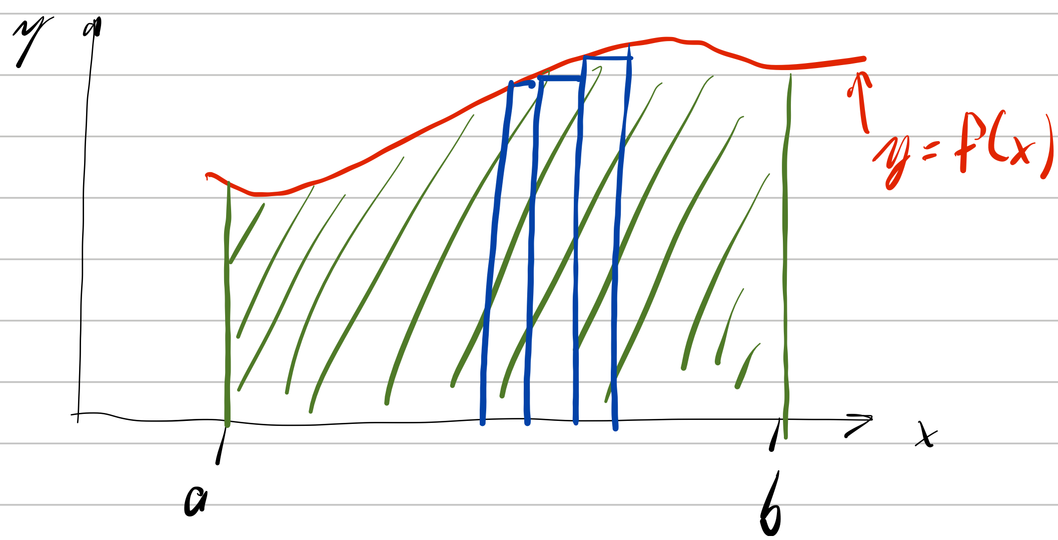
Numerical Integration (Quadrature)

We are probably all familiar with the idea of the definite integral

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

as the area under the curve $y = f(x)$ for x between $x=a$, $x=b$.



In the language of mathematics, the area (or I) is defined by a Riemann sum

$$I = \lim_{\substack{N \to \infty \\ \Delta x \to 0}} \sum_{i=1}^{N} f(x_i)\,\Delta x$$

if the limit exists, then its value is I.

Say now we want to approximate I numerically, the basic idea is to truncate the infinite sum, replace with a finite sum which leads to some error.

$$I = \underbrace{\sum_{i=1}^{N} a_i f(x_i)}_{\text{numerical quadrature.}} + R$$

remainder or error

One common approach to finding quadrature rules is to fit a polynomial interpolant through data and then integrate this.

Let $P(x)$ be the unique $(n-1)$ degree poly that fits the data $(x_i, f(x_i))$ $i=1,2,\dots,n$

Using a Lagrange basis

$$P(x) = \sum_{i=1}^{n} f(x_i) L_i(x)$$

$$L_i(x) = \prod_{\substack{j=1 \\ j \neq i}}^{n} \frac{(x - x_j)}{(x_i - x_j)}$$

now use $P(x)$ in place of $f(x)$ to get

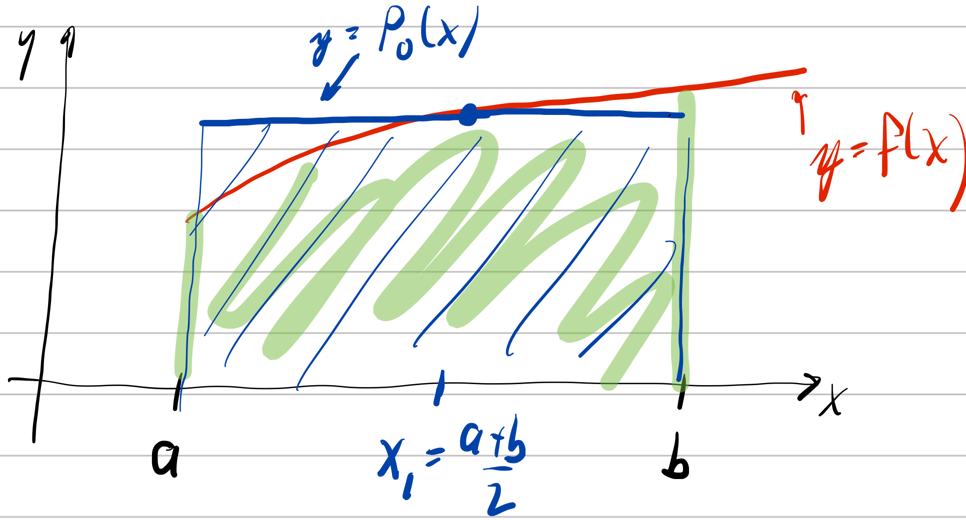
$$\int_a^b f(x)\,dx \approx \int_a^b P(x)\,dx$$

$$\int_a^b f(x)\,dx \approx \int_a^b \sum_{i=1}^{n} f(x_i) L_i(x)\,dx$$

$$\int_a^b f(x)\,dx \approx \sum_{i=1}^{n} f(x_i) \underbrace{\int_a^b L_i(x)\,dx}_{a_i}$$

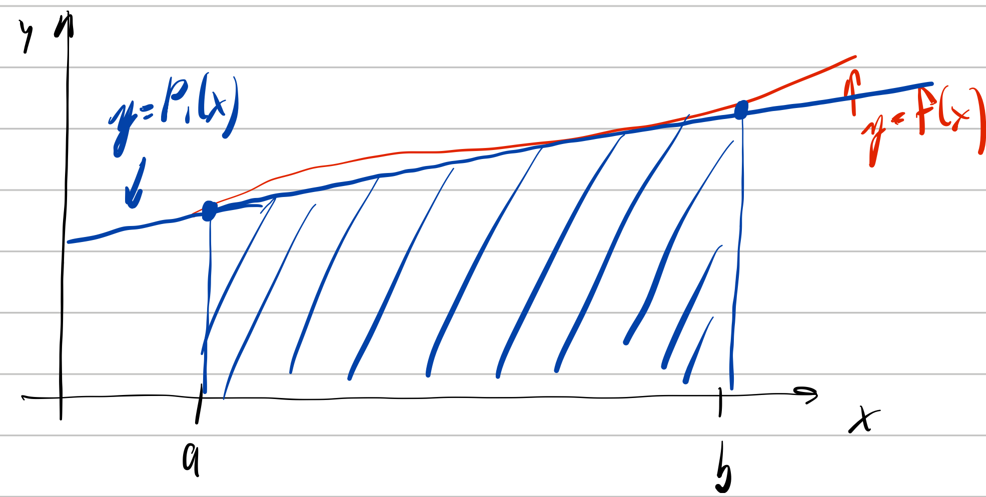
For example

1) constant interpolation



$$I \approx (b-a) f\left(\frac{a+b}{2}\right)$$ "midpt rule"

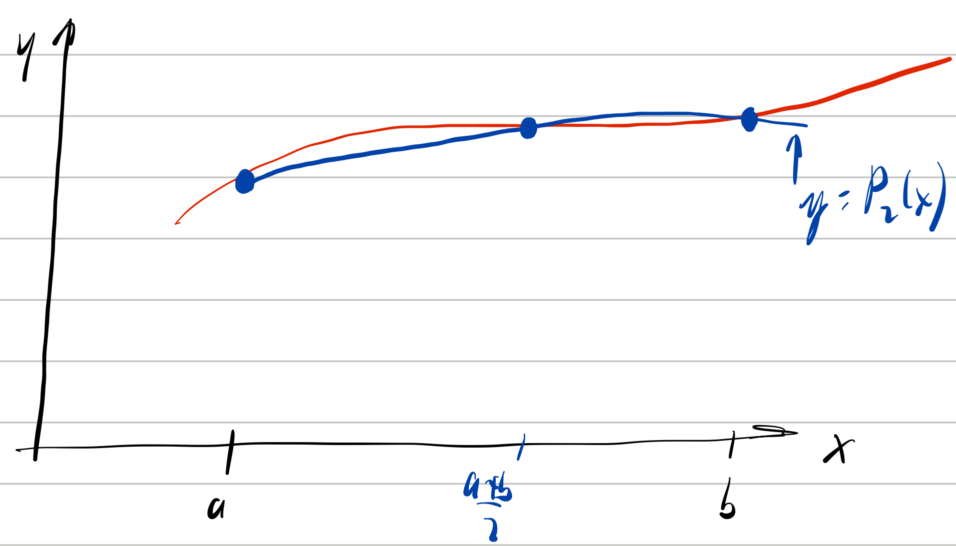
2) Linear interp



$$I \approx (b-a)\,\frac{f(a)+f(b)}{2}$$

"trapezoidal rule"

3)



$$I \approx \frac{(b-a)}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]$$

"Simpsons Rule"

Ex consider

$$I = \int_0^1 \sqrt{x}\, dx = \frac{x^{3/2}}{3/2}\Big|_0^1 = \frac{2}{3} x^{3/2}\Big|_0^1 = \frac{2}{3}$$

error

1) midpt: $I \simeq (1-0)\sqrt{\tfrac{1}{2}} = .7071\ldots$ .0404...

2) trap: $I \simeq \frac{(1-0)(\sqrt{1}+\sqrt{0})}{2} = \frac{1}{2}$ .166...

3) Simpson: $I \simeq \frac{1-0}{6}\left(\sqrt{0} + 4\sqrt{\tfrac{1}{2}} + \sqrt{1}\right) = .63807\ldots$

.0286...

Remark: Quadratures built on polynomial interpolation on equally spaced nodes are called Newton-Cotes formulas.

Quadrature Error

we want to understand the error in an approximate quadrature for a given function

As an example, consider the midpt rule

$$\int_a^b f(x)\,dx = (b-a) f\left(\tfrac{a+b}{2}\right) + R(f)$$

to discuss R, lets introduce the notion of polynomial precision. Recall that these quadratures are built on polynomial interpolation. If the interpolation is exact, the quadrature would be exact. The interpolant is exact if $f(x)$ is a low-degree polynomial i.e. degree $n-1$ or less.

e.g. $f(x) = 1$ (zeroth order poly)

$$\int_a^b 1\,dx = b-a = (b-a)f\left(\frac{a+b}{2}\right) + R(f)$$

$$= (b-a)\cdot 1 + \underbrace{R(f)}_{=0}$$

$\Rightarrow$ the error is zero for $f(x) = 1$

e.g. $f(x) = x$

$$\int_a^b x\,dx = \frac{b^2}{2} - \frac{a^2}{2} = (b-a)f\left(\frac{a+b}{2}\right) + R(f)$$

$$= (b-a)\left(\frac{a+b}{2}\right) + R(f)$$

$$= \frac{b^2-a^2}{2} + \underbrace{R(f)}_{=0}$$

$\Rightarrow$ the error is zero for $f(x) = x$!

e.g. $f(x) = x^2$

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

$$= \frac{1}{4}(b^2 - a^2)(a+b) + R(f)$$

$$= \frac{1}{4}\left[b^3 + ab^2 - a^2 b - a^3\right] + R(f)$$

$$= \frac{1}{3}(b^3 - a^3) - \frac{1}{12}(b^3 - 3ab^2 + 3a^2 b - a^3) + R(f)$$

$$= \frac{1}{3}(b^3 - a^3) - \frac{1}{12}(b-a)^3 + R(f)$$

$$\Rightarrow R(f) = \frac{1}{12}(b-a)^3$$

$\Rightarrow$ midpt was exact for polynomials of degree 0, or 1.

$\Rightarrow$ precision of midpt = 1

one can also show that

precision of trap = 1

precision of simpson = 3

the precision tells us which polynomials are exact for a given quadrature but it also tells us the precise form of the error!

If a quadrature has precision p $\Rightarrow$

$$\int_a^b f(x)\,dx = \sum_{i=1}^{n} a_i f(x_i) + c\,(b-a)^{p+2} f^{(p+1)}(u)$$

const $\qquad\qquad$ $u \in [a,b]$

e.g. midpt rule, $p = 1$

$$\int_a^b f(x)\,dx = (b-a) f\left(\frac{a+b}{2}\right) + c\,(b-a)^3 f''(u)$$

to compute c, let $f(x) = x^2$

$$\int_a^b f(x)\,dx = (b-a)\left(\frac{a+b}{2}\right)^2 + \frac{1}{12}(b-a)^3$$

$$c\cancel{(b-a)^3} f''(u) = \frac{1}{12}\cancel{(b-a)^3}$$

$$c \cdot 2 = \frac{1}{12}$$

$$c = \frac{1}{24}$$

$$\Rightarrow \int_a^b f(x)\,dx = (b-a) f\left(\frac{a+b}{2}\right) + \frac{1}{24}(b-a)^3 f''(u)$$

$u \in [a,b]$

for the other 2 quadratures we discussed.

trap: $\int_a^b f(x)dx = (b-a)\frac{f(b)+f(a)}{2} - \frac{(b-a)^3}{12} f''(u)$

simpson:

$$\int_a^b f(x)dx = \frac{b-a}{6}\left[f(a)+4f\left(\frac{a+b}{2}\right)+f(b)\right] - \frac{(b-a)^5}{90\cdot 2^5} f''''(u)$$

Remarks:

1) midpt, trap, & simpsons rule are just 3 of many Newton-Cotes formulas.

2) if n is odd

$$\int_a^b f(x)dx = \sum_{i=1}^{n} a_i f(x_i) + c(b-a)^{n+2} f^{(n+1)}(u)$$

if n is even

$$\int_a^b f(x)dx = \sum_{i=1}^{n} a_i f(x_i) + c(b-a)^{n+1} f^{(n)}(u)$$

Last time we discussed Qudrature

- midpt, trap, Simpson,
- Newton Cotes (and error)

Gaussian Quadrature

Consider the general quadrature

$$\int_a^b f(x)dx = \sum_{i=1}^{n} a_i f(x_i) + E(f)$$

with Newton-Cotes we used a uniform partition of $x \in [a,b]$. The weights were then found to maximize precision. There are n degrees of freedom $a_1, a_2, \dots, a_n$. The basic idea of Gaussian Quadrature is to let $x_1, x_2, \dots, x_n$ vary as well. This gives

2n degrees of freedom

e.g. consider 2-pt formula

$$\int_a^b f(x)\,dx = c_1 f(x_1) + c_2 f(x_2) + E(f)$$

to make algebra simpler take $[a,b] = [-1,1]$

then use (Linear) change of variables to

map to arbitrary interval.

$$\int_{-1}^{1} f(x)\,dx = c_1 f(x_1) + c_2 f(x_2) + E(f)$$

there are 4 degrees of freedom that can

be used to force $E(f)=0$ for $f = 1, x, x^2, x^3$

$f(x)=1: \Rightarrow \int_{-1}^{1} 1\,dx = 2 = c_1 + c_2$ (1)

$f(x)=x: \Rightarrow \int_{-1}^{1} x\,dx = 0 = c_1 x_1 + c_2 x_2$ (2)

$f(x) = x^2 \Rightarrow \int_{-1}^{1} x^2\,dx = \frac{2}{3} = c_1 x_1^2 + c_2 x_2^2$ (3)

$f(x) = x^3 \Rightarrow \int_{-1}^{1} x^3\,dx = 0 = c_1 x_1^3 + c_2 x_2^3$ (4)

This is 4 nonlinear eqns in 4 unknowns

notice that (2) & (4) are satisfied if

$$c_1 = c_2 \quad \& \quad x_1 = -x_2$$

then (1) tells us $c_1 = c_2 = 1$

and (3) $\frac{2}{3} = x_1^2 + x_1^2 = 2x_1^2$

$$x_1 = \sqrt{1/3} \qquad x_2 = -\sqrt{1/3}$$

$$\Rightarrow \int_{-1}^{1} f(x)\,dx = \underbrace{f\left(-\tfrac{1}{\sqrt{3}}\right) + f\left(\tfrac{1}{\sqrt{3}}\right)}_{\text{exact for polys of degree 3 or less}} + E(f)$$

the 2-point Gaussian quadrature has precision $p = 3$, compared to 2-pt Newton Cotes (trap) with precision $p = 1$.

Ex. Approximate the integral

$$I = \int_1^{3/2} e^{-x^2}\,dx$$

using 2-pt Gauss quadrature.

we first need to get to interval $[-1, 1]$

this is basically scaling & translating.

Let $\xi(x) = \alpha x + \beta$

now require $\begin{cases} \xi(1) = -1 \\ \xi(3/2) = 1 \end{cases}$

$$\left.\begin{aligned} \alpha + \beta &= -1 \\ \tfrac{3}{2}\alpha + \beta &= 1 \end{aligned}\right\} \alpha = 4,\ \beta = -5$$

$\Rightarrow \xi = 4x - 5$ $\qquad x = \frac{1}{4}(\xi + 5) \Rightarrow dx = \frac{1}{4}d\xi$

$$I = \int_{x=1}^{x=3/2} e^{-x^2}\,dx$$

$$= \int_{\xi=-1}^{\xi=1} \underbrace{e^{-\left(\frac{1}{4}(\xi+5)\right)^2}\frac{1}{4}}_{g(\xi)}\,d\xi$$

this is now the fcn to integrate

Recall $I = \int_{-1}^{1} g(\xi)\,d\xi \approx g\left(-\frac{1}{\sqrt{3}}\right) + g\left(\frac{1}{\sqrt{3}}\right)$

$$I \approx \frac{1}{4} e^{-\left(\frac{1}{4}\left(-\frac{1}{\sqrt{3}}+5\right)\right)^2} + \frac{1}{4} e^{-\left(\frac{1}{4}\left(\frac{1}{\sqrt{3}}+5\right)\right)^2}$$

$$I \approx 0.10940026\ldots$$

Compare this to

1) trap $\quad I \approx \frac{3/2-1}{2}\left[e^{-(1)^2} + e^{-(3/2)^2}\right] = .11831967\ldots$

2) Simpson $\quad I \approx \frac{(3/2-1)}{6}\left[e^{-(1)^2} + 4e^{-(5/4)^2} + e^{-(3/2)^2}\right]$

$$= .10931035\ldots$$

for reference $\quad I = .1093643\ldots$

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to implement change of coords

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

$$\xi(x) = \alpha x + \beta \qquad \begin{cases} \xi(a) = -1 \\ \xi(b) = 1 \end{cases}$$

$$x = \frac{1}{\alpha}(\xi - \beta)$$
$$dx = \frac{1}{\alpha}\,d\xi$$

$$\left.\begin{aligned} \alpha a + \beta &= -1 \\ \alpha b + \beta &= 1 \end{aligned}\right\} \begin{aligned} \alpha &= \ldots \\ \beta &= \ldots \end{aligned}$$

$$I = \int_{x=a}^{x=b} f(x)\,dx$$

$$= \int_{\xi=-1}^{\xi=1} f(x(\xi))\,\frac{1}{\alpha}\,d\xi$$

Gaussian Quadratures of higher order can be derived as discussed ... but its complicated. But there is a graceful approach using orthogonal polynomials. Here we use Legendre polys

$P_n(x)$ is a degree n poly with the property

$$\int_{-1}^{1} P_n(x)\, P_m(x)\, dx = 0 \quad \text{if } n \neq m$$

this property implies

$$\int_{-1}^{1} f(x)\, P_n(x)\, dx = 0$$

for any $f(x)$ a poly of degree $n-1$ or less.

$$P_0(x) = 1$$

$$P_1(x) = x$$

$$P_2(x) = x^2 - 1/3$$

$$P_3(x) = x^3 - 3/5\, x$$

$$\vdots$$

these properties can be used to obtain

The n-pt Gaussian quadrature formula

$$\int_{-1}^{1} f(x)dx = \sum_{i=1}^{n} c_i f(x_i) + E(f)$$

is exact for polys of degree $2n-1$ or less

and the nodes x_i, $i=1,2,\dots,n$ are the

roots of the $P_n(x)$ and the weights by

$$c_i = \int_{-1}^{1} \prod_{\substack{j=1 \\ j\neq i}}^{n} \frac{(x-x_j)}{(x_i-x_j)}\,dx$$

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the proof outline is fairly straight forward.

Let $f(x)$ be a poly of degree $2n-1$ or less

This can be written

$$f(x) = Q(x)\,P_n(x) + R(x)$$ (see later)

Q & R are polys of degree $n-1$ or less

$$\int_{-1}^{1} f(x)\,dx = \underbrace{\cancel{\int_{-1}^{1} Q(x)P_n(x)\,dx}}_{=0} + \int_{-1}^{1} R(x)\,dx$$

Now let

$$R(x) = \sum_{i=1}^{n} R(x_i)\, L_i(x)$$

Lagrange basis

this is a unique poly

$$\Rightarrow \int_{-1}^{1} f(x)\,dx = \int_{-1}^{1} R(x)\,dx$$

$$= \int_{-1}^{1} \sum_{i=1}^{n} R(x_i) L_i(x)\,dx$$

$$= \sum_{i=1}^{n} R(x_i) \underbrace{\left[\int_{-1}^{1} L_i(x)\,dx\right]}_{= c_i}$$

but $R(x_i) = f(x_i) = Q(x_i)\overset{0}{\cancel{P_n(x_i)}} + R(x_i)$

so why can we do

$$f(x) = \underset{\text{degree } n-1}{Q(x)}\ \underset{n\text{th legendre poly}}{P_n(x)} + \overset{\text{degree } n-1}{R(x)}$$

$$Q(x) = q_{n-1}x^{n-1} + q_{n-2}x^{n-2} + \dots + q_1 x + q_0$$

$$P_n(x) = p_n x^n + p_{n-1}x^{n-1} + \dots \quad p_1 x + p_0$$

$$\Rightarrow P_n(x)Q(x) = p_n q_{n-1} x^{2n-1}$$

$$+ (p_n q_{n-2} + p_{n-1} q_{n-1}) x^{2n-2}$$

$$+ \dots + \left(\sum_{j=0}^{n-1} p_{n-j} q_j\right) x^n \ \underline{+ d_{n-1}x^{n-1} + \dots + d_1 x + d_0}$$

$$f(x) = f_{2n-1} x^{2n-1} + f_{2n-2} x^{2n-2} + \dots f_1 x^1 + f_0$$

set $p_n q_{n-1} = f_{2n-1}$

$p_n q_{n-2} + p_{n-1} q_{n-1} = f_{2n-2}$

$\vdots$

$$\sum_{j=0}^{n-1} p_{n-j} q_j = f_n$$

$$f(x) - Q(x) P_n(x) = \underbrace{\alpha_{n-1} x^{n-1} + \alpha_{n-2} x^{n-2} + \dots + \alpha_1 x + \alpha_0}_{\text{degree } n-1}$$

---

the values for x_i, c_i can be computed or looked up.

e.g. $n=3$

$x_1 = -\sqrt{3/5} = -.7746\dots$ $\quad c_1 = 5/9$

$x_2 = 0$ $\quad c_2 = 8/9$

$x_3 = -x_1$ $\quad c_3 = 5/9$

$n=4$

$x_1 = -.8611\dots$ $\quad c_1 = .3479\dots$

$x_2 = -.3400\dots$ $\quad c_2 = .6521\dots$

$x_3 = -x_2$ $\quad c_3 = c_2$

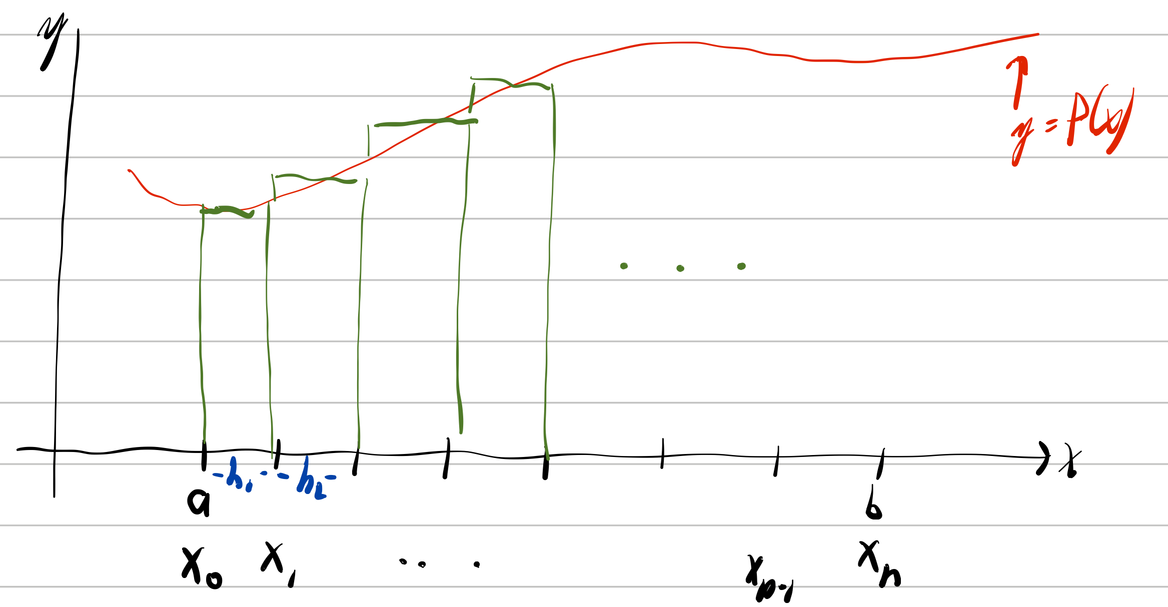
$x_4 = -x_1$ $\quad c_4 = c_1$

Composite Quadrature Formulas

consider the midpt formula

$$\int_a^b f(x)\,dx = (b-a)f\left(\frac{a+b}{2}\right) + \frac{(b-a)^3}{24} f''(u) \qquad u\in[a,b]$$

If $(b-a)$ is large, and we require small error, we might try to find a high-order quadrature. Alternately we could decompose $[a,b]$ into subintervals and then use midpt on each. Lets use midpt to illustrate



$$\int_a^b f(x)\,dx = \sum_{i=1}^{n} \int_{x_{i-1}}^{x_i} f(x)\,dx$$

now use midpt on each of these

$$\int_a^b f(x)\,dx = \sum_{i=1}^{n} h_i f(\bar{x}_i) + \sum_{i=1}^{n} \frac{h_i^3}{24} f''(u_i)$$

$h_i = x_i - x_{i-1}$ $\qquad \bar{x}_i = \frac{x_i + x_{i-1}}{2}$ $\qquad u_i \in [x_{i-1}, x_i]$

now assume a uniform grid ... $h_i = h$

$$\int_a^b f(x)\,dx = h \sum_{i=1}^{n} f(\bar{x}_i) + \frac{h^3}{24} \underbrace{\sum_{i=1}^{n} f''(u_i)}_{= n f''(u)} \qquad u \in [a,b]$$

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

$$\frac{h^2}{24} h n f''(u)$$

$\Rightarrow nh = b-a$

$$\int_a^b f(x)\,dx = h \sum_{i=1}^{n} f(\bar{x}_i) + \frac{(b-a)}{24} h^2 f''(u) \qquad u \in [a,b]$$

This is the composite midpt rule

Similarly for trap

$$\int_a^b f(x)\,dx = \frac{h}{2} \sum_{i=1}^{n} [f(x_{i-1}) + f(x_i)] - \frac{(b-a)}{12} h^2 f''(u)$$

$$= \frac{h}{2}\left[f(a) + f(b) + 2\sum_{i=1}^{n-1} f(x_i)\right] - \frac{(b-a)}{12} h^2 f''(u)$$

for Simpson

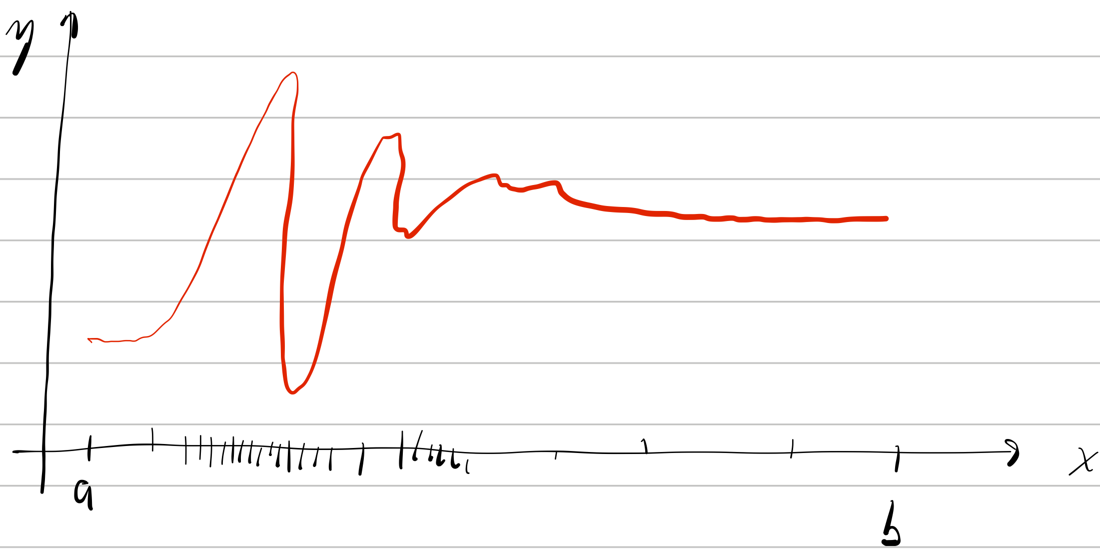
$$\int_a^b f(x)\,dx = \frac{h}{6}\sum_{i=1}^{n}\left[f(x_{i-1})+4f(\bar{x}_i)+f(x_i)\right] + \frac{(b-a)}{180}h^4 f''''(\eta)$$

$$= \frac{h}{6}\left[f(a)+f(b)+2\sum_{i=1}^{n-1}f(x_i)+4\sum_{i=1}^{n}f(\bar{x}_i)\right] + \frac{b-a}{180}h^4 f''''(\eta)$$

The basic idea is that we can controll the accuracy by using more or less intervals ...

Error estimation & adaptive quadrature

What types of situations might it be advantageous to take a non-uniform partition



To see how this might be done automatically lets use trapezoidal rule and define

$$T(a,b) = \frac{b-a}{2}[f(a)+f(b)]$$

we know for a single interval

$$\int_a^b f(x)\,dx = T(a,b) + c_1 h^2 \qquad c_1 = -\frac{(b-a)}{12} f''(u_1)$$

$$h = b-a$$

now with 2 intervals

$$\int_a^b f(x)\,dx = T\left(a, \frac{a+b}{2}\right) + T\left(\frac{a+b}{2}, b\right) + c_2\left(\frac{h}{2}\right)^2$$

$$c_2 = -\frac{(b-a)}{12} f''(u_2)$$

Note that $c_1 \approx c_2$ so assume they are the same and then find a way to estimate it

$$\int_a^b f(x)\,dx \approx T(a,b) + c h^2$$

$$\int_a^b f(x)\,dx \approx T\left(a, \frac{a+b}{2}\right) + T\left(\frac{a+b}{2}, b\right) + c\left(\frac{h}{2}\right)^2$$

Subtracting gives

$$0 \approx T(a,b) - T\left(a, \frac{a+b}{2}\right) - T\left(\frac{a+b}{2}, b\right) + \frac{3}{4} c h^2$$

$$\Rightarrow \left|\frac{ch^2}{4}\right| \approx \left|\frac{1}{3}\left[T\left(a,\tfrac{a+b}{2}\right) + T\left(\tfrac{a+b}{2}, b\right) - T(a,b)\right]\right|$$

$\Uparrow$

approximate error in 2-interval composite trap quadrature.

The idea is to pick a tolerance tol

Then if $\left|\frac{1}{3}\left[T\left(a,\tfrac{a+b}{2}\right) + T\left(\tfrac{a+b}{2}, b\right) - T(a,b)\right]\right| \leq tol$

$\Rightarrow$ done. If it doesn't then refine

The basic mechanics might look like.