

# CS 3200

## Introduction to Scientific Computing

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Instructor: Martin Berzins

Topic: Numerical Integration

Application of polynomial theory already covered

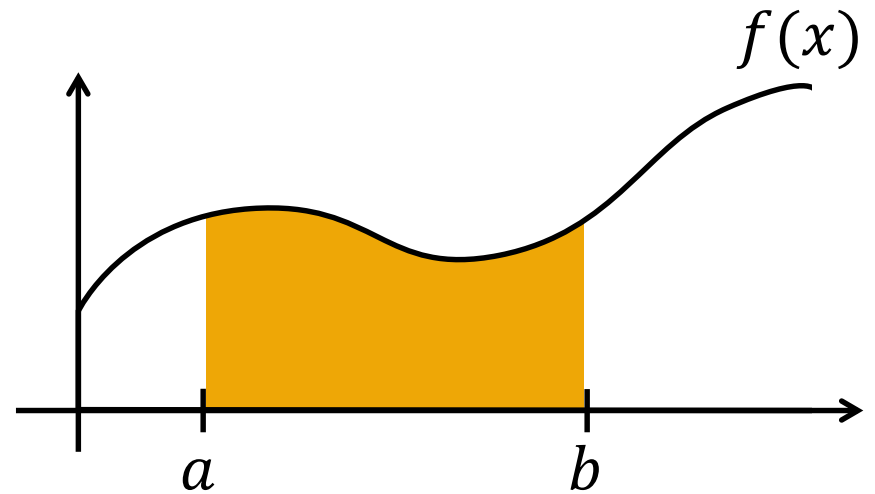
# Numerical Integration

- Goal: find the area under the curve


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

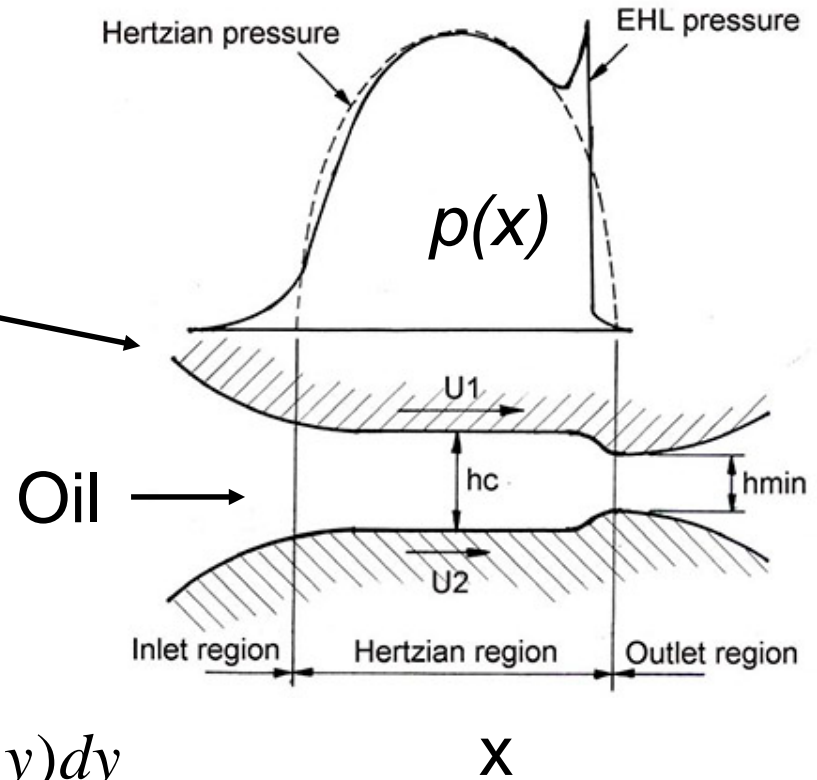
This application occurs with great frequency e.g. in the clean coal boiler or in finance

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.

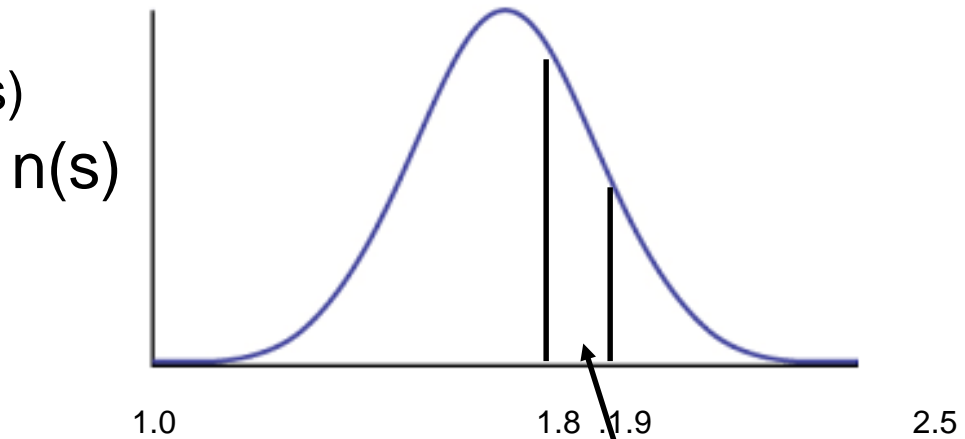


$$h(x) = h_{00} + \frac{x^2}{2R_x} - \frac{4}{\pi E} \int_{-\infty}^{\infty} \ln \left| \frac{x-y}{x_0} \right| p(y) dy$$

# Quadrature Example – Normal Distribution

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

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



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

$$M = 200$$

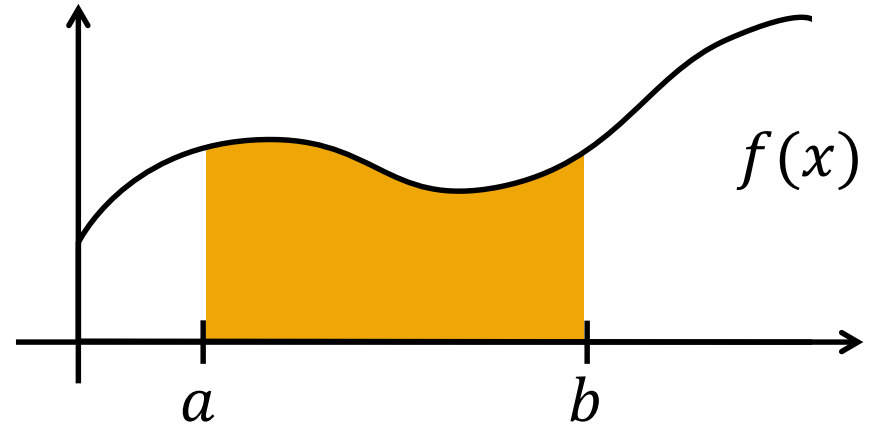
We need to calculate this area to estimate how many of the 200 are between 1.8m and 1.9m tall

# 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

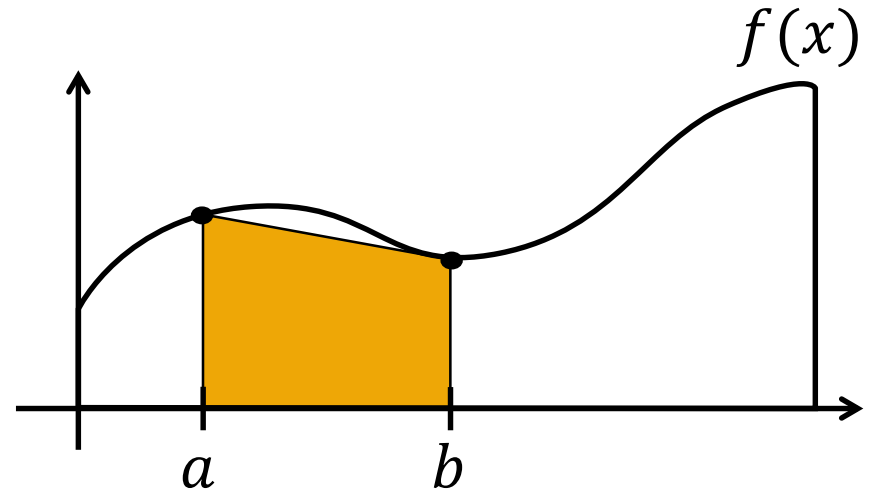
# Trapezoidal Rule

- 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:

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



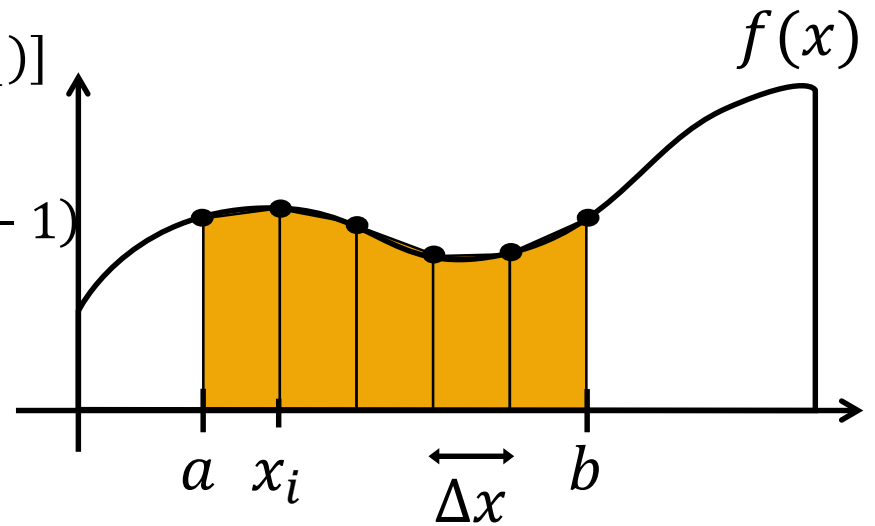
# Composite Trapezoidal Rule

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

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

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

- Can we simplify this to fit Quadrature Notation?





# Composite Trapezoidal Rule

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

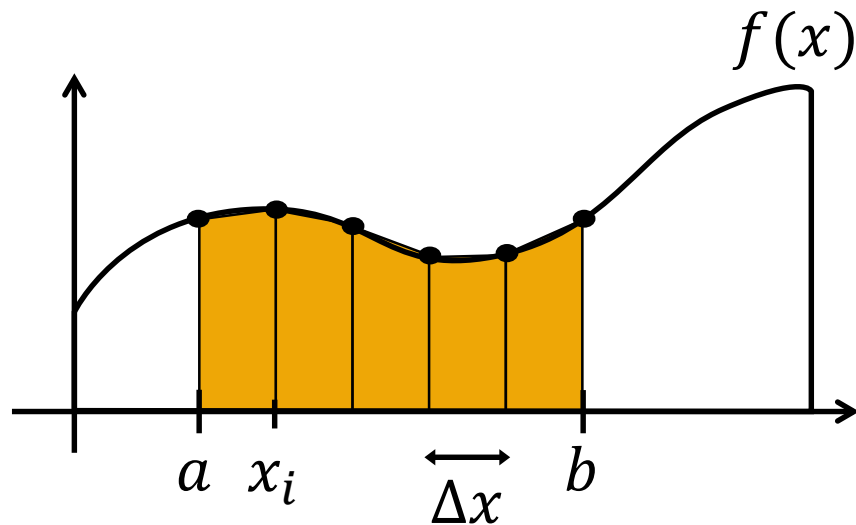
$$\int_a^b f(x) dx \approx \sum_{i=1}^{N-1} \frac{1}{2} \frac{b-a}{N} [f(x_i) + f(x_{i+1})]$$

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

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

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

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



# Composite Trapezoidal Rule

- Quadrature notation

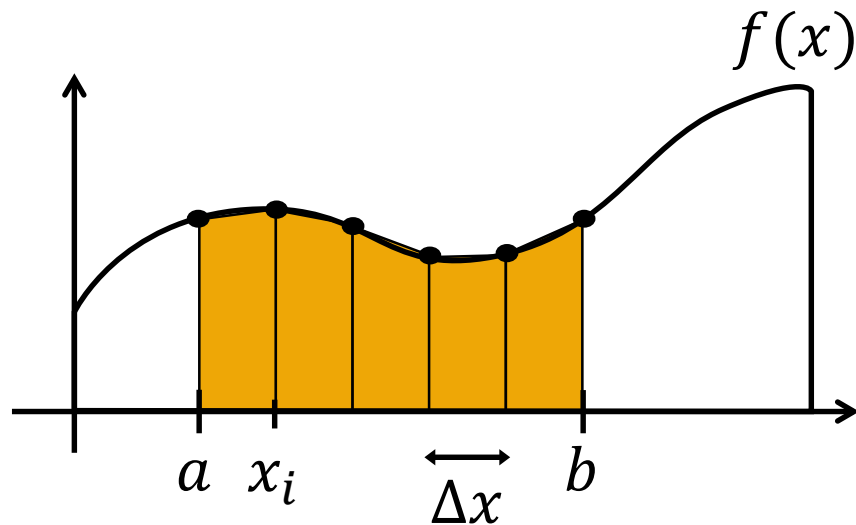
$$\int_a^b f(x)dx \approx \sum_{i=1}^N w_i f(x_i)$$

- This can be written as

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

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

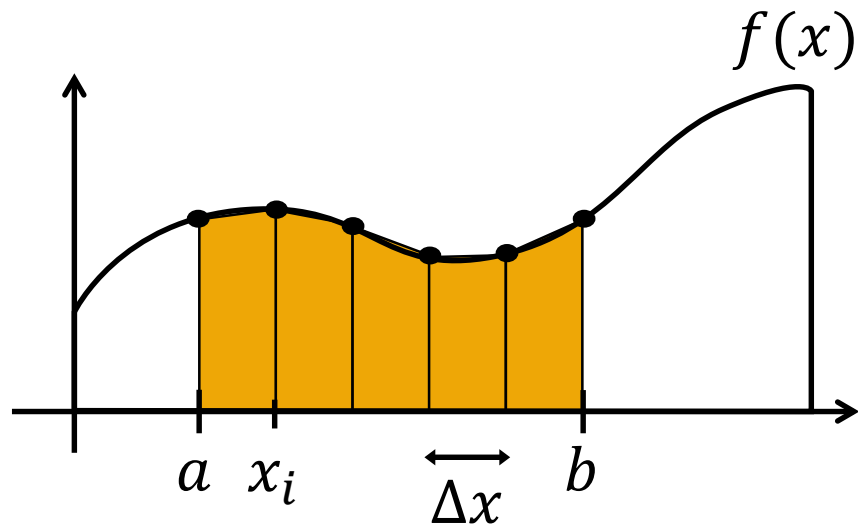
$$\text{where } \Delta x = \frac{b-a}{N-1}$$



# Composite Trapezoidal Rule

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

$$\begin{aligned}\epsilon &\leq \frac{N\Delta x^3}{12} f''(\zeta) \\ &= \frac{(b-a)\Delta x^2}{12} f''(\zeta) \\ &= \mathcal{O}(\Delta x^2)\end{aligned}$$



# Estimating the error?

# Estimating the error?

- Linear polynomial has error

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

# 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?

- 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

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

- Problem  $\xi_i$  depends on  $x$  – use **Mean Value Thm** 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

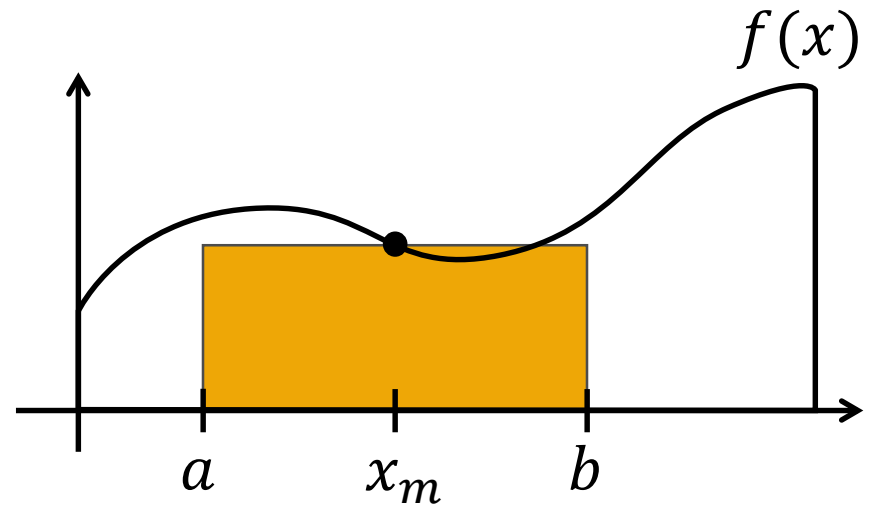
- Approximate the integral by a rectangle defined by the midpoint between  $a$  and  $b$ :

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

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

- The rule's error is given by:

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



# Composite Midpoint Rule

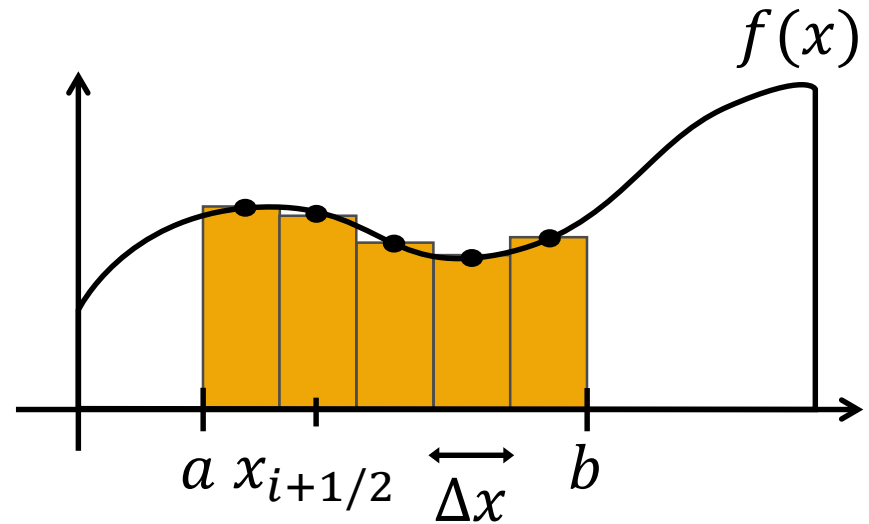
- Approximate the integral by  $N$  applications of the midpoint rule between  $a$  and  $b$ :

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

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

$$x_{i+1/2} = a + (i - .5)\Delta x$$

$$w_i = \Delta x$$



# Estimating the error using Taylors Series

Expand the function being integrated about the **midpoint**  
Error =

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

where  $\xi \in (x_i, x_{i+1})$  and  $x_{i+1/2} = \frac{x_i + x_{i+1}}{2}$

# Estimating the error using Taylors Series

General idea:

- (i) Expand the function being integrated about the points used in the numerical method ( **here the midpoint**) using Taylors series
- (ii) Evaluate the expression for the error by looking carefully at which terms cancel
- (iii) Obtain an expression involving  $h$  or  $\Delta x$  the step width or mesh spacing of the numerical method.

# Estimating the error using Taylors Series

Expand the function being integrated about the **midpoint**

$$f(x) - f\left(\frac{x_i + x_{i+1}}{2}\right) = \left(x - \frac{x_i + x_{i+1}}{2}\right) f'\left(\frac{x_i + x_{i+1}}{2}\right) + 0.5\left(x - \frac{x_i + x_{i+1}}{2}\right)^2 f''(\xi_i)$$

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

$$\text{As True Value} = \int_{x_i}^{x_{i+1}} f(x) dx \quad \text{Approx} = f\left(\frac{x_i + x_{i+1}}{2}\right)h = \int_{x_i}^{x_{i+1}} f\left(\frac{x_i + x_{i+1}}{2}\right) dx$$

Comparing the two gives an expression for the error

$$\int_{x_i}^{x_{i+1}} f(x) - f\left(\frac{x_i + x_{i+1}}{2}\right) dx \approx 0.5 \int_{x_i}^{x_{i+1}} \left(x - \frac{x_i + x_{i+1}}{2}\right)^2 f''(\xi_i) dx$$

# Estimating the error using Taylors Series

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

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

$$\begin{aligned} \int_{x_i}^{x_{i+1}} f(x) - f\left(\frac{x_i + x_{i+1}}{2}\right) dx &= 0 + \int_{x_i}^{x_{i+1}} \left(x - \frac{x_i + x_{i+1}}{2}\right)^2 f''(\xi_i) dx \\ &= f''(\xi^*) 0.5 \int_{x_i}^{x_{i+1}} \left(x - \frac{x_i + x_{i+1}}{2}\right)^2 dx, \quad \text{MVT for integrals} \\ &= f''(\xi^*) \frac{\Delta x^3}{24}, \quad \text{where } \Delta x = x_{i+1} - x_i \end{aligned}$$

# Composite Midpoint Rule

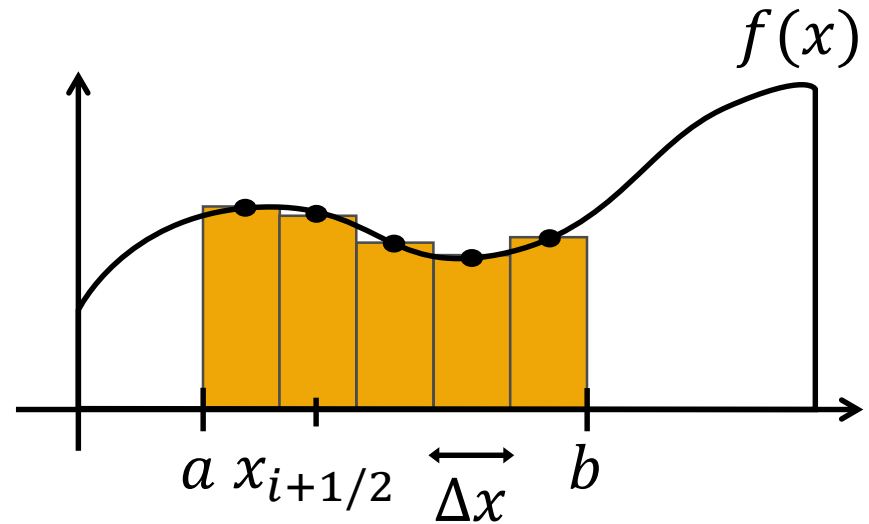
- This rule's error is given by summing over the intervals:

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

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

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

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



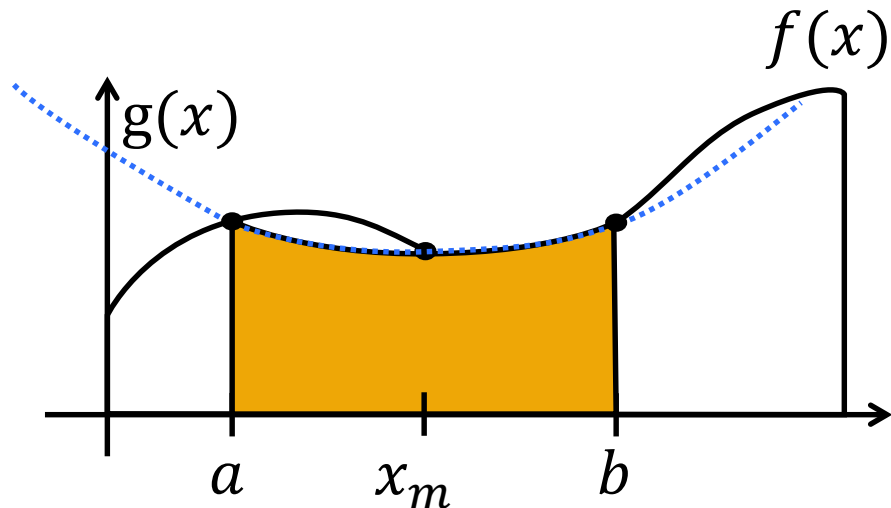


# Simpson's Rule

- 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

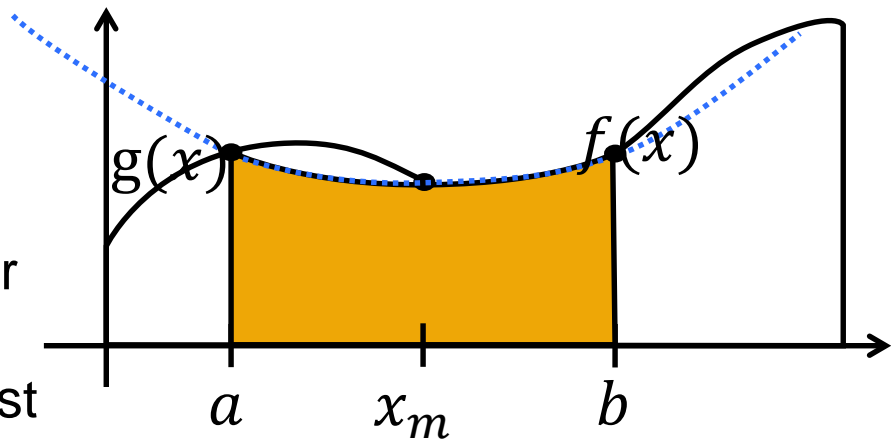
Thus Simpson's Rule defines the integral by:

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

The error is defined by

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

Note there is one extra power of  $(b-a)$  over what is expected from interpolating the polynomial error. This is because the lowest interpolation error term integrates to zero...



# Composite Simpson's Rule

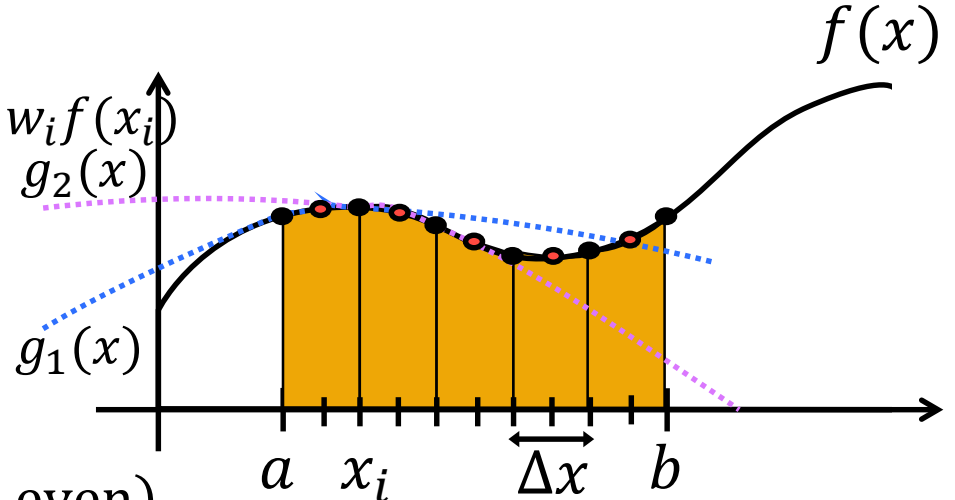
- In quadrature notation:

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

- Simpson Quadrature:

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

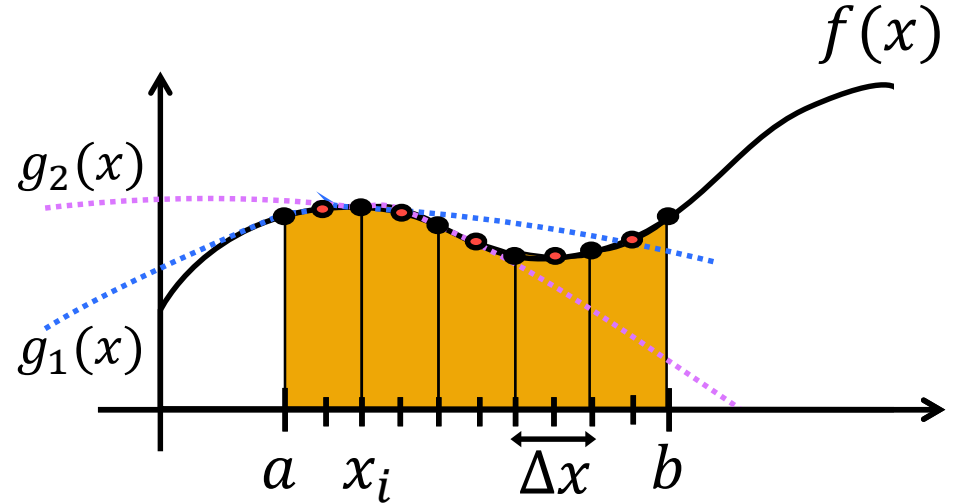
$$x_i = a + (i - 1)\Delta x \quad \text{where } \Delta x = \frac{b-a}{2N}$$



# Composite Simpson's Rule

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

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



# Example

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

Ignore this  
For now

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

# Example

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

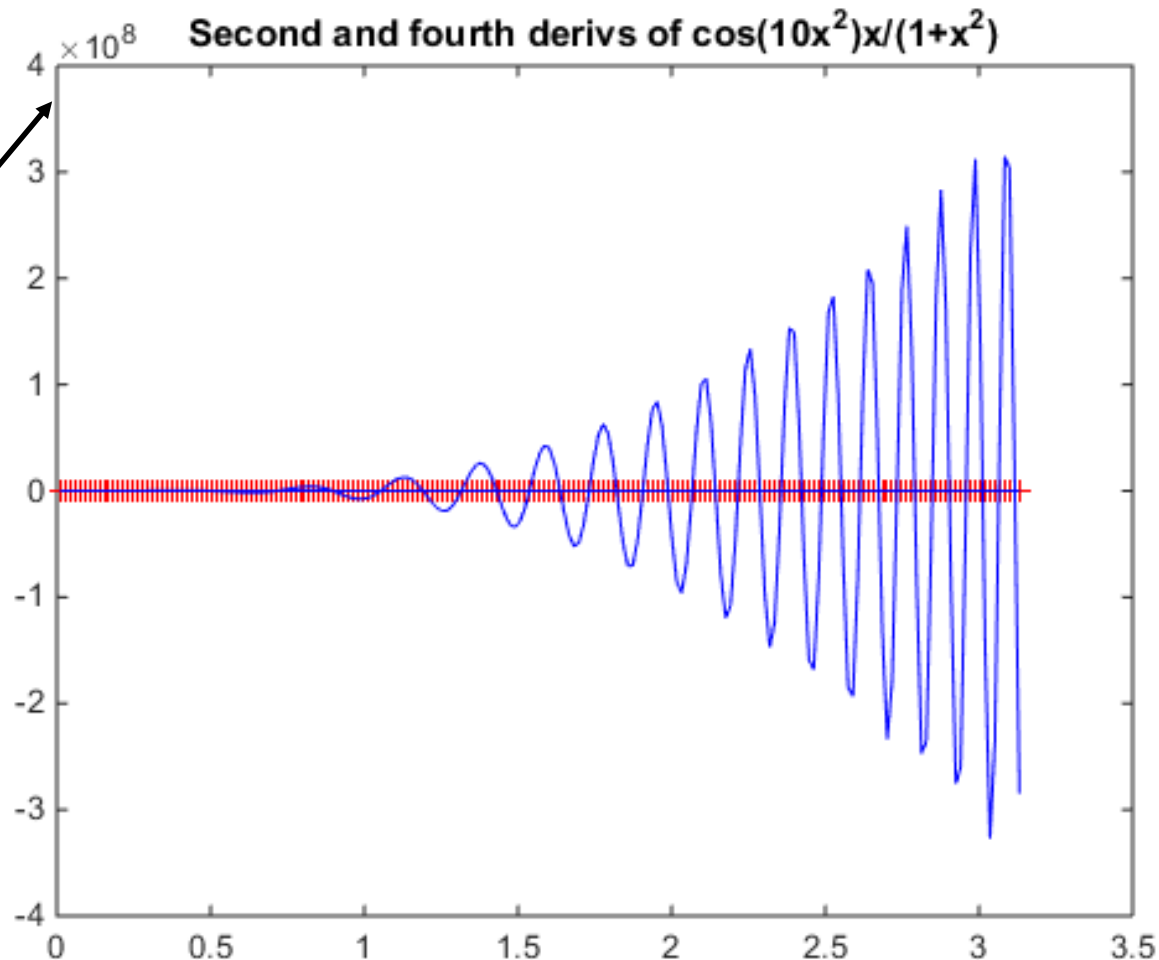
n	Trapez .	Simpson	Monte Carlo
64	0.004360	-0.013151	0.081207
128	0.001183	-0.001110	0.155946
256	0.000526	-0.000311	0.071404
512	0.000368	0.000006	0.002110
1024	0.000329	0.000161	-0.004525
2048	0.000319	0.000238	-0.010671
4096	0.000316	0.000277	0.000671
8192	0.000316	0.000296	-0.009300
16384	0.000316	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  $-\frac{0.25}{12} p(p-1)$  We need to pick  $\xi$  with more care  $\xi = 1/2$  ?

$p$	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	-0.125
		-0.0625	
4	9/32	9/45-9/32	-0.25
		-0.0812	
5	17/64	1/6-17/64	-0.41
		-0.0989	

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

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  $\frac{p(p-1)(p-2)(p-3)}{2880}$

$p$	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.
- Not used with higher order generally as weights can be negative.
- Gaussian quadrature creates a polynomial with non-uniform sampling.
- By picking both the weights and sample points we can get much greater accuracy.

# Gaussian Quadrature

- Gaussian quadrature is developed with the idea that we want to specify  $N$  points and  $N$  weights to integrate a polynomial of  $2N - 1$  degree polynomial
- A polynomial of degree  $2N - 1$  has  $2N$  coefficients:

$$p_{2N-1}(x) = a_0 + a_1x + a_2x^2 + \cdots + a_{2N-1}x^{2N-1}$$

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

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

$$a_0 : \int_{-1}^1 1 dx = [x]_{-1}^1 = 2 = \sum_{i=1}^N w_i,$$

$$a_1 : \int_{-1}^1 x dx = \left[\frac{x^2}{2}\right]_{-1}^1 = 0 = \sum_{i=1}^N w_i x_i$$

$$a_2 : \int_{-1}^1 x^2 dx = \left[\frac{x^3}{3}\right]_{-1}^1 = \frac{2}{3} = \sum_{i=1}^N w_i x_i^2$$

$$a_3 : \int_{-1}^1 x^3 dx = \left[\frac{x^4}{4}\right]_{-1}^1 = 0 = \sum_{i=1}^N w_i x_i^3$$

⋮

$$a_{2N-2} : \int_{-1}^1 x^{2N-2} dx = \left[\frac{x^{2N-1}}{2N-1}\right]_{-1}^1 = \frac{2}{2N-1} = \sum_{i=1}^N w_i x_i^{2N-2}$$

$$a_{2N-1} : \int_{-1}^1 x^{2N-1} dx = \left[\frac{x^{2N}}{2N}\right]_{-1}^1 = 0 = \sum_{i=1}^N w_i x_i^{2N-1}$$

Making sure that the polynomial is integrated exactly gives us 2N nonlinear equations in the 2N variables

$w_i$  ,  $i = 1 \dots N$  and  $x_i$ ,  $i = 1 \dots N$

Although we could solve these equations ,in fact we use Legendre polynomials and their properties

## Example N = 1

$$a_0 : \int_{-1}^1 1dx = [x]_{-1}^1 = 2 = \sum_{i=1}^N w_i = w_1,$$

$$a_1 : \int_{-1}^1 xdx = \left[\frac{x^2}{2}\right]_{-1}^1 = 0 = \sum_{i=1}^N w_i x_i = w_1 x_1$$

From top equation  $w_1 = 2$

From second equation  $w_1 x_1 = 0$ , giving  $x_1 = 0$

Example  $N = 1$

$$a_0 : \int_{-1}^1 1dx = [x]_{-1}^1 = 2 = \sum_{i=1}^N w_i = w_1,$$

$$a_1 : \int_{-1}^1 xdx = \left[\frac{x^2}{2}\right]_{-1}^1 = 0 = \sum_{i=1}^N w_i x_i = w_1 x_1$$

From top equation  $w_1 = 2$

From second equation  $w_1 x_1 = 0$ , giving  $x_1 = 0$

Hence we have derived the midpoint rule with  $h = 2$

$$\int_{-1}^1 f(x)dx \approx 2f(0)$$

# Gauss-Legendre Quadrature Table

- In practice, Gaussian quadrature points and weights are tabulated for small  $N$
- In some scientific computing applications we rarely use  $N$  larger than about 5

$N$	$x_i$	$w_i$
1	0	2
2	$\pm 1/\sqrt{3}$	1
3	0	8/9
	$\pm \sqrt{3/5}$	5/9
4	$\pm \sqrt{(3 - 2\sqrt{6/5})/7}$	$(18 + \sqrt{30})/36$
	$\pm \sqrt{(3 + 2\sqrt{6/5})/7}$	$(18 - \sqrt{30})/36$
5	0	128/225
	$\pm \frac{1}{3} \sqrt{5 - 2\sqrt{10/7}}$	$(322 + 13\sqrt{70})/900$
	$\pm \frac{1}{3} \sqrt{5 + 2\sqrt{10/7}}$	$(322 - 13\sqrt{70})/900$



# Gauss-Legendre Quadrature

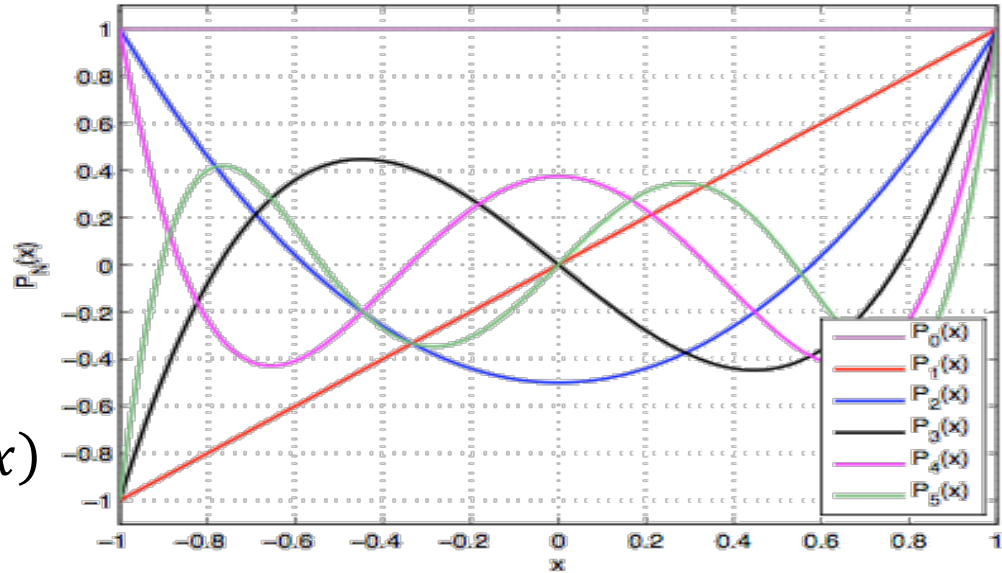
Normalized Legendre polynomials are defined by the following recurrence relation:

$$P_0(x) = 1$$

$$P_1(x) = x$$

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

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

$$w_i = \frac{2}{(1 - x_i^2)(P'_N(x_i))^2}$$

# Gaussian Quadrature - Transforming Intervals

- Gaussian quadrature rules, as presented, only works 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:

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

# Gaussian Quadrature - Transforming Intervals

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

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

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

# Gaussian Quadrature - Transforming Intervals

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

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# 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:

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

# Gaussian Quadrature – Example

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

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	4e-16	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?

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

# Quadrature Summary

- A number of methods for integration of a function may be derived by using polynomial theory
- Methods based upon linear or quadratic polynomials work well for low accuracy
- Methods based based upon high order legendre (or other) polynomials work well at high accuracy if the function being integrated is smooth enough
- Error estimates typically depend on some derivative of the function being integrated and the stepsize used in the formula
- How do we estimate the error without, in many cases, knowing the function itself other than its value at the quadrature points?

# 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>