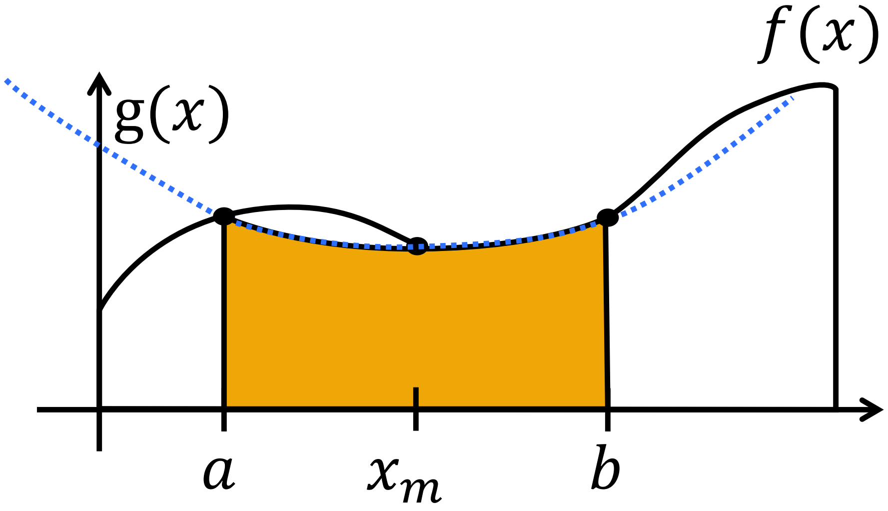


Simpson’s Rule

- Evaluate the function at a, b, and the midpoint
- Find a quadratic polynomial with known integral that interpolates the three points
- Approximate the integral by the exact integral of the interpolating polynomial:

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

- We’ll use a Quadratic Lagrange Polynomial



Lagrange Polynomial

Quadratic Lagrange Polynomial

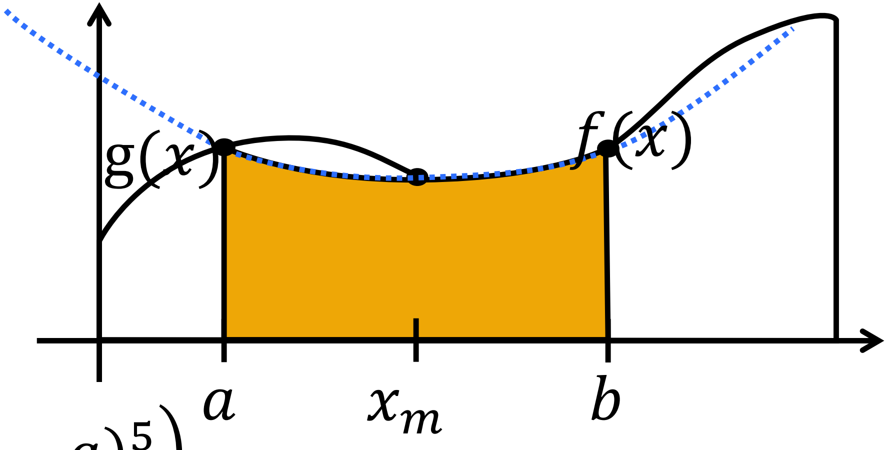
- Given known a, x_m, b, and $f(x)$
- $g(x) = f(a)\frac{(x-x_m)(x-b)}{(a-x_m)(a-b)} + f(x_m)\frac{(x-a)(x-b)}{(x_m-a)(x_m-b)} + f(b)\frac{(x-a)(x-x_m)}{(b-a)(b-x_m)}$
- Integral of which is:

$$\int_a^b g(x)dx = \frac{1}{6}(b-a)[f(a) + 4f(x_m) + f(b)]$$

Simpson's Rule

Thus Simpson's Rule defines the integral by:

$$\int_a^b f(x)dx \approx \frac{1}{6}(b-a)[f(a) + 4f(x_m) + f(b)]$$



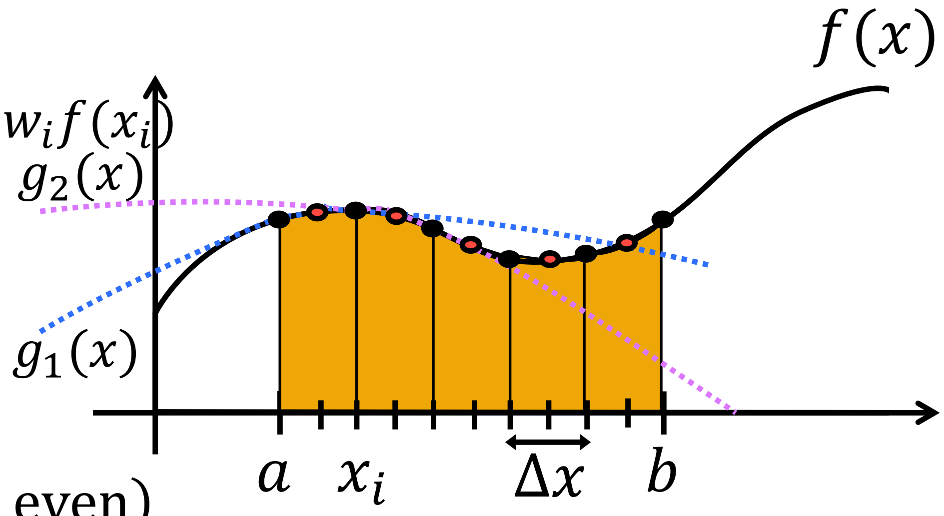
The error is defined by

$$\epsilon \leq \frac{(b-a)^5}{2880} f^{(4)}(\varphi) = \mathcal{O}\left((b-a)^5\right)$$

Composite Simpson's Rule

- In quadrature notation:

$$\int_a^b f(x)dx \approx \sum_{i=1}^{N} \int_a^b g(x)dx = \sum_{i=1}^{2N+1} w_i f(x_i)$$



- Simpson Quadrature:

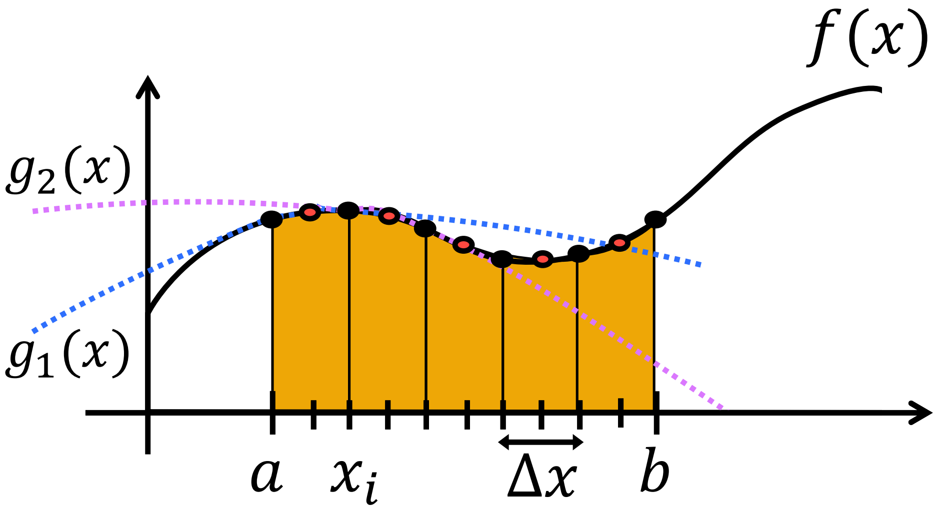
$$w_i = \begin{cases} \frac{\Delta x}{3} & : \quad i = 1, 2N+1 \\ \frac{4\Delta x}{3} & : \quad i = 2, \ldots, 2N \quad (i \text{ even}) \\ \frac{2\Delta x}{3} & : \quad i = 3, \ldots, 2N-1 \quad (i \text{ odd}) \end{cases}$$

$$x_i = a + (i-1)\Delta x \qquad \text{where } \Delta x = \frac{b-a}{2N}$$

Composite Simpson's Rule

- The error in composite Simpson's rule is governed by:

$$\epsilon \leq \frac{N\Delta x^5}{2880} f^{(4)}(\varphi)$$
$$= \frac{(b-a)\Delta x^4}{2880} f^{(4)}(\varphi)$$
$$= \mathcal{O}(\Delta x^4)$$



Example

$$\int_0^{\pi} \sin(x)\, dx = 2.0$$

Ignore this
For now

n	Trapez.	Simpson	Monte Carlo
2	1.570796	2.094395	2.483686
4	1.896119	2.004560	2.570860
8	1.974232	2.000269	2.140117
16	1.993570	2.000017	1.994455
32	1.998393	2.000001	2.005999
64	1.999598	2.000000	2.039970
128	1.999900	2.000000	2.000751
256	1.999975	2.000000	2.065036
512	1.999994	2.000000	2.037365
1024	1.999998	2.000000	1.988752
2048	2.000000	2.000000	1.989458
4096	2.000000	2.000000	1.991806
8192	2.000000	2.000000	2.000583
16384	2.000000	2.000000	1.987582
32768	2.000000	2.000000	1.991398
65536	2.000000	2.000000	1.997360

Example

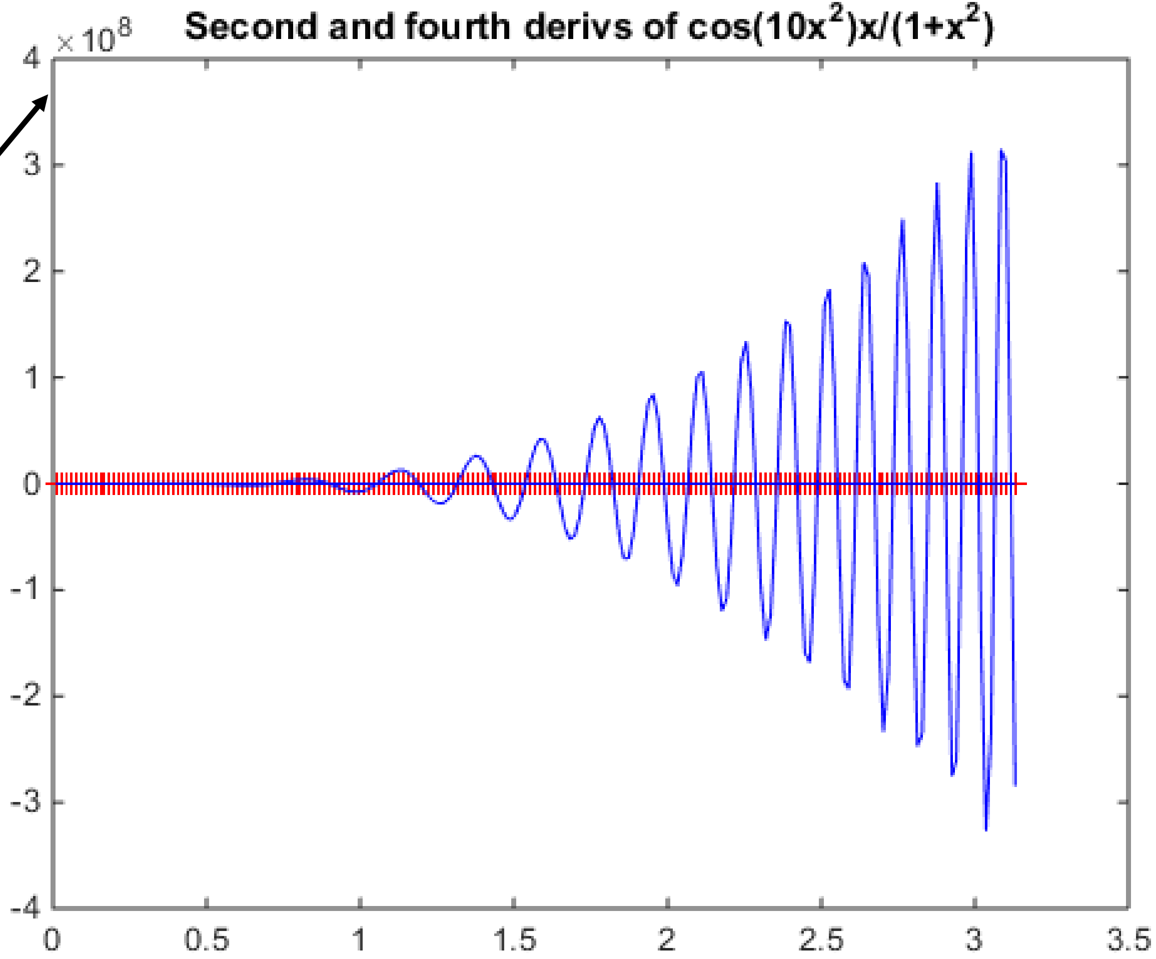
$$\int_0^{\pi} \frac{x}{x^2+1} \cos(10x^2)\, dx = 0.0003156$$

n	Trapez.	Simpson	~~Monte Carlo~~
64	0.004360	−0.013151	~~0.081207~~
128	0.001183	−0.001110	~~0.155946~~
256	0.000526	−0.000311	~~0.071404~~
512	0.000368	0.000006	~~0.002110~~
1024	0.000329	0.000161	~~−0.004525~~
2048	0.000319	0.000238	~~−0.010671~~
4096	0.000316	0.000277	~~0.000671~~
8192	0.000316	0.000296	~~−0.009300~~
16384	0.000316	0.000306	~~−0.009500~~
32768	0.000316	0.000311	~~−0.005308~~
65536	0.000316	0.000313	~~−0.000414~~
131072	0.000316	0.000314	~~0.001100~~
262144	0.000316	0.000315	~~0.001933~~
524288	0.000316	0.000315	~~0.000606~~
1048576	0.000316	0.000315	~~−0.000369~~
2097152	0.000316	0.000316	~~0.000866~~
4194304	0.000316	0.000316	~~0.000330~~

Why might trapezoidal be better than Simpson?

Comparison of Second and Fourth Derivatives

Note scale



Trapezoidal error involves second derivatives while Simpson’s error involves fourth derivatives

Example

Consider $\int_0^1 x^p dx = \frac{1}{p+1}$

Trapezoidal rule with $h = 0.5$ gives

$$0.5(0.5(0+\frac{1}{2^p})+0.5(\frac{1}{2^p}+1)) = 1 \text{ if } p = 0$$

$$= (\frac{1}{2^{p+1}}+\frac{1}{4})$$

error estimate is $-\frac{0.25}{12}p(p-1)(\xi)^{p-2}$

Use $\xi = 1$ giving $-\frac{0.25}{12}p(p-1)$

p	value	error	estimate
0	1	0	
1	1 /2	0	
2	3/8	3/9-3/8 -0.041	-0.041
3	5/16	4/16-5/16 -0.0625	-0.125
4	9/32	9/45-9/32 -0.0812	-0.25
5	17/64	1/6-17/64 -0.0989	-0.41

We need to pick ξ with more care ξ=1/2 ?

Consider $\int_0^1 x^p dx = \dfrac{1}{p+1}$

Simpsons rule with $h = 1.0$ gives

$$\frac{1}{6}(0 + \frac{4}{2^p} + 1) = 1 \text{ if } p = 0$$

$$= \frac{1}{6}(\frac{1}{2^{p+2}} + 1)$$

error estimate is

$$\frac{(1.0)^4}{2880} p(p-1)(p-2)(p-3)(\xi)^{p-4}$$

Use $\xi = 1$ giving $\dfrac{p(p-1)(p-2)(p-3)}{2880}$

p	value	error	estimated
0	1	0	
1	1 /2	0	
2	1/3	0	
3	1/4	0	
4	5/24	1/5-5/24	0.0083
		0.0083	
5	9/48	8/48-9/48	0.0208
		0.02	

Gaussian Quadrature

- Newton-Cotes formulae use regular spaced sample points
- Gaussian quadrature creates a polynomial with non-uniform sampling

Gaussian Quadrature

- Gaussian quadrature is developed with the idea that we want to find an $N - 1$ degree polynomial to represent the curve
- A polynomial of degree $N - 1$ has N coefficients:

$$p_{N-1}(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_{N-1} x^{N-1}$$

- For simplicity, Gaussian quadrature is specified over a fixed interval $[-1,1]$:

$$\int_{-1}^{1} f(x)dx = \sum_{i=1}^{N} w_i f(x_i)$$

Gauss-Legendre Quadrature

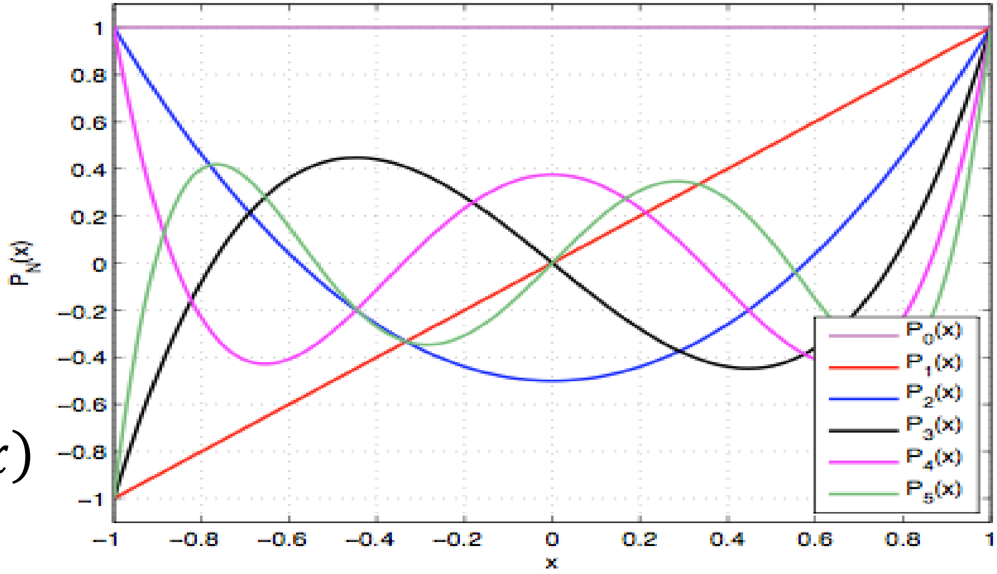
Normalized Legendre polynomials are defined by the following recurrence relation:

$$P_0(x) = 1$$

$$P_1(x) = x$$

$$(N+1)P_{N+1}(x)$$
$$= (2N+1)xP_N(x) - NP_{N-1}(x)$$

This graph shows the first six normalized Legendre polynomials:



Gauss-Legendre Quadrature

- Formulating quadrature:
  - Points are found by setting

$$P_n(x) = 0$$

  - Weights are determined by

$$w_i = \frac{2}{\left(1 - x_i^2\right)\left(P_N'(x_i)\right)^2}$$

Gaussian Quadrature - Transforming Intervals

- Gaussian quadrature rules, as presented, only work for integrating a function on the interval $[-1,1]$, but we are typically interested in an interval $[a, b]$
- Change of variables will let us accomplish this. Recall from calculus:

$$\int_{g(t_1)}^{g(t_2)} f(x)dx = \int_{t_1}^{t_2} f\big(g(t)\big)g'(t)dt$$

Gaussian Quadrature - Transforming Intervals

$$\int_{g(t_1)}^{g(t_2)} f(x)dx = \int_{t_1}^{t_2} f\big(g(t)\big)g'(t)dt$$

$$g(t) = \frac{t+1}{2}, g'(t) = \frac{1}{2}$$

$$\int_0^1 f(x)dx = \int_{-1}^1 f(\frac{t+1}{2})\frac{1}{2}dt$$

Gaussian Quadrature - Transforming Intervals

- Substituting for Gaussian quadrature along the interval $[a, b]$ produces the following formula:

$$\int_a^b f(x)dx \approx \frac{b-a}{2}\sum_{i=1}^{N} w_i f\left(\frac{b-a}{2}x_i + \frac{a+b}{2}\right)$$

- This quadrature method's error is governed by the following relation:

$$\epsilon \leq \frac{(b-a)^{2N+1}(N!)^4}{(2N+1)\big((2N)!\big)^3} f^{(2N)}(\varphi) = \mathcal{O}\big((b-a)^{2N+1}\big)$$

Gaussian Quadrature – Example

$$\int_0^1 (\mathrm{p}+1)\mathrm{x}^\wedge\mathrm{p}\,dx \approx \frac{1}{2}\sum_{i=1}^{5} w_i(p+1)\left(\frac{1}{2}x_i+\frac{1}{2}\right)^\wedge p$$

Exact value = 1 Matlab results for different values of p

P	2	3	4	5	6	7	8	9	10
Error	2e-16	2e-16	2e-16	4e1-6	4e-16	4e-16	4e-16	4e-16	2e-5

P	11	12	13	14	15	16	17	18	19
Error	9e-5	3e-4	8e-4	2e-3	3e-3	5e-3	8e-3	1e-2	2e-2

```
%  Gauss Quad Example 5 point formula.   applied to integral from 0 to 1 of (p+1)x^p dx
x(1) = -1/3*sqrt(5.0+2.0*sqrt(10./7.));   w(1)=(322-13.0*sqrt(70))/900.0;
x(2) = -1/3*sqrt(5.0-2.0*sqrt(10./7.));   w(2)=(322+13.0*sqrt(70))/900.0;
x(3) = 0.0;                               w(3)= 128.0/225.0;
x(4) = -x(2);                             w(4)= w(2);
x(5) = -x(1);                             w(5)=w(1);
for p = 2:20
    int = 0.0;
    for i = 1:5
        int = int + 0.5*w(i)*(p+1)*(0.5*x(i)+0.5)^p;     end
    error = abs(1.0-int);     disp(p);disp(error);
end
```

Simple Scientific Computing Example

- I'm driving a car.
  - First, I go 0-45 mph in 15 seconds. My velocity is $f_1(t)$.
  - Second, I go 45-60 mph in another 45 seconds. My velocity is $f_2(t)$.
  - What distance have I travelled?

$$\boldsymbol{x} = \int_0^{15} f_1(t)dt + \int_{15}^{60} f_2(t)dt$$

Recommended Reading

- Additional Explanation of the:
  - Trapezoidal rule
  - Simpson's rule
  - Gaussian quadrature
- Error Analysis for Midpoint, Trapezoid, and Simpson Rules
  - http://pages.cs.wisc.edu/~amos/412/lecture-notes/lecture19.pdf