Numerical Integration

A. Donev, Spring 2021

Most integrals cannot be computed analytically using standard functions, and require introducing special functions such as the error function

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$$

How do we compute

$$J = \int_a^b f(x)\, dx$$

numerically — called numerical integration or quadrature

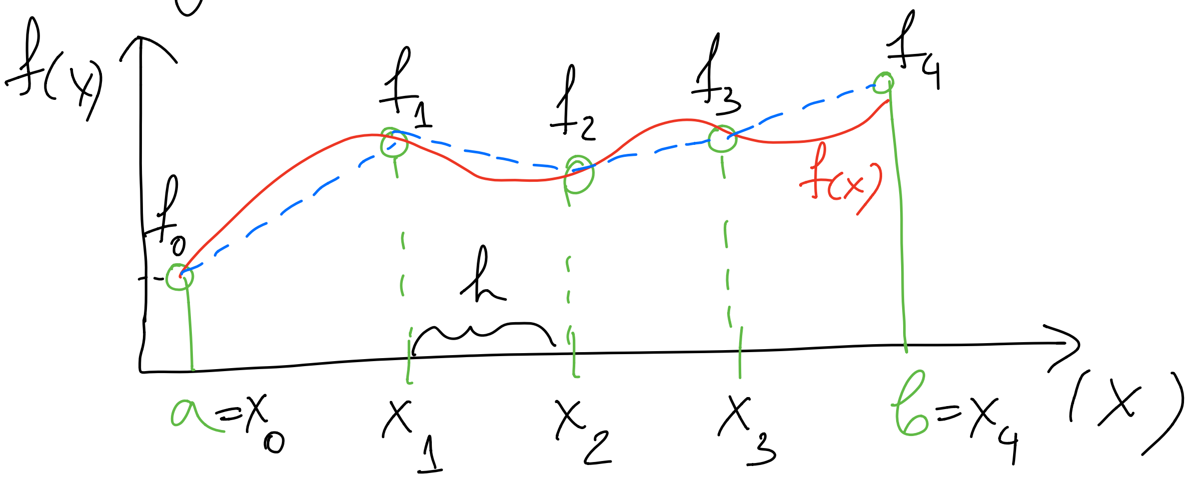
(comes from old days when gridded paper was used to count number of squares under a graph)

<u>Simple idea</u>:

Approximate function by (piecewise or global) polynomial and integrate polynomial

<u>Note</u>: Same works for numerical differentiation, as you saw in Worksheets. But, differentiation is easy so we mostly use numerical differentiation for solving differential equations (<u>not</u> covered in this course)

E.g. Piecewise linear interpolation:



$$x_k = a + k \cdot h$$

$$h = \frac{b-a}{n} = \text{grid spacing}$$

Since we approximate area under the graph of $f(x)$ by a sum of areas of trapezoids we call this the composite trapezoidal rule:

$$I \simeq h \cdot \left(\frac{f_0+f_1}{2} + \frac{f_1+f_2}{2} + \frac{f_2+f_3}{2} + \frac{f_3+f_4}{2} \right)$$

$$I \simeq h\left(\frac{f_0+f_n}{2}+\sum_{j=1}^{n-1} f_j\right)$$

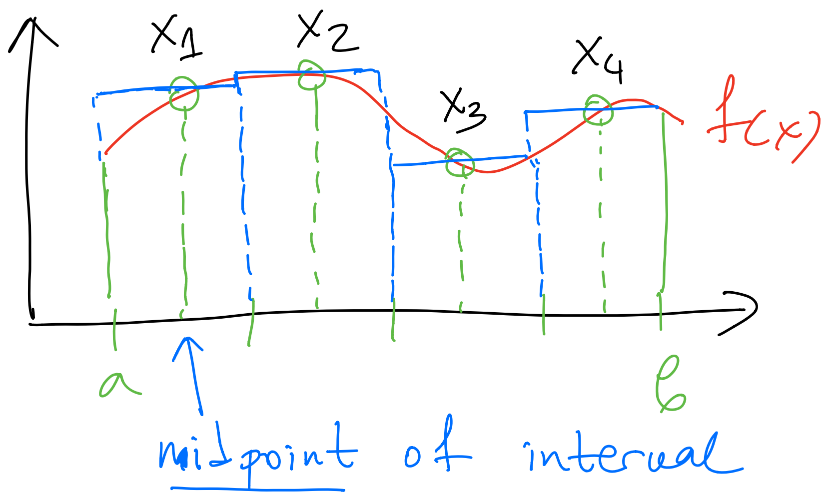
where $f_j = f(x_j)$

Usually written as

$$I=\int_a^b f(x)\,dx \simeq h\sum_{j=0}^{n} f(x_j) - \frac{h}{2}\left(f(a)+f(b)\right)$$

$\boxed{\text{Trapezoidal}}$

It is very common to see student codes that miss this endpoint correction. If you don't want a correction at the end points, use instead the midpoint quadrature rule



Here $$x_j = a + (j - 1/2)\,h \,, \; j = 1, .., n$$

$$h = \frac{b-a}{n}$$

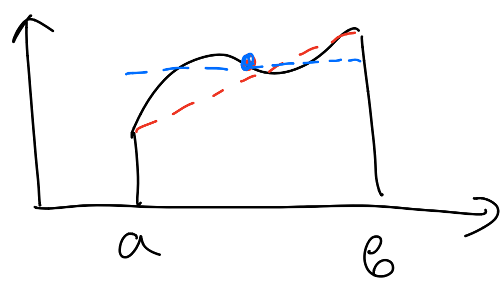
and now we approximate the area by a sum of areas of rectangles

$$I \simeq h \sum_{j=1}^{n} f(x_j) \quad \boxed{\text{midpoint}}$$

The trapezoidal & midpoint rules are equally accurate & are the most basic formulas

How accurate are these quadrature rules?

Let's consider a single interval / trapezoid / rectangle first:



For midpoint rule: Expand $f(x)$ in a Taylor series around the midpoint, with remainder term, to show that

$$\mathcal{E} = \int_{x-h/2}^{x+h/2} f(t)\,dt - h\,f(x) = \frac{h^3}{24} f''(\xi)$$

where ξ is in inside interval.

$\boxed{\text{Do on your own!}}$

For trapezoidal rule, use formula for <u>error</u> of linear interpolant $p_1(x)$:

$$f(x) - p_1(x) = \frac{1}{2} f''(\xi(x))(x-a)(x-b)$$

$$\xi(x) \in [a, b]$$

$$\Rightarrow \mathcal{E} = \left(\int_a^b f(x)\,dx\right) - \left(\int_a^b p_1(x)\,dx\right)$$

$$= \frac{1}{2} \int f''(\xi(x))(x-a)(x-b)\,dx$$

$$= \frac{f''(\eta)}{2} \int_a^b (x-a)(x-b)\,dx$$

where $\eta \in [a,b]$ according to the mean-value theorem for integrals. Do intergral to get:

$$\begin{cases} \mathcal{E}_{trap} = -\frac{h^3}{12} f''(\xi) \\ \mathcal{E}_{mid} = \frac{h^3}{24} f''(\xi) \\ \xi \in [a,b], \quad b-a=h \end{cases}$$

Note these are similar to each other.

This was only <u>one</u> rectangle.

For many rectangles, i.e., for composite trapezoidal rule, in the <u>worst case scenario</u> all errors will have the <u>same</u> sign and will add up,

$$\left| I - I_{trap.} \right| = \left| -\frac{h^3}{12} \sum_{k=1}^{n} f''(\xi_k) \right|$$

where $\xi_k \in [x_{k-1}, x_k]$

Assume $|f''(x)| < M$ for $x \in [a,b]$

$$\Rightarrow e_{trap} = |I - I_{trap}| \leq \frac{h^3}{12} \cdot n \cdot M$$

$$= \frac{h^3}{12} \cdot \frac{(b-a)}{h} \cdot M$$

$$e_{trap} \leq \frac{(b-a)}{12} \cdot M \cdot h^2$$

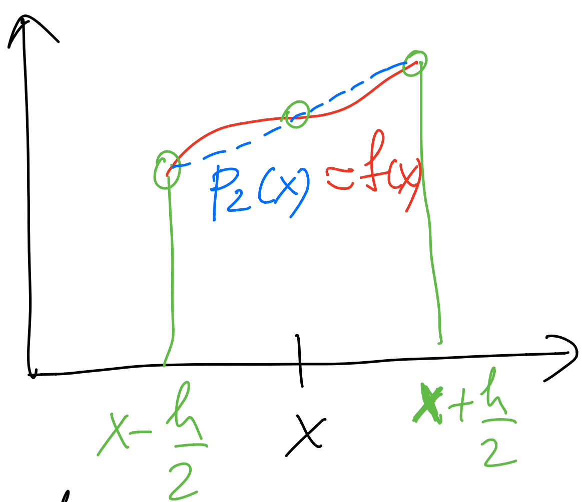
error $= O(h^2)$ for both composite trapezoidal & composite midpoint rules

Composite midpoint / trapezoidal rule is second-order accurate

This means that if you double the number of points/intervals, the error decreases by a factor of 4 !

Note that this is just an upper bound on error – a much more precise estimate is provided by the Euler-MacLaurin theorem (see Wikipedia if interested)

To get more accuracy, we can use piecewise quadratic interpolation: approximate function by a parabola over each interval. Let's take one interval only.



$$\int_{x-h/2}^{x+h/2} f(x)\,dx \approx \int_{x-h/2}^{x+h/2} P_2(x)\,dx$$

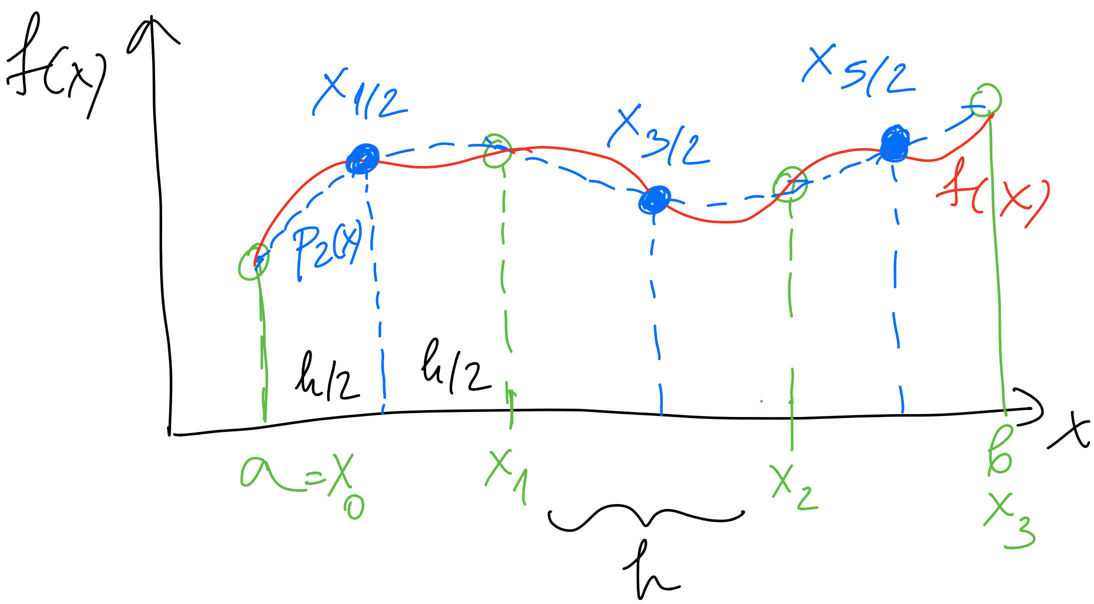
where P_2 is the quadratic interpolant.

You did this calculation in a worksheet, to get

$$\int_{x-h/2}^{x+h/2} f(x)\,dx = \frac{h}{6}\left[f(x-\tfrac{h}{2}) + 4f(x) + f(x+h/2)\right]$$

This is called Simpson's rule.

To make this a composite rule, split [a, b] into pieces (piecewise quadratic interpolation)



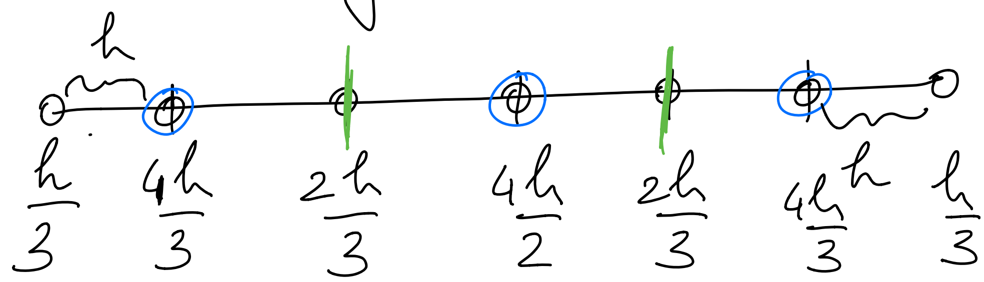
$$
\begin{aligned}
I \approx\ & \frac{h}{6}\left(f_0 + 4f_{1/2} + f_1\right) \\
& + \frac{h}{6}\left(f_1 + 4f_{3/2} + f_2\right) \\
& + \frac{h}{6}\left(f_2 + 4f_{5/2} \quad f_3\right)
\end{aligned}
$$

$$
\begin{aligned}
= \frac{h}{6}\Big[& f_0 + 4f_{1/2} + 2f_1 + 4f_{3/2} \\
& + 2f_2 + 4f_{5/2} + f_3 \Big]
\end{aligned}
$$

$$
\begin{aligned}
\int_a^b f(x)\,dx \approx\ & \frac{h}{6}\left(f(a) + f(b)\right) \\
& + \frac{h}{3}\sum_{k=1}^{n-1} f(x_k) \\
& + \frac{2h}{3}\sum_{k=0}^{n-1} f(x_{k+1/2})
\end{aligned}
$$

$\boxed{\text{Simpson quadrature}}$

Another way to write it



Give first and last point weight $h/3$, even points weight $4h/3$, and odd ones $2h/3$ (compare to midpoint which gave all points weight h, and trapezoidal which gave first and last point weight $h/2$ and all others weight h).

Simpson's rule is only slightly more complicated but 4th order accurate so use it!

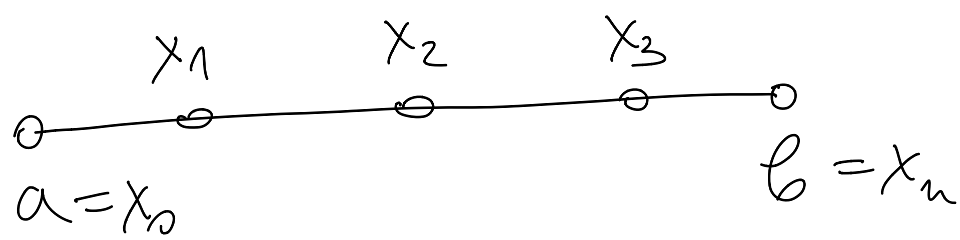
$$\mathcal{E}_{simp} = \left| \mathcal{I} - \mathcal{I}_{simp} \right| = \frac{b-a}{2880} h^4 M$$

$$M = \max_{a \le x \le b} \left| f^{(4)}(x) \right|$$

Double number of points, 16 times smaller error!

We can get even better accuracy by using higher-degree polynomial approximants.

Let's focus on only one interval, but of course one can always split $[a, b]$ into pieces for composite quadrature



Choose interpolation nodes in $[a, b]$ (not necessarily equi-spaced!) and use Lagrange interpolation

$$f(x) \approx p_n(x) = \sum_{j=0}^{n} f(x_j) L_j(x)$$

Lagrange polynomial

$$\Rightarrow \int_a^b f(x)\,dx \approx \int_a^b p_n(x)\,dx$$

$$= \int_a^b f_j L_j(x)\,dx$$

$$\int_a^b f(x)\,dx \simeq \sum_{j=0}^{n} \underbrace{\left(\int_a^b L_j(x)\,dx\right)}_{w_j} f_j$$

$$J = \int_a^b f(x)\,dx \simeq \sum_{j=0}^{n} w_j\, f(x_j)$$

quadrature weights

quadrature nodes

$$(*) \ldots \quad w_j = \int_a^b L_j(x)\,dx$$

All quadrature rules have this form, but different weights & nodes. Note that once we choose the nodes we can <u>pre-compute the weights $\vec{w}$</u>

(see Newton-Cotes quadrature on Wiki for tables)

The midpoint, trapezoidal & Simpson's rule were just special cases for $n=0$, $n=1$ and $n=2$. For these small n it is <u>obvious</u> where to place the nodes by symmetry, if we want to include the endpoints.

But what is the <u>best</u> choice of nodes & weights?

Note that once we choose the nodes, the weights are given by (*), so really the question is what are the "best" nodes?

Let us first clarify about what we mean by "best":

We want the most accurate integral for a generic smooth function for a given number of nodes.

And "most accurate" we define (but this choice is not unique or necessarily "optimal") to be the highest order of accuracy:

$$\text{error} = O\left(\frac{1}{n^p}\right)$$

where p is as large as possible for a given number of nodes n

Now let's observe the following:

A method that is p^{th} order accurate is exact for polynomials of degree at least up to $p-1$

This is a pretty useful way to check (validate) & derive formulas quickly and intuitively.

For example, we can derive Simpson's rule (quadratic interpolation, so exact for quadratic polynomials) which has $p = 2+1 = 3$

[note that Simpson's rule actually has error $\sim 1/n^4$ but this is "luck" and is why we need "at least" in red above]

$$\int_a^b p(x)\,dx = w_1 p(a) + w_2\, p\left(\frac{a+b}{2}\right) + w_3\, p(b) \leftarrow \underline{\text{unknown}}\ w_1, w_2, w_3$$

for $p(x) \in \mathcal{P}_2$

This is <u>equivalent</u> [make sure you understand why, i.e., can prove both directions of equivalence] to saying equation above is true for every element of a basis of $\mathcal{P}_2$.

If we choose the monomials as a basis

$$p_1 = 1, \quad p_2 = x, \quad p_3 = x^2$$

we get 3 linear equations:

$$\int_a^b 1\,dx = w_1 + w_2 + w_3 = b - a$$

$$\int_a^b x\,dx = w_1 a + w_2 \frac{a+b}{2} + w_3 b = \frac{b^2 - a^2}{2}$$

$$\int_a^b x^2\,dx = w_1 a^2 + w_2 \left(\frac{a+b}{2}\right)^2 + w_3 b^2$$
$$= \frac{b^3 - a^3}{3}$$

Solve to get <u>Simpson's rule</u>

$$w_1 = w_3 = \frac{b-a}{6}, \quad w_2 = \frac{4(b-a)}{6}$$

<u>Note</u>:
In general, you can check if some formula you derived using polynomial interpolation of degree p is correct by testing it on the monomials $\{1, x, \dots, x^p\}$

Now, observe that the formula

$$(*) \ldots \quad w_j = \int_a^b L_j(x)\,dx$$

ensures that the quadrature rule is exact for all of the Lagrange polynomials up to degree $n-1$ if we have n points [note switch in notation – n points not $n+1$ points like for interpolation]

Therefore the quadrature rule is exact for all polynomials of degree up to $n_{\text{points}} - 1$ regardless of the choice of nodes.

But we can also choose the n nodes/points at will, so we have n additional degrees of freedom. Therefore we can hope that we can make the quadrature rule exact for polynomials of degree up to

$$(n-1) + n = 2n-1$$

How can we find the nodes?
Just plug all monomials of degree up to $2n-1$ into quadrature to get a nonlinear system of $2n$ equations for the $2n$ unknowns $\vec{w}$ and $\vec{x}$.
See homework for $n=3$!

It turns out, however, that one can find a solution of this system of equations <u>analytically</u> by using orthogonal polynomials.

<u>Theorem</u>: If $x_1, \dots, x_n$ are the zeros / roots of the Legendre polynomial of degree n, then the Gaussian quadrature rule

$$\int_a^b f(x)\,dx \simeq \sum_{j=1}^{n} w_j f(x_j)$$

with w_j given by (*) is exact for polynomials of degree $2n-1$ or less.

Nodes $\vec{x}$ are called Gaussian nodes and are in $[-1,1]$

as we mentioned at the end of the lecture on orthogonal polynomials. So these special points/nodes are good not only for interpolation but also for quadrature.

You can find tables of values or explicit formulas for the Gaussian nodes & weights for $n \leq 5$ on Wikipedia, and a code on the webpage for computing them numerically for any (modest) n.

This concludes our search for the "best" quadrature rule on $[-1,1]$ – easy to change to $[a,b]$

Proof of theorem:

Let $p \in \mathcal{P}_{2n-1}$ and denote the Legendre polynomials with $\{P_0, P_1, P_2, \dots, P_n\}$

$$p = q\, P_n + r$$

where $q(x) \in \mathcal{P}_{n-1}$

$$P_n(x) \in \mathcal{P}_n$$

$$r(x) \in \mathcal{P}_{n-1}$$

residual of "polynomial long division

Since x_j is a root of P_j,

$$p(x_j) = q(x_j)\, \underbrace{\cancel{P_n}(x_j)}_{0} + r(x_j) = r(x_j)$$

$$\int_{-1}^{1} p(x)\,dx = \int_{-1}^{1} q(x)\,P_n(x)\,dx$$

$$+ \int_{-1}^{1} r(x)\,dx$$

Now, since $P_n(x)$ was constructed (using Gram-Schmidt) to be orthogonal to all $q(x) \in \mathcal{P}_{n-1}$,

$$(q, P_n) = \int q(x)\,P_n(x)\,dx = 0$$

$$\Rightarrow \int p(x)\,dx = \int r(x)\,dx =$$

$$\left(\begin{array}{l}\text{since } r \in \mathcal{P}_{n-1} \\ \text{and } (*)\end{array}\right) = \sum w_j\, r(x_j)$$

$$= \sum w_j\, f(x_j)$$

which is Gaussian quadrature.