Chapter 7: Numerical Integration

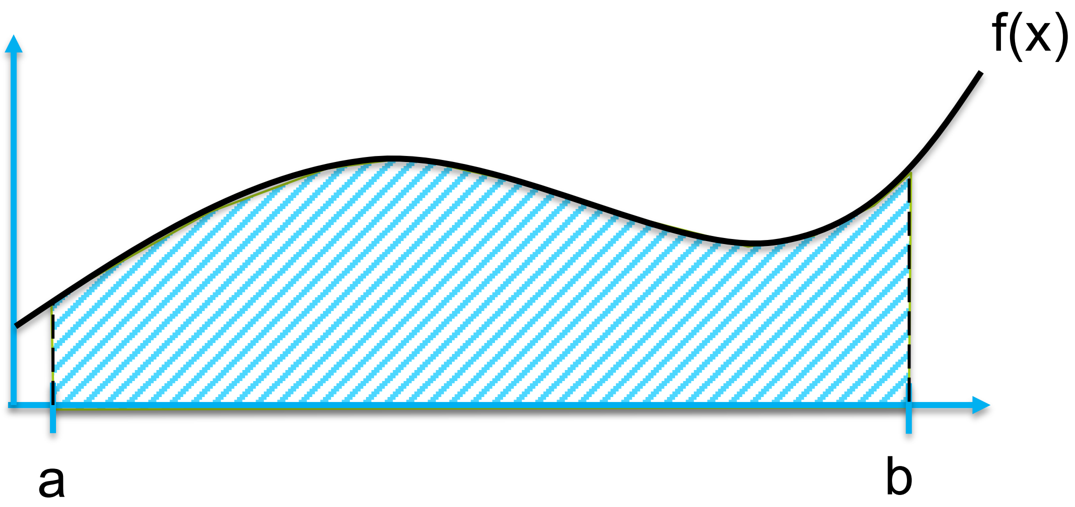
Contents:

- Quadrature Rules
- Degree of Precision (DoP)
- Interval Transformation

Chapter 7: Numerical Integration

Suppose we want to know the integral of f(x) over the interval [a, b]:

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



But we do not have an analytical expression for f(x), or the exact integration of f(x) is too difficult:

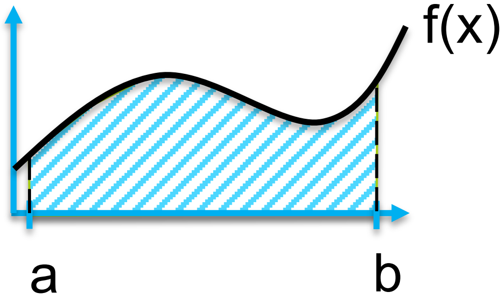
- Method to approximate the integral of a function f(x)

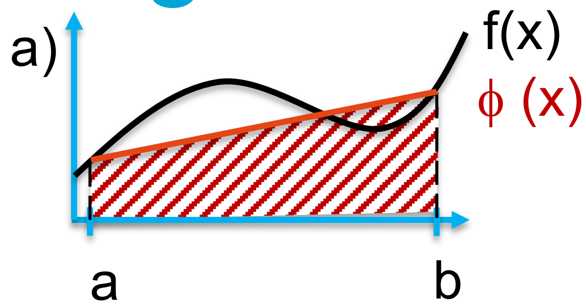
TU Delft

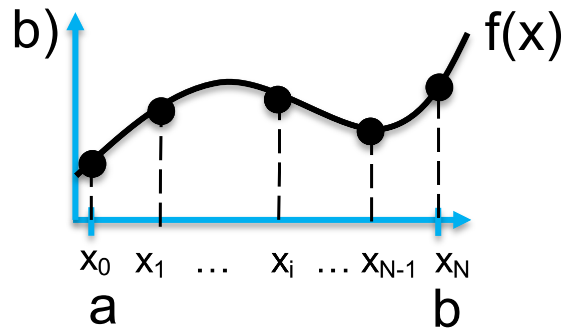
Chapter 7: Numerical Integration

Method to approximate the integral of f(x) over the interval [a, b]:

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







Two approaches:

a) Approximate f(x) by an interpolation $\phi(x)$ and integrate $\phi(x)$, i.e. I(f; a,b) ≈ I(ϕ; a,b)

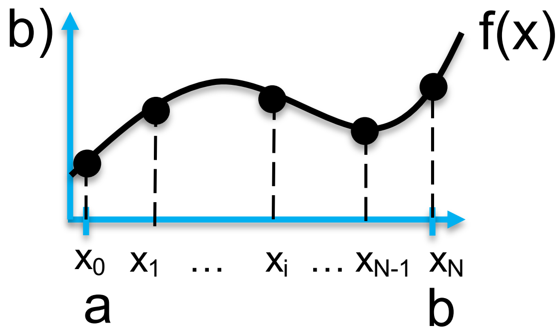
b) Define a <u>quadrature rule</u> by:

- Number of <u>nodes</u> $x_0, x_1, \dots, x_N$
- Number of <u>weights</u> $\omega_0, \omega_1, \dots, \omega_N$

} ⟹ Q(f; a,b) = $\sum_{j=0}^{N} \omega_j f(x_j)$

Chapter 7: Degree of Precision

Q(f; a,b) =$\sum_{j=0}^{N} \omega_j f(x_j)$



Goal is to construct quadrature rule with a high degree of precision (DoP)

Definition:

Q(f; a,b) has a DoP *d* if and only if:

Q(p; a,b) = I(p; a,b) for all polynomials p ∈ $\mathbb{P}^d$

Q(q; a,b) ≠ I(q; a,b) for some polynomial q ∈ $\mathbb{P}^{d+1}$

Note: Q(f; a,b) is exact for all $f(x) = a_d x^d + a_{d-1} x^{d-1} + \cdots + a_1 x + a_0$

Ch. 7
Numerical
Integration

Chapter 7: Degree of Precision

Q(f; a,b) is exact for all:

$$f(x) = a_d x^d + a_{d-1} x^{d-1} + \cdots + a_1 x + a_0 = \sum_{i=0}^{d} a_i x^i$$

Also:

I(*c* p + *d* q; a,b) = *c* I(p; a,b) + *d* I(q; a,b)

Q(*c* p + *d* q; a,b) = *c* Q(p; a,b) + *d* Q(q; a,b)

Hence:

I($\sum_{i=0}^{d} a_i x^i$; a,b) = $\sum_{i=0}^{d} a_i$I(x^i; a,b)

Q($\sum_{i=0}^{d} a_i x^i$; a,b) = $\sum_{i=0}^{d} a_i$Q(x^i; a,b)

For arbitrary values of a_i this is true if:

I(x^i; a,b) = Q(x^i; a,b) $0 \le i \le d$

Chapter 7: Degree of Precision

Q(f; a,b) = $\sum_{j=0}^{N} \omega_j f(x_j)$

Q(f; a,b) is exact for all:

$$f(x) = a_d x^d + a_{d-1} x^{d-1} + \cdots + a_1 x + a_0 = \sum_{i=0}^{d} a_i x^i$$

when:

I(x^i; a,b) = Q(x^i; a,b) $0 \leq i \leq d$

i = 0 $\int_a^b 1dx$ = I(1; a,b) = Q(1; a,b) = $\sum_{j=0}^{N} \omega_j$

i = 1 $\int_a^b xdx$ = I(x; a,b) = Q(x; a,b) = $\sum_{j=0}^{N} \omega_j x_j$

i = 2 $\int_a^b x^2 dx$ = I(x^2; a,b) = Q(x^2; a,b) = $\sum_{j=0}^{N} \omega_j x_j^2$

⋮

i = d $\int_a^b x^d dx$ = I(x^d; a,b) = Q(x^d; a,b) = $\sum_{j=0}^{N} \omega_j x_j^d$

TUDelft

Ch. 7
Numerical
Integration

Chapter 7: Degree of Precision

Q(f; a,b) $=\sum_{j=0}^{N} \omega_j f(x_j)$

Q(f; a,b) is exact for all:

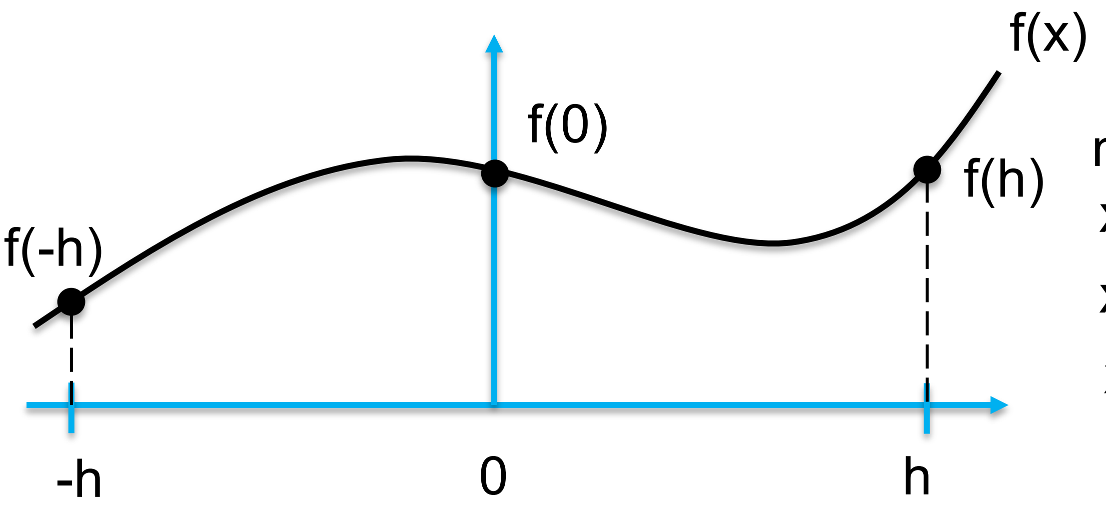
$$f(x) = a_d x^d + a_{d-1}x^{d-1} + \cdots + a_1 x + a_0 = \sum_{i=0}^{d} a_i x^i$$

When we solve the weights ω_j through solving the linear system:

$$\begin{bmatrix} 1 & 1 & \dots & 1 \\ x_0 & x_1 & \dots & x_N \\ \vdots & & \ddots & \\ x_0^d & x_1^d & \dots & x_N^d \end{bmatrix} \begin{bmatrix} \omega_1 \\ \omega_2 \\ \vdots \\ \omega_N \end{bmatrix} = \begin{bmatrix} \int_a^b 1dx \\ \int_a^b xdx \\ \vdots \\ \int_a^b x^d dx \end{bmatrix}$$

TU Delft

Example: derivation of Simpson's rule



nodes

$x_0 = -h$

$x_1 = 0$

$x_2 = h$

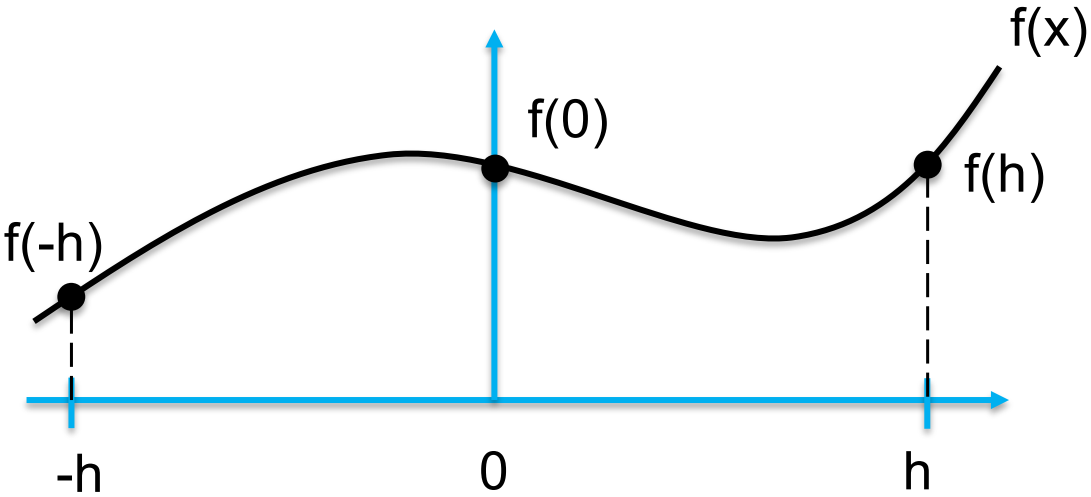
quadrature

$Q[f] = \omega_0 f(-h) +$
$\omega_1 f(0) +$
$\omega_2 f(h)$

Find weights ω_i such that Q[f] has a DoP 2: i.e. exact for any $p \in \mathbb{P}^2$

$$\begin{bmatrix} \quad & \quad & \quad \\ \quad & \quad & \quad \\ \quad & \quad & \quad \end{bmatrix} \begin{bmatrix} \omega_0 \\ \omega_1 \\ \omega_2 \end{bmatrix} = \begin{bmatrix} \quad \\ \quad \\ \quad \end{bmatrix} = \begin{bmatrix} \quad \\ \quad \\ \quad \end{bmatrix}$$

Example: derivation of Simpson's rule



nodes

$x_0 = -h$

$x_1 = 0$

$x_2 = h$

quadrature

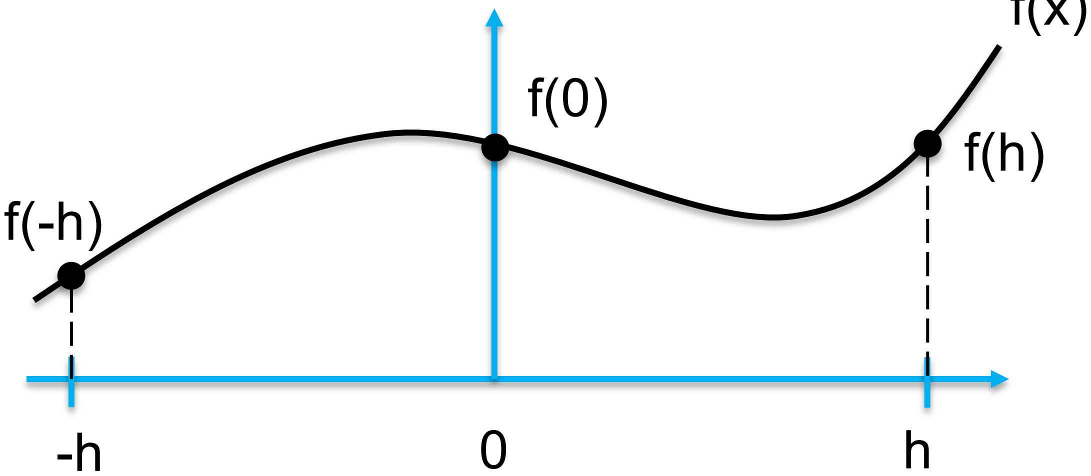
$Q[f] = \omega_0\, f(-h) + \omega_1\, f(0) + \omega_2\, f(h)$

Find weights ω_i such that Q[f] has a DoP 2: i.e. exact for any $p \in \mathbb{P}^2$

(0) $p = 1$

$$\begin{bmatrix}1 & 1 & 1\\ & & \\ & & \end{bmatrix}\begin{bmatrix}\omega_0\\ \omega_1\\ \omega_2\end{bmatrix} = \begin{bmatrix}\int_{-h}^{h} 1\, dx\\ \\ \end{bmatrix} = \begin{bmatrix} \\ \\ \end{bmatrix} = \begin{bmatrix}2h\\ \\ \end{bmatrix}$$

Example: derivation of Simpson's rule



nodes

$x_0 = -h$

$x_1 = 0$

$x_2 = h$

quadrature

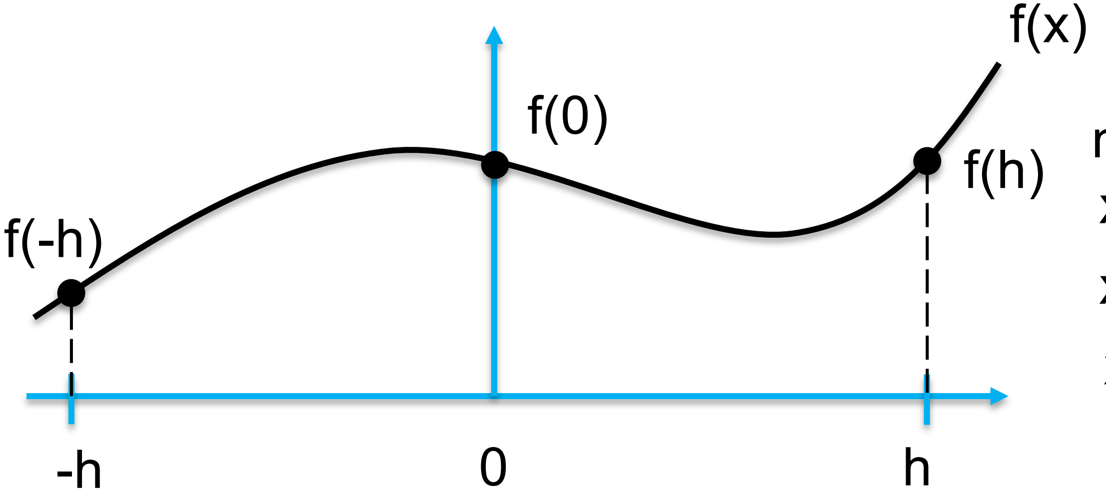
$Q[f] = \omega_0 \, f(-h) + \omega_1 \, f(0) + \omega_2 \, f(h)$

Find weights ω_i such that Q[f] has a DoP 2: i.e. exact for any $p \in \mathbb{P}^2$

(0) p = 1
(1) p = x

$$\begin{bmatrix} 1 & 1 & 1 \\ -h & 0 & h \end{bmatrix} \begin{bmatrix} \omega_0 \\ \omega_1 \\ \omega_2 \end{bmatrix} = \begin{bmatrix} \int_{-h}^{h} 1 \, dx \\ \int_{-h}^{h} x \, dx \end{bmatrix} = \begin{bmatrix} 2h \\ 0 \end{bmatrix}$$

Example: derivation of Simpson’s rule



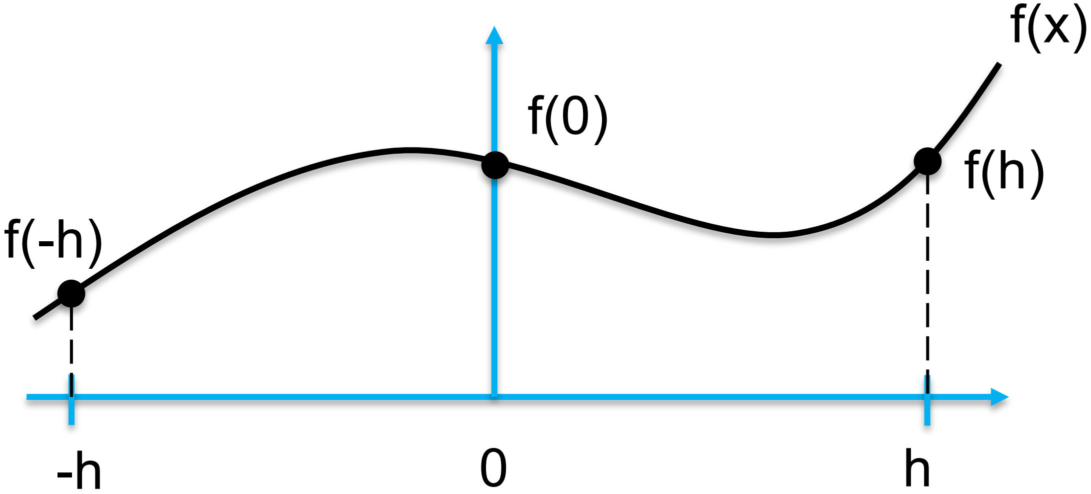
nodes	quadrature
$x_0 = -h$	$Q[f] = \omega_0 f(-h) +$
$x_1 = 0$	$\omega_1 f(0) +$
$x_2 = h$	$\omega_2 f(h)$

Find weights ω_i such that Q[f] has a DoP 2: i.e. exact for any $p \in \mathbb{P}^2$

(0) $p = 1$
(1) $p = x$
(2) $p = x^2$

$$\begin{bmatrix} 1 & 1 & 1 \\ -h & 0 & h \\ h^2 & 0 & h^2 \end{bmatrix} \begin{bmatrix} \omega_0 \\ \omega_1 \\ \omega_2 \end{bmatrix} = \begin{bmatrix} \int_{-h}^{h} 1\, dx \\ \int_{-h}^{h} x\, dx \\ \int_{-h}^{h} x^2\, dx \end{bmatrix} = \begin{bmatrix} 2h \\ 0 \\ \frac{2}{3}h^3 \end{bmatrix}$$

Example: derivation of Simpson's rule



nodes

$x_0 = -h$

$x_1 = 0$

$x_2 = h$

quadrature

$Q[f] = \omega_0 f(-h) + \omega_1 f(0) + \omega_2 f(h)$

Find weights ω_i such that Q[f] has a DoP 2: i.e. exact for any $p \in \mathbb{P}^2$

(0) $p = 1$
(1) $p = x$
(2) $p = x^2$

$$\begin{bmatrix} 1 & 1 & 1 \\ -h & 0 & h \\ h^2 & 0 & h^2 \end{bmatrix} \begin{bmatrix} \omega_0 \\ \omega_1 \\ \omega_2 \end{bmatrix} = \begin{bmatrix} 2h \\ 0 \\ \frac{2}{3}h^3 \end{bmatrix}$$

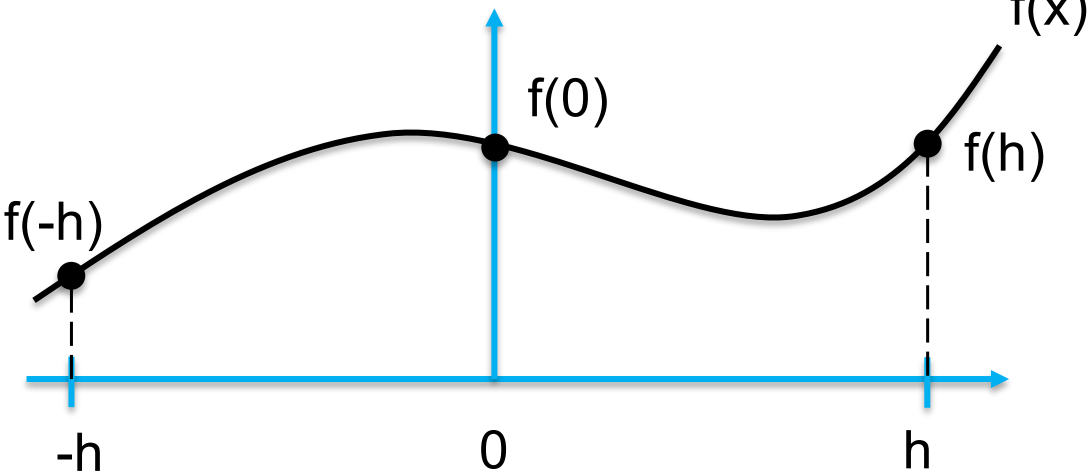
$(1) \Rightarrow \omega_0 = \omega_2$

$(2) \Rightarrow \omega_0 = \omega_2 = \frac{h}{3}$

$(0) \Rightarrow \omega_1 = \frac{4}{3}h$

TU Delft

Example: derivation of Simpson's rule



nodes

$x_0 = -h$

$x_1 = 0$

$x_2 = h$

quadrature

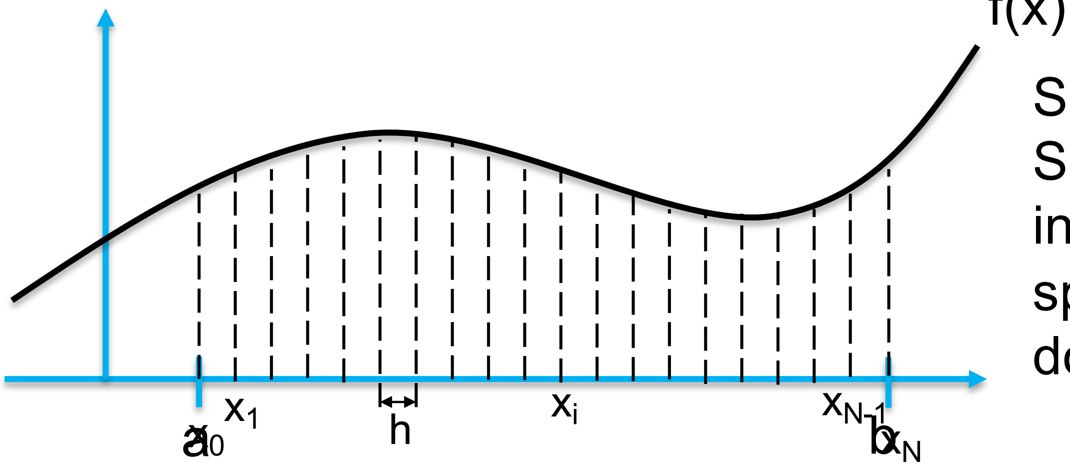
$Q[f] = \omega_0 f(-h) + \omega_1 f(0) + \omega_2 f(h)$

Therefore, the quadrature:

$$Q(f; -h, h) = \frac{h}{3}[f(-h) + 4f(0) + f(h)]$$

Which is known as "Simpson's Rule" has a DoP of 2

Example: Interval transformation



Suppose we want to use Simpson's rule to integrate domain [a,b] by splitting into *N* sub-domains with equal size *h*

$$\int_a^b f(x)dx = \sum_{i=0}^{N-1} \int_{x_i}^{x_{i+1}} f(x)dx \approx \sum_{i=0}^{N-1} Q(f;\ x_i, x_{i+1})$$

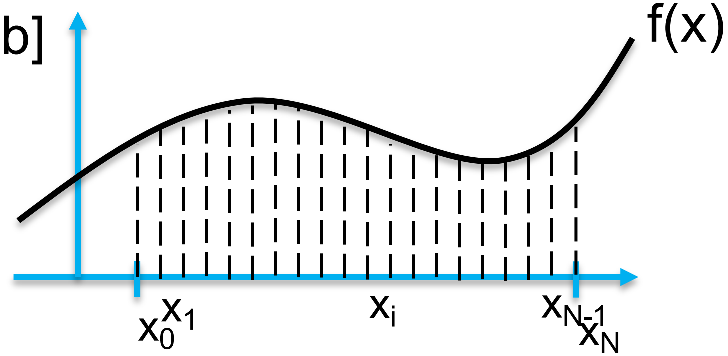
Using Simpson's rule quadrature (in computational space):

$$Q_\xi(f;-1,1) = \tfrac{1}{3}[f(-1) + 4f(0) + f(1)]$$

Example: Interval transformation

Approximate the integral of *f(x)* over [a, b]

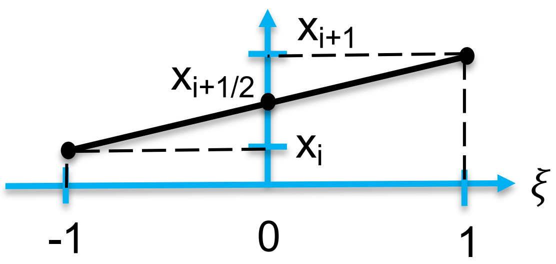
$$\int_a^b f(x)dx \approx \sum_{i=0}^{N-1} Q(f;\, x_i, x_{i+1})$$



Using Simpson's rule quadrature:

$$Q_\xi(f;-1,1) = \tfrac{1}{3}[f(-1) + 4f(0) + f(1)]$$

Map "computational space" onto "physical space":



$$\Rightarrow \begin{cases} \xi = -1 \Rightarrow x = x_i \\ \xi = 0 \quad \Rightarrow x = x_{i+1/2} \\ \xi = 1 \quad \Rightarrow x = x_{i+1} \end{cases}$$

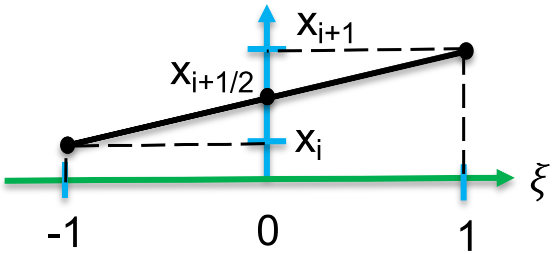
Slope:

$$\frac{dx}{d\xi} = \frac{x_{i+1} - x_i}{2} = \frac{h}{2}$$

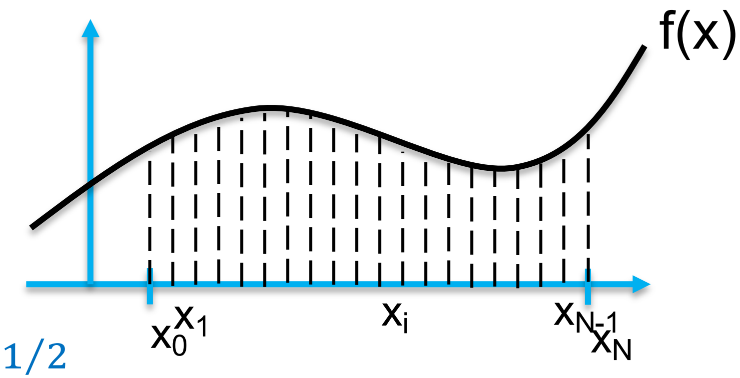
Example: Interval transformation

Simpson's rule quadrature:

$$Q_\xi(f; -1, 1) = \frac{1}{3}[f(-1) + 4f(0) + f(1)]$$



$$\begin{cases} \xi = -1 \Rightarrow x = x_i \\ \xi = 0 \Rightarrow x = x_{i+1/2} \\ \xi = 1 \Rightarrow x = x_{i+1} \end{cases}$$



Slope: $\frac{dx}{d\xi} = \frac{h}{2}$

$$Q(f(x); x_i, x_{i+1}) = \frac{dx}{d\xi} Q_\xi(f(x(\xi)); -1, 1)$$

$$= \frac{h}{2}\frac{1}{3}\left[f(x_i) + 4f\left(x_{i+1/2}\right) + f(x_{i+1})\right]$$

$$\int_a^b f(x)dx \approx \sum_{i=0}^{N-1} Q(f; x_i, x_{i+1}) = \sum_{i=0}^{N-1} \frac{h}{6}\left[f(x_i) + 4f\left(x_{i+1/2}\right) + f(x_{i+1})\right]$$