
# Introduction to Scientific Computing

(Lecture 9: Numerical integration)

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December 12, 2017

# Solving ODE

In last lecture we have shown that the proces of solving

$$\dot{x}(t) = f(t, x(t)),$$

for $t \in [t_0, T], x(t_0) = x_0$, where $f : \mathbb{R}_+ \times \mathbb{R}^n \to \mathbb{R}^n$ is a given function and $x_0$ is the given initial condition, is equivalent to the process of evaluating the solution of the following integral equation

$$x(T) = x_0 + \int_{t_0}^{T} f(t, x(t))\, dt$$

# Problem

The main issue appearing in the previous equation is that the integral cannot be always computed in an analytical way. In order to avoid this, we may perform numerical integration

$$\text{integral} = \text{area under curve}$$

which further means that we need to compute the area under curve

$$\int_{t_0}^{T} f(t, x(t))\, dt$$

However, this is not an easy task since the term under integral $f(t, x(t))$ depends on the unknown $x$.

# Numerical integration

In practice, there are many situations in which the previous integrand can be respesented as a function of time only

$$\int_{t_0}^{T} f(t, x(t))\, dt = \int_{t_0}^{T} g(t)\, dt$$

which further makes our problem easier to treat. As analytical solution of the previous integral is not always possible, one may try to numerically compute the value by approximating the function $g$ by something simpler such as a polynomial $P_n(t)$ of order $n$—polynomial interpolation.

# Polynomial interpolation

The polynomial

$$P_n(t) = a_0 + a_1 t + ... + a_n t^n$$

can be integrated instead of $g(t)$ in one of following ways

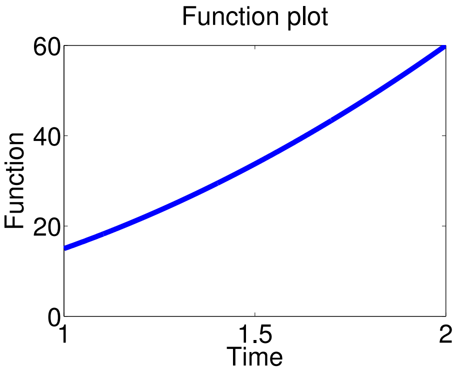
- globally: compute the area under the curve directly

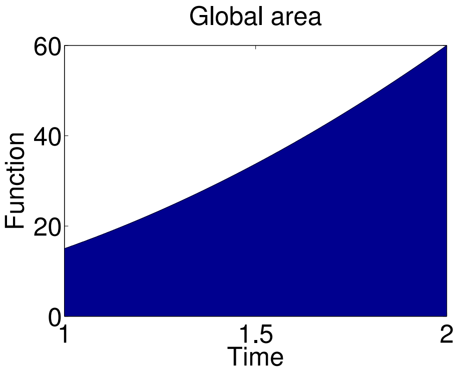
$$\int_{t_0}^{T} g(t)\, dt \approx \int_{t_0}^{T} P_n(t)\, dt$$

- locally: compute the area under curve by cutting it into pieces (composite rule)

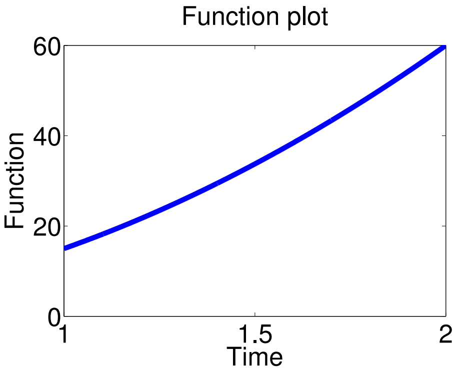
$$\int_{t}^{t+h} g(t)\, dt \approx \sum_{i=0}^{N-1} \int_{t_i}^{t_i+h} P(t)\, dt$$

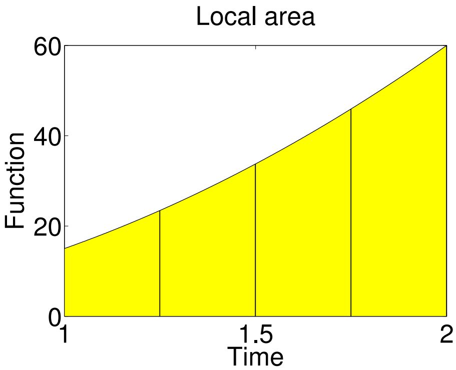
# Global integration



# Local integration



# How to choose polynomial?

Let us choose $n$ pairwise distinct points $t_i$ in time interval $I = [t_0, T]$, and let us compute the value of function $g_i := g(t_i)$ in these points. Then the polynomial can be found by global interpolation

$$g(t_i) = P(t_i) = \sum_{j=0}^{n} a_j t_i^j$$

The last relation is equivalent to the process of solving

$$Qa = w$$

in which

$$Q = [t_i^j], \quad a = [a_j], \quad w = [g(t_i)]$$

# Polynomial interpolation

The matrix $Q$ is of the form

$$Q = \begin{pmatrix} 1 & t_0 & \dots & t_0^n \\ 1 & t_1 & \dots & t_1^n \\ \vdots & \vdots & & \vdots \\ 1 & t_n & \dots & t_n^n \end{pmatrix}$$

and hence is regular. This further means that one may compute the vector of unknown coefficients $a$ by solving

$$Qa = w$$

To solve the previous equation one may use one of the iterative methods introduced to you before.

# Newton-Cotes integration

Once the coefficients $a_j$ are known the integration becomes simple

$$\int_{t_0}^{T} g(t)\; dt \approx \int_{t_0}^{T} P(t)\; dt = \int_{t_0}^{T} \sum_{j=0}^{n} a_j t_i^j dt$$

Before we give general expression for the previous interval, let us first focus on specific polynomiall approximations:

- piecewise constant interpolation
- linear interpolation
- quadtratic interpolation

# Global piecewise constant interpolation

To compute the integral

$$\int_{t_0}^{T} g(t)\, dt$$

we approximate the function $g$ by a zero order polynomial

$$P_1(t) = a_0$$

such that for given point $(t_i, g_i := g(t_i))$ the following interpolation condition holds

$$P_1(t_i) = g(t_i) \Rightarrow a_0 = g(t_i)$$

# Global piecewise constant interpolation

This then leads to

$$\int_{t_0}^{T} g(t)\ dt = \int_{t_0}^{T} P(t)\ dt = \int_{t_0}^{T} a_0 dt = g_i(T - t_0)$$

Hence,

$$\int_{t_0}^{T} g(t) dt \approx g(t_i)(T - t_0)$$

In other words, one computes the integral as area of rectangle.

# Global piecewise constant interpolation

Depending on the choice of $g(t_i)$ one may distinguish

- left sum: $g_i = g(t_0) \Rightarrow \int_{t_0}^{T} g(t)dt \approx g_i(T - t_0)$
- right sum: $g_i = g(T) \Rightarrow \int_{t_0}^{T} g(t)dt \approx g_i(T - t_0)$
- lower sum: $g_i = \underset{t \in I}{min}\, g(t) \Rightarrow \int_{t_0}^{T} g(t)dt \approx g_i(T - t_0)$
- upper sum: $g_i = \underset{t \in I}{max}\, g(t) \Rightarrow \int_{t_0}^{T} g(t)dt \approx g_i(T - t_0)$
- mid-point rule: $\int_{t_0}^{T} g(t)dt \approx 0.5(g(t_0) + g(T))(T - t_0)$

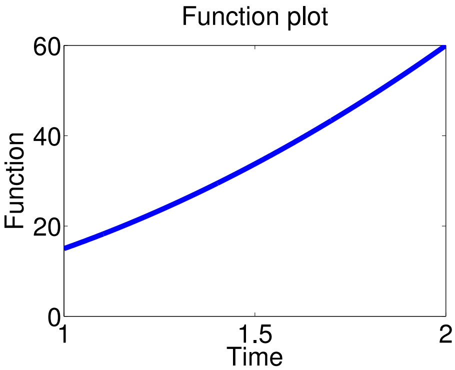
Pros:

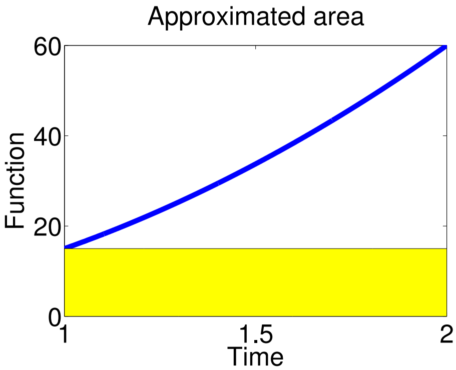
- easy to perfom numerical integration

Cons:

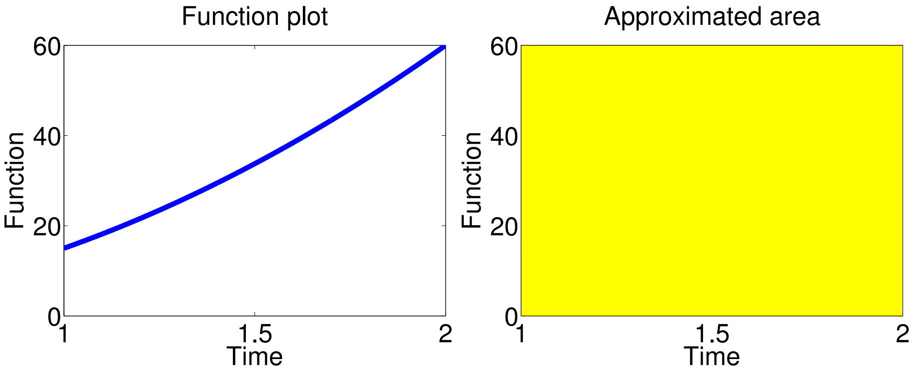
- not very much accurate

# Left (also lower) integration rule

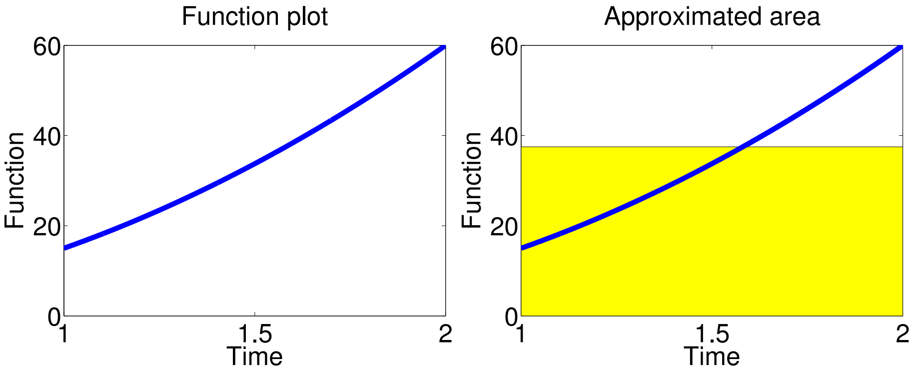


# Right (also upper) integration rule



# Mid-point integration rule



# Exercise: Global interpolation

Problem: Compute the integral of $g(t) = 15t^2$ on interval $[1, 2]$.

Answer: having

the

$$g(t_0) = 15, \quad g(t_1) = 15 \cdot 2^2 = 60$$

approximation of integral by left (here also lower) rule becomes

$$\int_{t_0}^{T} g(t)dt \approx g_{(}t_0)(T - t_0) = 15 \cdot (2 - 1) = 15$$

The correct value is

$$\int_1^2 15t^2 dt = 15\frac{t^3}{3}|_1^2 = \frac{15}{3}(2^3 - 1^3) = 5 \cdot 7 = 35$$

# Exercise: Global interpolation

Thus, global interpolation using this rule is not correct. The right/upper rule gives

$$\int_{t_0}^{T} g(t)dt \approx g_{(}T_0)(T - t_0) = 60 \cdot (2-1) = 60$$

and leads to overestimation. Finally, the mid-point rule

$$\int_{t_0}^{T} g(t)dt \approx 0.5(g(t_0) + g(T))(T - t_0) = 37.5 \cdot (2-1) = 37.5$$

is also not correct. However, it is the closest to the solution.

# Local piecewise constant interpolation

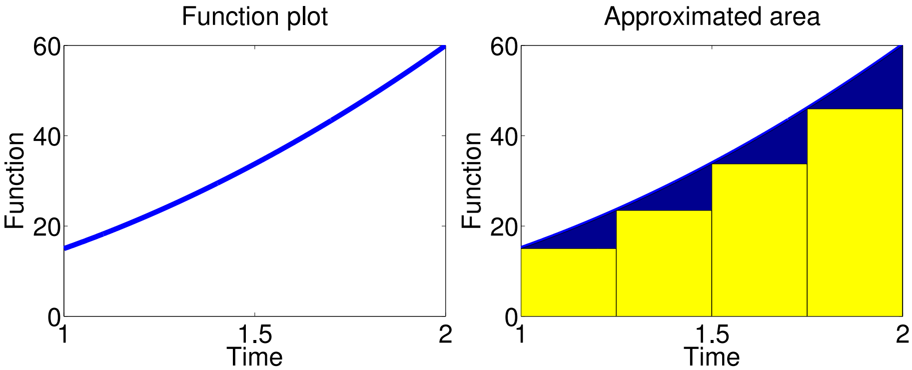
To increase accuracy one may apply the local piecewise interpolation. That is to divide the interval $[t_0, T]$ into $N$ subintervals such that the integral reads

$$\int_{t_0}^{T} g(t)\, dt \approx \sum_{i=0}^{N-1} \int_{t_i}^{t_i+h} g(t)\, dt$$

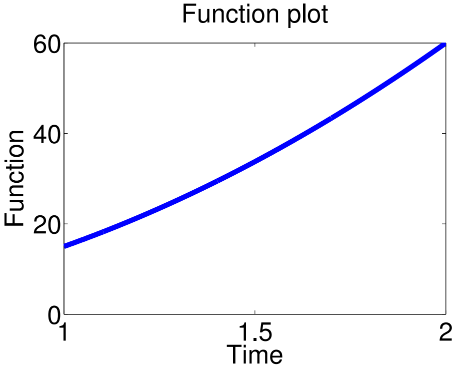
Then in each subinterval apply interpolation by

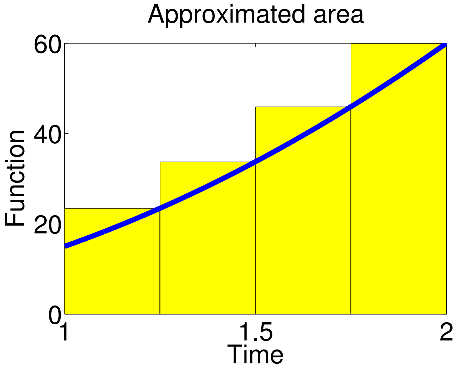
- left rule
- right rule
- lower sum
- upper sum
- mid-point rule

# Local left (here also lower) rule

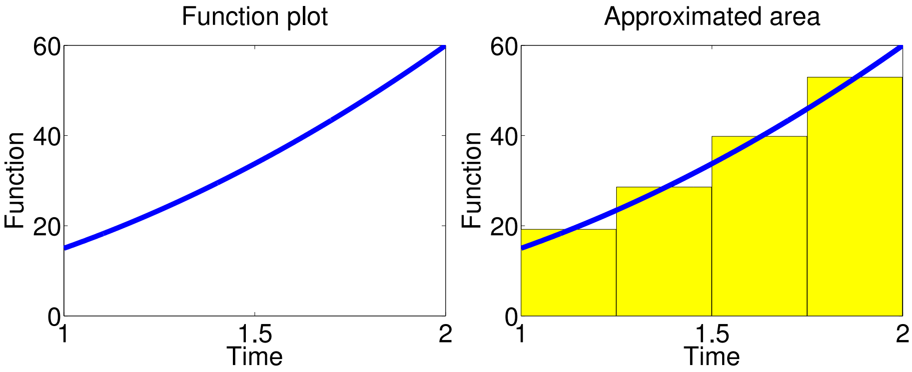


# Local right (here also upper) rule



# Local midpoint rule



# Exercise: Local interpolation

Problem: Compute the integral of $g(t) = 15t^2$ on interval $[1, 2]$ using composite left rule.

Answer: Divide the interval into $N$ small subintervals and take $h = \frac{2-1}{N}$. Then compute the values of function $g(t)$ in points $t_i = t_0 + hi, i = 0, 1, \cdots, N$. Let us take, for example, $N = 2$, then $h = 0.5$ and the points are $t_0 = 1, t_1 = 1.5, t_2 = 2$. The values of function in those points are:

$$g(t_0) = 15, \quad g(t_1) = 15 \cdot 1.5^2 = 33.75, \quad g(t_2) = 15 \cdot 2^2 = 60$$

Left rule reads:

$$\int_1^2 g(t)dt = \sum_{i=0}^{N-1} g(t_i)h$$

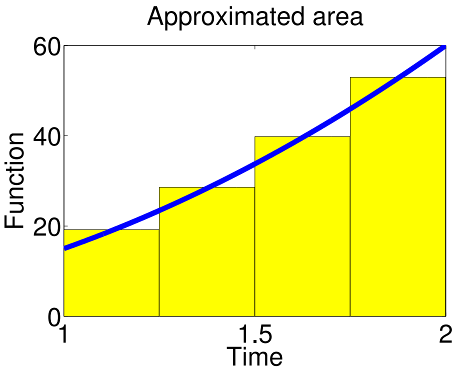
# Exercise: Local interpolation

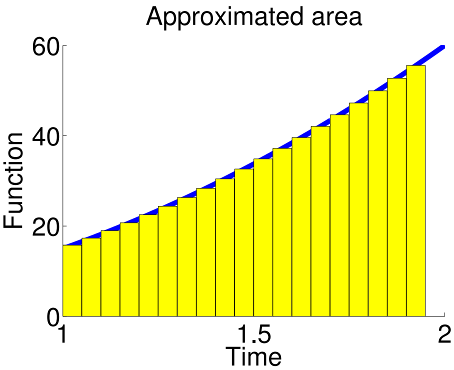
In our case $N = 2$ and hence

$$\int_1^2 g(t)dt = (15 + 33.75) \cdot 0.5 = 24.375$$

This value is closer to the correct one compared to the global rule. Precision will improve with the increase of number $N$. On the other side, with the increase of $N$ the number of function evaluations $g(t_i)$ will also increase (and hence the computation time).

# Local midpoint rule:coarser vs finer



# Global linear interpolation

To compute the integral

$$\int_{t_0}^{T} g(t)\, dt$$

we may approximate the function $g$ by a linear polynomial

$$P_1(t) = a_0 + a_1 t$$

such that for given two points $(t_i, g_i := g(t_i))$ and $(t_{i+1}, g_{i+1} := g(t_{i+1}))$ in $I$ the following interpolation conditions hold

$$P_1(t_i) = g(t_i), \quad P_1(t_{i+1}) = g(t_{i+1})$$

# Global linear interpolation

The last relation represents the system of equations

$$\begin{pmatrix} 1 & t_i \\ 1 & t_{i+1} \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \end{pmatrix} = \begin{pmatrix} g(t_i) \\ g(t_{i+1}) \end{pmatrix} = \begin{pmatrix} g_i \\ g_{i+1} \end{pmatrix}$$

After solving one obtains

$$a_1 = \frac{g_{i+1} - g_i}{t_i - t_{i+1}}$$

and

$$a_0 = g_i - \frac{g_{i+1} - g_i}{t_i - t_{i+1}} t_i$$

# Global linear interpolation

Now substitute back the coefficients into polynomial:

$$P_1(t) = a_1 t + a_0$$

$$\begin{aligned} P_1(t) &= \frac{g_{i+1} - g_i}{t_i - t_{i+1}} t + g_i - \frac{g_{i+1} - g_i}{t_i - t_{i+1}} t_i \\ &= \frac{(g_{i+1} - g_i)t - g_i t_{i+1} - g_{i+1} t_i}{t_i - t_{i+1}} \end{aligned}$$

$$P_1(t) = \frac{t - t_{i+1}}{t_i - t_{i+1}} g_i + \frac{t - t_i}{t_{i+1} - t_i} g_{i+1}$$

# Global linear interpolation

Note that in

$$P_1(t) = \frac{t - t_{i+1}}{t_i - t_{i+1}} g_i + \frac{t - t_i}{t_{i+1} - t_i} g_{i+1}$$

we have polynomials

$$\ell_i := \frac{t - t_{i+1}}{t_i - t_{i+1}}, \quad \ell_{i+1} := \frac{t - t_i}{t_{i+1} - t_i} g_{i+1}$$

These are known as **Lagrange polynomials**. Hence, our polynomial $P_1(t)$ is actually Lagrange expansion:

$$g(t) \approx P_1(t) = \ell_i g_i + \ell_{i+1} g_{i+1}$$

Once we know this, the integration can be performed.

# Properties of $\ell_i$

We have

$$\ell_i(t_k) := \delta_{ik} := \begin{cases} 1, & k = i \\ 0, & k \neq i \end{cases},$$

where $\delta_{ik}$ is the so-called Kronecker-product.

# Global linear interpolation

Integration reads

$$\int_{t_0}^{T} P_1(t)dt = \int_{t_0}^{T} \ell_i g_i dt + \int_{t_0}^{T} \ell_{i+1} g_{i+1} dt$$

i.e.

$$\int_{t_0}^{T} P_1(t)dt = g_i \int_{t_0}^{T} \ell_i dt + g_{i+1} \int_{t_0}^{T} \ell_{i+1} dt$$

$$\int_{t_0}^{T} P_1(t)dt = g_i w_i + g_{i+1} w_{i+1}$$

where

$$w_i := \int_{t_0}^{T} \ell_i dt, \quad w_{i+1} = \int_{t_0}^{T} \ell_{i+1} dt$$

# Global linear interpolation

Weights in last relation do not depend on the function $g(t)$. They read

$$w_0 := \int_{t_0}^{T} \frac{t - T}{t_0 - T} dt, \quad w_1 = \int_{t_0}^{T} \frac{t - t_0}{T - t_0} dt$$

However, they do depend on the interval $I = [t_0, T]$, which prevents us from precomputing them. To resolve this issue, one may transform interval $[t_0, T]$ to $[0, 1]$. To achieve this use the transformation formula

$$\tau := \frac{t - t_0}{T - t_0}$$

which for $t = t_0$ gives 0 and for $t = T$ gives 1.

# Global linear interpolation

From the transformation formula one has

$$d\tau = \frac{1}{T - t_0} dt$$

as well as

$$t = \tau(T - t_0) + t_0$$

This leads to

$$w_0 := \int_{t_0}^{T} \frac{t - t_0}{T - t_0} dt = \int_0^1 \frac{\tau(T - t_0) + t_0 - t_0}{T - t_0} (T - t_0) d\tau$$

i.e.

$$w_0 := (T - t_0) \int_0^1 \tau d\tau$$

# Global linear interpolation

in last relation

$$w_0 := (T - t_0)\int_0^1 \tau d\tau$$

integral $\int_0^1 \tau d\tau$ can be computed analytically. Let us denote its value as $\alpha_0$ such that

$$w_0 := (T - t_0)\int_0^1 \tau d\tau = (T - t_0)\alpha_0$$

holds. Note that $\alpha_0$ is the weigth which can be stored in a table. in a similar manner one may compute

$$w_1 = \int_{t_0}^{T} \frac{t - t_0}{T - t_0} dt$$

# Global linear interpolation

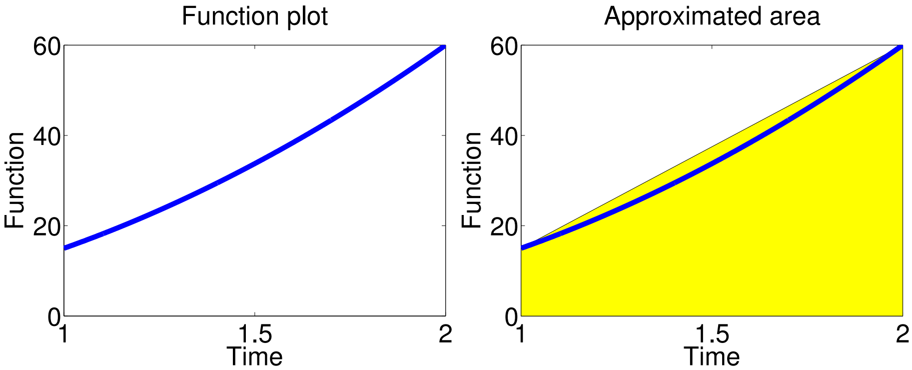
Once the weights are found, the final formula for linear numerical integration reads

$$\int_{t_0}^{T} g(t)dt = \int_{t_0}^{T} P_1(t)dt = g_0 w_0 + g_1 w_1$$

$$= (T - t_0) \sum_{i=0}^{1} \alpha_i g_i = 0.5(T - t_0)(g(t_0) + g(T)).$$

Hence, the integral is approximated by area of trapozoid. Thus, this numerical integration is named as **trapezoidal rule**.

# Global linear interpolation



# Exercise: Global interpolation

Compute the integral of $f(x) = 15x^2$ on interval $[1, 2]$. Hence, $t_0 = 1$, $t_1 = 2$.

$$\int_1^2 g(t)dt = \int_1^2 15t^2 = \frac{1}{2}(t_1 - t_0)[g(t_0) + g(t_1)]$$

$$\int_1^2 15t^2 dt = \frac{1}{2}(2-1)[15 \cdot 1^2 + 15 \cdot 2^2] = 0.5 \cdot 75 = 37.5$$

True value:

$$\int_1^2 15t^2 dt = 15\frac{t^3}{3}|_1^2 = \frac{15}{3}(2^3 - 1^3) = 5 \cdot 7 = 35$$

# Local linear interpolation

In similar manner as before the global linear interpolation can be translated to the local linear interpolation by using cummulative rule

$$\int_{t_0}^{T} g(t)\, dt \approx \sum_{i=0}^{N-1} \int_{t_i}^{t_i+h} g(t)\, dt$$

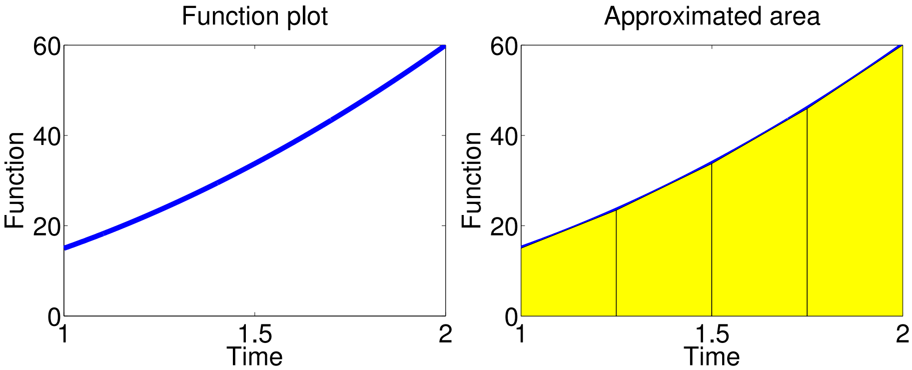
and in each subinterval interpolating function $g(t)$ by a linear polynomial

$$\int_{t_i}^{t_i+h} P_1(t) dt = \int_{t_i}^{t_i+h} \ell_i g_i dt + \int_{t_i}^{t_i+h} \ell_{i+1} g_{i+1} dt$$

Finally,

$$\int_{t_0}^{T} g(t)\, dt \approx \sum_{i=0}^{N-1} 0.5h(g_i + g_{i+1})$$

# Local linear interpolation



# Exercise: Local interpolation

Compute the integral of $g(t) = 15t^2$ on interval $[1, 2]$ by composite rule. Hence, let us take $N = 2$. Then, $t_0 = 1, t_1 = 1.5, t_2 = 2$.

$$\int_1^2 g(t)dt = \int_1^{1.5} 15t^2 + \int_{1.5}^2 15t^2$$

$$= \frac{1}{2}(t_1 - t_0)[g(t_0) + g(t_1)] + \frac{1}{2}(t_2 - t_1)[g(t_2) + g(t_1)]$$

$$\int_1^2 15t^2 dt = \frac{1}{2}(1.5 - 1)[15 \cdot 1^2 + 15 \cdot (1.5)^2]$$

$$+\frac{1}{2}(2 - 1.5)[15 \cdot (1.5)^2 + 15 \cdot (2)^2] = 12.1875 + 23.4375 = 35.625$$

# Global quadratic interpolation

To compute the integral

$$\int_{t_0}^{T} g(t)\, dt$$

we approximate the function $g$ by a quadratic polynomial

$$g(t) \approx P_2(t) = a_2 t^2 + a_1 t + a_0$$

where

$$P_2(t_i) = g_i$$
$$P_2(t_{i+1}) = g_{i+1}$$
$$P_2(t_{i+2}) = g_{i+2}$$

Here, points $t_i$ are equidistant in the interval $[t_0, T]$.

# Global quadratic interpolation

Having that $t_{i+1} = \frac{t_i + t_{i+2}}{2}$ and after solving previous system for $a_2, a_1$ and $a_0$ one obtains

$$a_2 = \frac{(2g_i - 4g_{i+1} + 2g_{i+2})}{(t_i^2 - 2t_i t_{i+2} + t_{i+2}^2)}$$

$$a_1 = -\frac{(g_i t_i - 4g_{i+1} t_i + 3g_i t_{i+2} + 3g_{i+2} t_i - 4g_{i+1} t_{i+2} + g_{i+2} t_{i+2})}{(t_i^2 - 2t_i t_{i+2} + t_{i+2}^2)}$$

$$a_0 = \frac{(g_i t_{i+2}^2 + g_{i+2} t_i^2 + g_i t_i t_{i+2} - 4g_{i+1} t_i t_{i+2} + g_{i+2} t_i t_{i+2})}{(t_i^2 - 2t_i t_{i+2} + t_{i+2}^2)}$$

# Global quadratic interpolation

After substitution in $P_2(t)$ one obtains:

$$P_2(t) = \frac{(t-t_{i+1})(t-t_{i+2})}{(t_i-t_{i+1})(t_i-t_{i+2})}g_i + \frac{(t-t_i)(t-t_{i+2})}{(t_{i+1}-t_i)(t_{i+1}-t_{i+2})}g_{i+1}$$
$$+\frac{(t-t_i)(t-t_{i+2})}{(t_{i+2}-t_i)(t_{i+2}-t_{i+1})}g_{i+2}.$$

in which the quadratic Lagrange polynomials read

$$\ell_i = \frac{(t-t_{i+1})(t-t_{i+2})}{(t_i-t_{i+1})(t_i-t_{i+2})}, \quad \ell_{i+1} = \frac{(t-t_i)(t-t_{i+2})}{(t_{i+1}-t_i)(t_{i+1}-t_{i+2})}$$

$$\ell_{i+2} = \frac{(t-t_i)(t-t_{i+2})}{(t_{i+2}-t_i)(t_{i+2}-t_{i+1})}$$

# Global quadratic interpolation

Hence,

$$P_2(t) = \ell_i g_i + \ell_{i+1} g_{i+1} + \ell_{i+2} g_{i+2}$$

which after integration leads to

$$\int_{t_0}^{T} P_2(t)dt = g_i \int_{t_0}^{T} \ell_i dt + g_{i+1} \int_{t_0}^{T} \ell_{i+1} dt + g_{i+2} \int_{t_0}^{T} \ell_{i+2} dt$$

If we employ transformation of the interval $[t_0, T]$ into $[0, 1]$ in a similar manner as for linear interpolation one obtains

$$\int_{t_0}^{T} P_2(t)dt = (T - t_0) \sum_{i=0}^{n} g(t_i) \underbrace{\int_0^1 \prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{nt - j}{i - j}\, dt}_{=:\alpha_i}$$

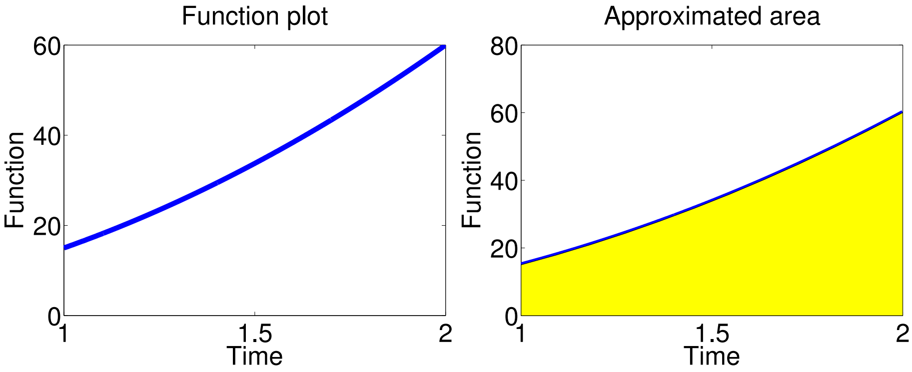
# Global quadratic interpolation

After simple mathematical operations one finally obtains:

$$\int_{t_0}^{T} g(t)dt = \int_{t_0}^{T} P_2(t)dt = \frac{T - t_0}{6}(g_i + 4g_{i+1} + g_{i+2})$$

which is known as Simpson's rule.

# Global quadratic interpolation



# Exercise: Global interpolation

Compute the integral of $g(t) = 15t^2$ on interval $[1, 2]$. Hence, $t_0 = 1$, $t_1 = 1.5$, $t_2 = 2$.

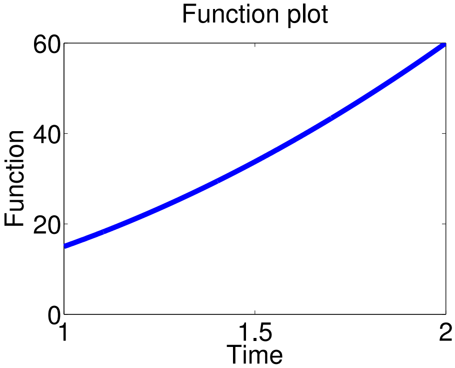
$$\int_1^2 g(t)dt = \frac{T - t_0}{6}(g_i + 4g_{i+1} + g_{i+2})$$

$$\int_1^2 g(t)dt = \frac{1}{6}(15(1)^2 + 4 \cdot 15 \cdot (1.5)^2 + 15 \cdot (2)^2 = 35$$

This shows us that the global quadratic interpolation is exact for the function of polynomial order 2. Namely, this method is exact for function of polynomial order 3 or less.

# Local quadratic interpolation

Quadratic interpolation applied on each subinterval $h$ of interval $I$ is called local. And can be applied in a similar manner as previous interpolations.



# Exercise: Local interpolation

Compute the integral of $g(t) = 15t^2$ on interval $[1, 2]$ by composite rule. Hence, $N = 2$ and $t_0 = 1$, $t_1.25$ $t_2 = 1.5$, $t_3 = 1.75$ $t_4 = 2$.

$$\int_1^2 g(t)dt = \int_{t_0}^{t_2} g(t)dt + \int_{t_2} t_3 g(t)dt$$

$$\int_1^2 g(t)dt = \frac{0.5}{6}(15(1)^2 + 4 \cdot 15 \cdot (1.25)^2 + 15 \cdot (1.5)^2)$$
$$+\frac{0.5}{6}(15(1.5)^2 + 4 \cdot 15 \cdot (1.75)^2 + 15 \cdot (2)^2)$$
$$= 35$$

Hence, the same conclusion as for global interpolation.

# Error of polynomial approximation

Let us define the function

$$\phi(t) = g(t) - P_n(t) - \frac{g(t_p) - P_n(t_p)}{v(t_p)} v(t)$$

in which $g(t)$ is the function we would like to integrate (belongs to $C^{n+1}(I)^a$) and $P_n(t)$ is the $n$-th order interpolation polynomial (through $t_i, i = 0, .., n$ interpolation points). Argument $t_p$ is some chosen (fixed) point in interval of definition $I$, not neccessary the interpolation point. Here,

$$v(t) = \prod_{i=0}^{n}(t - t_i), v(t_p) = \prod_{i=0}^{n}(t_p - t_i)$$

[a] $g$ is in the interval $I$ $n+1$-times continuously differentiable

# Error of polynomial approximation

The function

$$\phi(t) = g(t) - P_n(t) - \frac{g(t_p) - P_n(t_p)}{v(t_p)} v(t)$$

has the following properties

- $\phi(t) = 0$ when $t = t_i$ or $t = t_p$, i.e. it has $(n+2)$ roots
- $\phi'(t)$ has $n+1$ roots
- $\phi^{(n+1)}(t)$ has only one root denoted by $\xi$, i.e. $\phi^{(n+1)}(\xi) = 0$

# Error of polynomial approximation

This allows us to write

$$\phi^{(n+1)}(t) = \frac{d^{(n+1)}}{dt^{(n+1)}}(g(t) - P_n(t) - \frac{g(t_p) - P_n(t_p)}{v(t_p)} v(t)$$

$$= g^{(n+1)}(t) - P_n^{(n+1)}(t) - \frac{g(t_p) - P_n(t_p)}{v(t_p)} v^{(n+1)}(t)$$

$$= g^{(n+1)}(t) - P_n^{(n+1)}(t) - \frac{g(t_p) - P_n(t_p)}{v(t_p)} (n+1)!$$

Furthermore,

$$\phi^{(n+1)}(\xi) = 0 \Rightarrow g^{(n+1)}(\xi) - P_n^{(n+1)}(\xi) - \frac{g(t_p) - P_n(t_p)}{v(t_p)} (n+1)! = 0$$

Here note that $P_n^{(n+1)}(\xi) = 0$ since $P_n$ is polynomial of order $n$

# Error of polynomial approximation

Thus,

$$g^{(n+1)}(\xi) - \frac{g(t_p) - P_n(t_p)}{v(t_p)}(n+1)! = 0$$

from which one obtains the estimate of the error

$$g(t_p) - P_n(t_p) = \frac{1}{(n+1)!}g^{(n+1)}(\xi)v(t_p) = \frac{1}{(n+1)!}g^{(n+1)}(\xi)\prod_{i=0}^{n}(t_p - t_i)$$

in point $t_p$ of interval.

# Error of polynomial approximation

Theorem

*Let $g \in C^{n+1}(I)$, then there exists for every $t$ a $\xi \in I_s$ (smallest interval which contains points) such that*

$$g(t) - P_n(t) = \frac{1}{(n+1)!} g^{(n+1)}(\xi) \prod_{j=0}^{n} (t - t_j)$$

*holds. Since $\xi$ is unknown, the error is estimated by*

$$|g(t) - P_n(t)| \leq \frac{1}{(n+1)!} \max_{\xi \in I_s} |g^{(n+1)}(\xi)| \left| \prod_{j=0}^{n} (t - t_j) \right|.$$

# Error of numerical integration

Aim: Find an error estimator for

$$E_n^I(g) := \int_{t_0}^{T} g(t)dt \; - \sum_{j=0}^{n} \alpha_j g(t_j)$$

*Theorem: Let $H := \frac{T-t_0}{n}$ and $g$ be sufficiently often differentiable in $I$. Then there exists a constant $c_n$ independent of the interval $I$ such that*

$$|E_n^I(g)| \leq \frac{c_n}{(n+1)!} \max_{\xi \in I} \left| g^{(n+1)}(\xi) \right|, \quad c_n := |\int_{t_0}^{T} \prod_{i=0}^{n} (t - t_i)|$$

*holds. If $n$ is even, then there exists a constant $d_n$ independent of the interval $I$ such that*

$$|E_n^I(g)| \leq \frac{d_n}{(n+2)!} \max_{\xi \in I} \left| g^{(n+2)}(\xi) \right|, \quad d_n := |\int_{t_0}^{T} t \prod_{i=0}^{n} (t - t_i)|$$

*holds.*

# Exercise: error

Before we have used linear global interpolation to compute the value of intergral of a function $f(x) = 15t^2$ on interval $[1, 2]$.

We got the following result

| exact | approximated |
|---|---|
| 35 | 37.5 |

Let us now compute the error using error estimate

$$|E_n^I(g)| \leq \frac{c_n}{(n+1)!} \max_{\xi \in I} \left| g^{(n+1)}(\xi) \right|, \quad c_n := \left| \int_{t_0}^{T} \prod_{i=0}^{n} (t - t_i) \right|$$

in which $n + 1 = 2$.

# Exercise: error

Having

$$g^{'} = 30t, g^{''} = 30$$

one concludes that

$$\max_{\xi \in I} \left| g^{(n+1)}(\xi) \right| = 30$$

Furthermore,

$$\int_{t_0}^{T} \prod_{i=0}^{n} (t - t_i) = \int_{0}^{1} (t-0)(t-1)dt = \frac{t^3}{3} - \frac{t^2}{2} = -\frac{1}{6}$$

Thus,

$$|E_n^I(g)| \leq \frac{\frac{1}{6}}{(2)!} 30 = 2.5$$

# Exercise: error

Let us compute the error of linear global interpolation to compute the value of intergral of a function $f(x) = 15t$ on interval $[1, 2]$. by applying linear integration one gets the following result

| exact | approximated |
|---|---|
| $\frac{45}{2}$ | $\frac{45}{2}$ |

Let us now compute the error using error estimate

$$|E_n^I(g)| \leq \frac{c_n}{(n+1)!} \max_{\xi \in I} \left| g^{(n+1)}(\xi) \right|, \quad c_n := | \int_{t_0}^{T} \prod_{i=0}^{n} (t - t_i) |$$

in which $n + 1 = 2$.

# Exercise: error

Having

$$g^{'} = 15, g^{''} = 0$$

one concludes that

$$\max_{\xi \in I} \left| g^{(n+1)}(\xi) \right| = 0$$

and hence

$$|E_n^I(g)| \leq 0$$

Thus, our integration is exact for linear polynomials (as well as for constant).

# What we know so far?

So far we have learned that given any set of $n$ points $t_i$ over the time interval $I$ we may build Newton-Cotes quadrature rule

$$w_i, t_i$$

which can be used to **exactly integrate polynomials of order** $n-1$ **or less** by using the formula

$$\int_{t_0}^{T} P(t)\, dt = \sum_{i=0}^{n-1} P(t_i) w_i$$

The question is: can we do better than that?

# Yes, we can

- Newton-Cotes formula
    - one chooses $n$ points $t_i$ in which the value of function will be evaluated (uniformly distributed)
    - weigths are computed according to given points $t_i$
    - accurate for polynomials of order $n-1$ given $n$ points
- improvement: Gauss quadrature
    - vary both $n$ points $t_i$ and $n$ weights $w_i$ (both are unknown)
    - make the integration formula exact for polynomials of order $2n-1$

# Gauss quadrature

The Gauss quadrature has for a goal to vary the placements $t_i$ such that the integration is more accurate. In general Gauss formula approximates:

$$\int_{-1}^{1} g(t)dt \approx \int_{-1}^{1} P(t)dt = \sum_{i=0}^{n} g(t_i)w_i, \quad w_i = \int_{-1}^{1} \ell_i(t)dt$$

in the same way as Newton-Cotes. But, $t_i$ are unknown and have to be found. Additionaly to them are also unknown the coefficients of a polynomial $P(t)$.

# 1 point Gauss quadrature

Let us have 1 point formula in which $t_i$ and hence $w_i$ are unknown. Having two unkowns, one has to build the system of two equations. This can be achieved by letting the formula to exactly integrate constant and linear polynomial. One does not loose on generality by letting

$$\int_{-1}^{1} 1dt = w_i g(t_i) = w_i \cdot 1.$$

$$\int_{-1}^{1} tdt = w_i g(t_i) = w_i \cdot t_i.$$

Having that $\int_{-1}^{1} 1dt = 2$ and $\int_{-1}^{1} tdt = 0$, the last system reduces to

$$t_i w_i = 0$$

$$w_i = 2$$

# 1 point Gauss quadrature

Hence, $t_i = 0, w_i = 2$ is 1 point Gauss rule which exactly integrates constant and linear polynomials over $[-1, 1]$. Do not forget that in Newton-Cotes formula we needed two points, i.e. two function evaluations.

# 2 point- Gauss quadrature

Let us have 2 point formula in which $t_{i-1}, t_i$ and hence $w_{i-1}, w_i$ are unknown. Having four unkowns, one has to build the system of four equations. This can be achieved by letting the formula to exactly integrate polynomial up to third order. One does not loose on generality by letting

$$\int_{-1}^{1} 1 dt = w_{i-1} + w_i$$

$$\int_{-1}^{1} t dt = t_{i-1} w_{i-1} + t_i w_i$$

$$\int_{-1}^{1} t^2 dt = t_{i-1}^2 w_{i-1} + t_i^2 w_i$$

$$\int_{-1}^{1} t^3 dt = t_{i-1}^3 w_{i-1} + t_i^3 w_i$$

# 2 point- Gauss quadrature

This leads to a system of equatons whose solution is

$$t_{i-1} = -\sqrt{\frac{1}{3}}, w_{i-1} = 1$$

$$t_i = \sqrt{\frac{1}{3}}, w_i = 1$$

Hence, the two point Gauss-quadrature rule approximates exactly the polynomials of order 3. Newton Cotes formula needed 4 evaluations.

# Generalisation

We need generalisation of 1-point and 2-pont rule. For this, note that 1-point rule

$$t_0 = 0, w_0 = 2$$

is placed in $t_0 = 0$ which is the root of a first order polynomial $q(t) = t$. Two point rule

$$t_0 = -\sqrt{\frac{1}{3}}, w_0 = 1, \quad t_1 = \sqrt{\frac{1}{3}}, w_1 = 1$$

is placed at roots of second order polynomial $q(t) = 0.5(3t^2 - 1)$. These two polynomials are known as **Legendre polynomials**.

$$What \quad about \quad n - point \quad rule?$$

# Generalisation

Let us express $2n-1$ order polynomial $P(t)$ over the $n$-th order Lagrange polynomial $q(t)$ whose roots are the integration points $t_i$ such that

$$P(t) = q(t)\phi(t) + r(t)$$

holds. Here, $\phi(t)$ and reminder $r(t)$ are at most of order $n-1$ or less. By applying integration rule

$$\int_{-1}^{1} g(t)dt \approx \int_{-1}^{1} P(t)dt = \int_{-1}^{1} (q(t)\phi(t) + r(t))dt \Rightarrow \int_{-1}^{1} g(t)dt = \int_{-1}^{1} r(t)dt$$

one may conclude that the last expression reduces only to $\int_{-1}^{1} r(t)dt$ having that the polynomial $q(t)$ is equal to zero in integration points (its own roots) $t_i$. Since $r(t)$ is of most $n-1$ order, the last integration is exact given $n$ points.

# Error estimation

In a similar manner as for Newton-Cotes formula, one may derive the error estimate:

$$\left| E_n^{[a,b]}(g) \right| \leq (b-a)^{2n+1} \frac{(n!)^4}{[(2n)!]^3(2n+1)} \max_{\xi \in [a,b]} \left| g^{(2n)}(\xi) \right|$$

Note that Gauß-formulas can be also made composite in a similar manner as Newton-Cotes formula.

# Another interval

So we know how to compute

$$\int_{-1}^{1} g(t)dt$$

What to do if

$$\int_{a}^{b} g(t)dt = ?$$

Then one may apply the **transformation formula**

$$\int_{a}^{b} g(t)dt = \int_{-1}^{1} f(p)dp$$

in which

$$t = qp + s, dt = qdp$$

such that $p = -1$ for $t = a$ and $p = 1$ for $t = b$.

# Another interval

By solving one obtains that

$$q = \frac{b-a}{2}, \quad s = \frac{a+b}{2}.$$

Hence,

$$\int_a^b g(t)dt = \int_{-1}^1 g(\frac{b-a}{2}p + \frac{a+b}{2})\frac{b-a}{2}dp = \int_{-1}^1 f(p)dp$$

and now you are ready to use the quadrature formula on $[-1, 1]$.

# Other Gauss quadratures

Note that Gauss-Legendre formula is the most often used, but it is not the only one. Integration points can also be selected as roots of other kind of polynomials. If the integral

$$\int_a^b g(t)dt$$

can be represented as

$$\int_a^b g(t)dt = \int_a^b v(t)f(t)dt = \sum_{i=0}^{n-1} w_i f(t_i)$$

in which $v(t)$ is the weight, then integration rule will depend on the type of weight $v(t)$ as given in the following slide.

# Other Gauss quadratures

Some of Gauss quadrature rules:

| Weight $v(t)$ | Interval $(a, b)$ | Polynomial |
|---|---|---|
| $1$ | $[-1, 1]$ | Lagrange |
| $e^{-t^2}$ | $(-\infty, \infty)$ | Hermite |
| $e^{-t}$ | $(0, \infty)$ | Laguerre |
| $\sqrt{1-t^2}$ | $[-1, 1]$ | Chebishev (I kind) |