Numerical Integration

A. Donev, Spring 2021

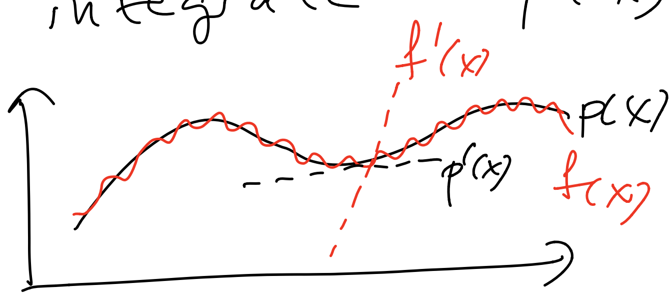
$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2}\, dt$$

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

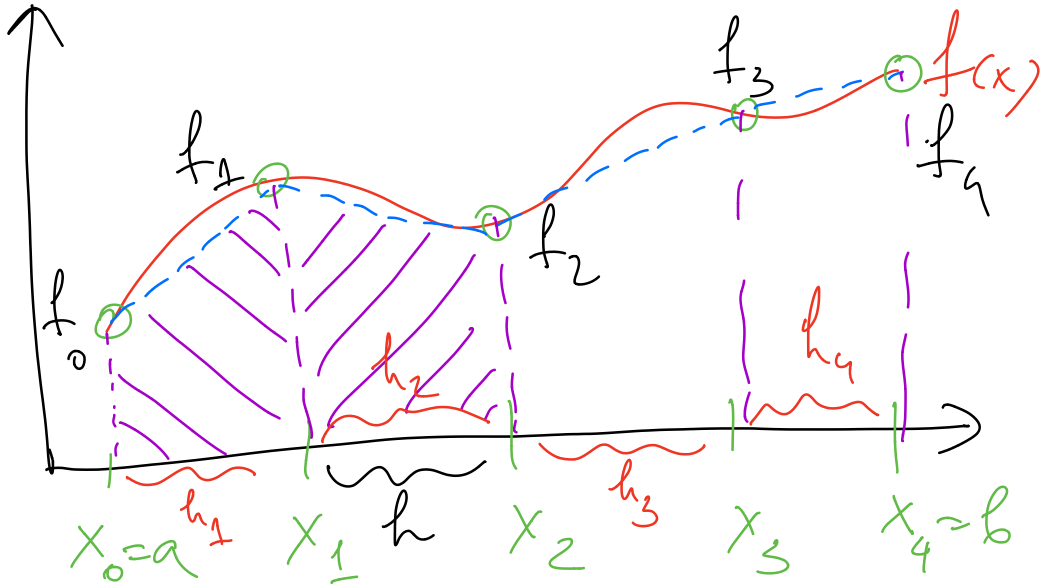
quadrature

Idea:

Approximate $f(x)$ by $p(x)$, and integrate $p(x)$ instead



E.g. Piecewise linear interp.



$$\begin{cases} x_k = a + k \cdot h, & k = 0, \dots, n \\ h = \dfrac{b-a}{n}, & f_k = f(x_k) \end{cases}$$

Area under $f \simeq$ sum of areas of four trapezoids

$$I \simeq \cancel{h} \cdot \left(\frac{f_0 + f_1}{2} h_1 + \frac{f_1 + f_2}{2} h_2 + \frac{f_2 + f_3}{2} h_3 + \frac{f_3 + f_4}{2} h_4 \right)$$

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

$$I = \int_a^b f(x)\,dx \approx h \cdot \sum_{j=0}^{n} f(x_j)$$

Don't forget this

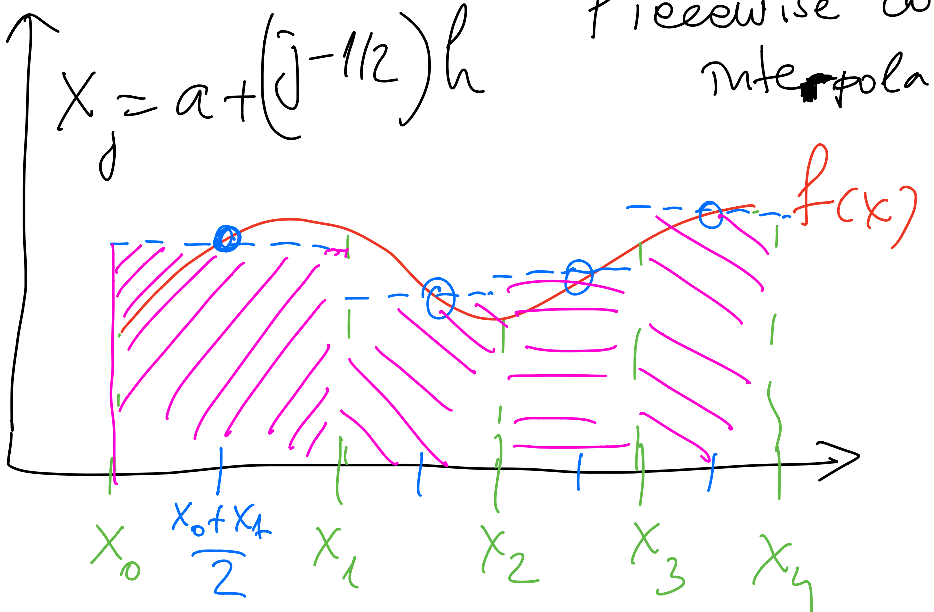
$$\boxed{-\frac{h}{2}\,\frac{f(x_0)+f(x_n)}{2}}$$

Composite trapezoidal rule

Composite midpoint rule

Piecewise constant interpolation

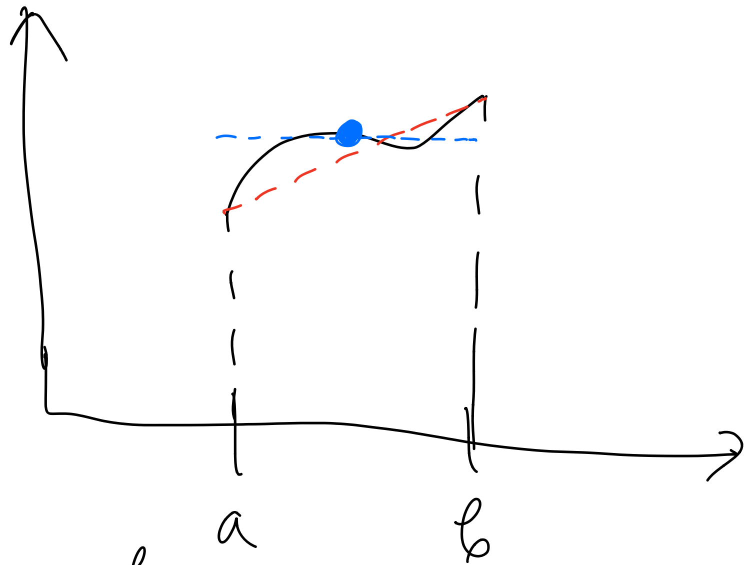
$$x_j = a + \left(j - 1/2\right) h$$



$$\int_a^b f(x)\,dx = \int_a^{x_1} f\,dx + \int_{x_1}^{x_2} f\,dx + \int_{x_2}^{x_3} f\,dx + \int_{x_3}^{x_4} f\,dx$$

$$I = h \sum_{j=1}^{n} f(x_j)$$

Composite midpoint rule



error? $\displaystyle\int_a^b f(x)\,dx \simeq \frac{f(a)+f(b)}{2}\cdot(b-a)$

#1 Taylor series

For midpoint $\qquad x_{mid} = \dfrac{a+b}{2}$

$$f(x) \simeq f(x_{mid}) + f'(x_{mid})(x - x_{mid}) + \frac{1}{2} f''(\xi(x))(x - x_{mid})^2$$

ξ between x and x_{mid}

Do this at home

$$\mathcal{E} = \int_{x-h/2}^{x+h/2} f(t)\,dt - \underbrace{f(x)\cdot h}_{\text{midpoint}}$$

$$= \frac{h^3}{24} f''(\xi)$$

$$\xi \in \left[x-\frac{h}{2},\ x+\frac{h}{2}\right)$$

#2 Use formula for error of polynomial interpolant for trapezoidal rule

$$\mathcal{E}_1(x) = f(x) - P_1(x) = \frac{1}{2} f''(\xi(x))(x-a)(x-b)$$

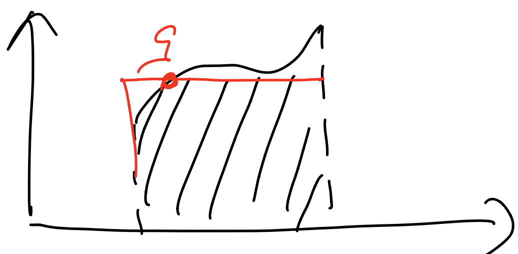
linear interpolant $\quad \xi(x) \in [a,b]$

$$\mathcal{E} = \int f(x)\,dx - \underbrace{\int p_1(x)\,dx}_{\text{trapezeidal rule}} =$$

$$\mathcal{E} = \int_a^b \varepsilon_1(x)\,dx = \frac{1}{2}\int_a^b f''(\overset{\xi}{\nearrow}\xi(x))(x-a)(x-b)\,dx$$

Mean-value theorem for integrals

$$\text{continuous} \rightarrow \int_a^b f(x)\,dx = f(\xi)(b-a)$$



$$\mathcal{E} = \frac{f''(\xi)}{2}\int_{x=a}^{b}(x-a)(x-b)\,dx\,, \quad \xi\in[a,b]$$

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

$$\mathcal{E}_{mid/trap} \sim O(h^3) \cdot f''(\xi)$$

<u>Composite rule error</u>

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

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

$$\left| f''(x) \right| < M, \; x \in [a,b]$$

$$|\mathcal{I} - \mathcal{I}_{trap}| < \frac{M}{12} h^3 \cdot n$$

$$= \frac{M}{12} h^{\cancel{3}\,2} \cdot \frac{b-a}{\cancel{h}}$$

$$\mathcal{E}_{\text{comp. trap}} \leq \frac{h^2}{12} \cdot M = O(h^2)$$

Same for composite midpoint.

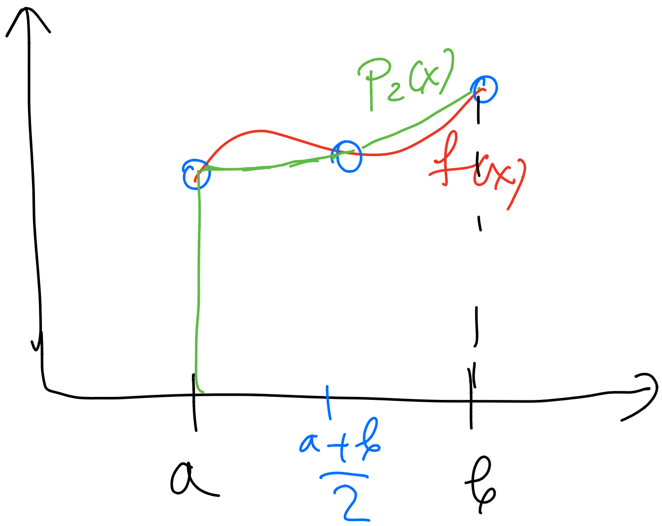
Composite midpoint / trapezoidal rule are second-order accurate

$$\mathcal{E} \sim \frac{1}{n^2}$$

$$\begin{cases} n \to 2n \\ \mathcal{E} \to \frac{\mathcal{E}}{4} \end{cases}$$

Warning: This is an <u>overestimate</u>. See Euler-MacLaurin theorem (trap. rule)

More accurate: Piecewise quadratic interpolation

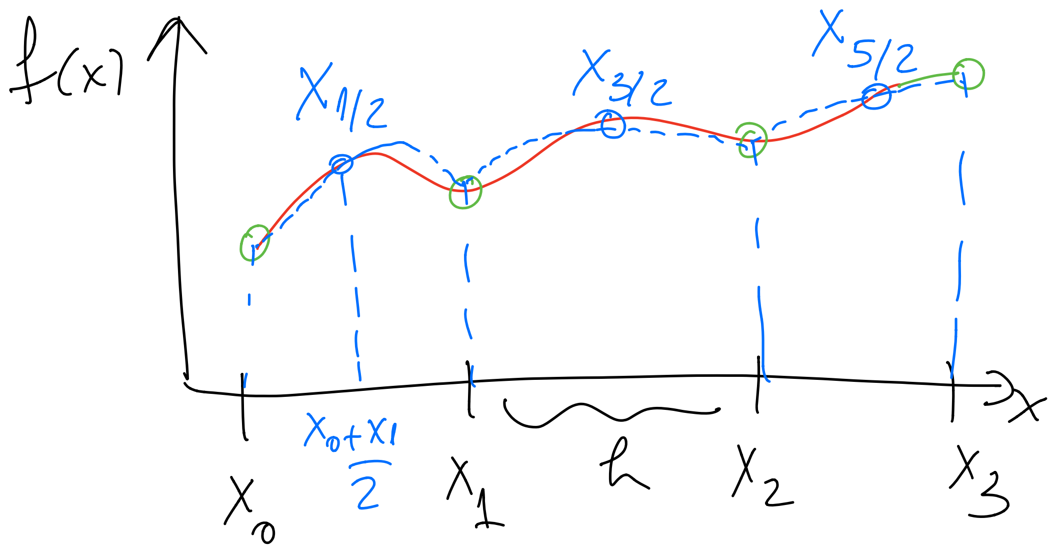


$$\int_a^b f(x)\,dx \approx \int_a^b P_2(x)\,dx$$

$$\int_a^b f(x)\,dx \approx \frac{b-a}{6}\left[f(a)+f(b)+4f\left(\frac{a+b}{2}\right)\right]$$

Simpson's rule

Composite Simpson's rule



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

$$+2f_2+4f_{5/2}+f_3]$$

$$\int_a^b f(x)\,dx \approx \frac{h}{6}\left[f(a)+f(b)\right]$$

$$+\frac{h}{3}\sum_{k=1}^{n-1} f(x_k)$$

$$+\frac{2h}{3}\sum_{k=0}^{n-1} f(x_{k+1/2})$$

Composite Simpson's rule

$$\mathcal{E}_{\substack{comp\\ Simp}} = \frac{b-a}{2880}\, h^4 \cdot M$$

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

$$\mathcal{E}_{comp.\,simp.} = O(h^4)$$

A method is p^{th} order accurate iff it is <u>exact</u> for polynomials of degree (at least) up to $p-1$

Use this to:

1) validate / test formulas

2) derive formulas faster

$$\int_a^b P_2(x)\,dx = w_1 f(a) + w_2 \cdot f\left(\frac{a+b}{2}\right) + w_3 \cdot f(b)$$

unknown weights

$\forall\, P(x) \in \mathcal{P}_2$

Formula is exact for $\{1, x, x^2\}$

(understand why)

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

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

$$= \frac{b^2-a^2}{2}$$

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

$$+ w_3 b^2$$

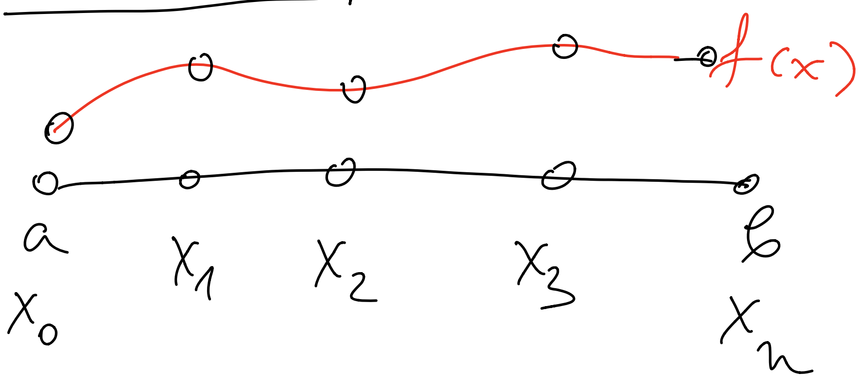
3 linear eqs for 3 unknowns

w_1, w_2, w_3

Solution is $w_1 = w_3 = \frac{b-a}{6}$

$$w_2 = \frac{4}{6}(b-a)$$

Gauss quadrature



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

Lagrange polynomial

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

$$\sum_{j=0}^{n} \int f_j \, L_j(x)\, dx$$

$$\int_a^b f(x)\, dx \approx \sum_{j=0}^{n} f_j \underbrace{\int_a^b L_j(x)\, dx}_{\text{constant}}$$

weight w_j

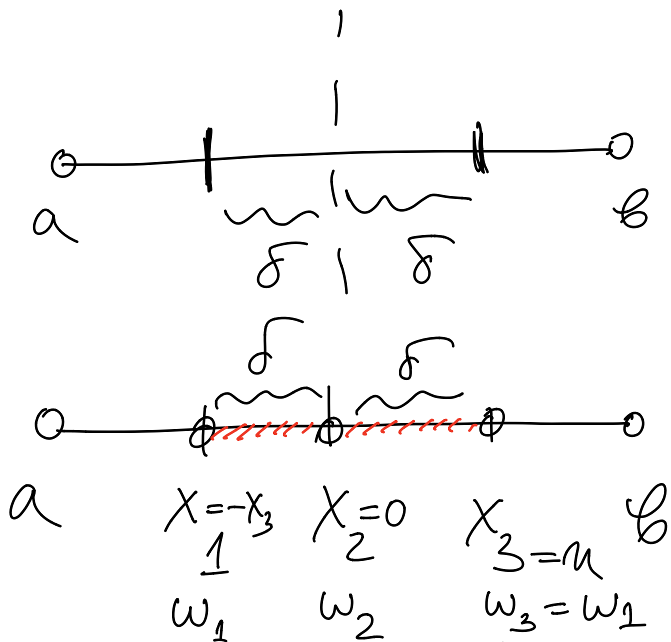
$$\int_a^b f(x)\, dx = \sum_{j=0}^{n} w_j f(x_j)$$

nodes

General quadrature formula

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

Newton-Cotes quadrature



What is the "best" choice of n nodes for quadrature

best $\equiv$ most "accurate" for a generic (analytic function) smooth function

means error $\sim O\left(\frac{1}{n^p}\right)$

p largest possible

Recall:

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

Conclusion: We want to find quadrature formula with n nodes that is exact for polynomials up to some degree p as large as possible.

Choose n nodes $\{x_j\}_{j=1,\dots,n}$

Set

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

polynomial interpolation of degree $n-1$

then quadrature rule will be exact for polynomials of degree up to $n-1$.

We have n unknown positions $x_1, \dots, x_n$

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

Require $\int f(x)\,dx \approx \sum w_j f(x_j)$ to be exact for monomials

$$f \in \{1, x, x^2, \dots, x^{2n-1}\}$$

Equations are nonlinear but polynomial.

Homework : 3 points, $n=3$

e.g. Exact $x^3 = f(x)$

$$\int_{-1}^{1} x^3\,dx = \frac{2}{4} = \frac{1}{2} = w_1 x_1^3 + w_2 x_2^3 + w_3 x_3^3$$

Theorem: If $x_1, \dots, x_n$ are (has to be) the roots of the Legendre polynomial of degree n, then the Gaussian quadrature formula/rule

$$\int_{-1}^{1} f(x)\,dx \approx \sum_{j=1}^{n} f(x_j) \underbrace{\int_{-1}^{1} L_j(x)\,dx}_{w_j}$$

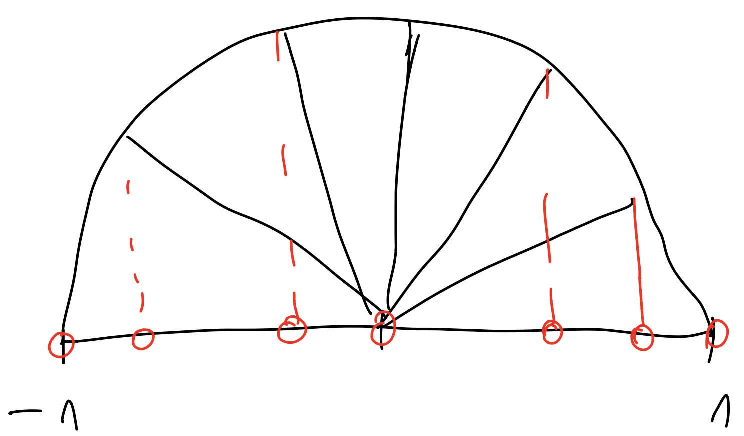
is exact for polynomials of degree $2n-1$ or less.

Also, $x_j \in [-1, 1]$
$j = 1, \dots, n$

Nodes are called Gaussian nodes

& w_j's Gaussian weights

(easy to change to $[a, b]$ using coordinate transformation)



Chebyshev

Aside

Roots of any set of orthogonal polynomials are good to use for polynomial interpolation, and also good in practice for quadrature.

Proof of first part of theorem.

Let $p \in \mathcal{P}_{2n-1}$ and denote the Legendre polynomials

$$\{p_0, p_1, \dots, p_n\}$$

$$p_{2n-1} / p_n = q \in \mathcal{P}_{n-1} + \text{remainder } r \in \mathcal{P}_{n-1}$$

$$\to p(x) = q(x) \cdot p_n(x) + r(x)$$

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

$$p(x_j) = r(x_j) \quad \ldots\ldots (1)$$

$$\int_{-1}^{1} p(x)\,dx \overset{?}{=} \sum_{j=1}^{n} w_j\, p(x_j)$$

$$= \int_{-1}^{1} \underbrace{\cancel{q(x)\,P_n(x)}}_{\text{zero}}\,dx + \int_{-1}^{1} r(x)\,dx$$

$$P_n(x) \perp \mathcal{P}_{n-1}$$

$$(q \in \mathcal{P}_{n-1}, P_n) = \int_{-1}^{1} q(x)\,P_n(x)\,dx = 0$$

$$\int p(x)\,dx = \int \underset{\substack{\uparrow \\ r \in \mathcal{P}_{n-1}}}{r}(x)\,dx$$

Because $w_j = \int L_j(x)\,dx$

$$\Rightarrow \int r(x)\,dx = \sum w_j\, r(x_j)$$

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

$$\int p(x)\,dx = \sum w_j\, r(x_j)$$

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

$\Rightarrow$ Gauss quadrature is exact for any $p(x) \in \mathcal{P}_{2n-1}$ QED $\blacksquare$

ASIDE on ODEs

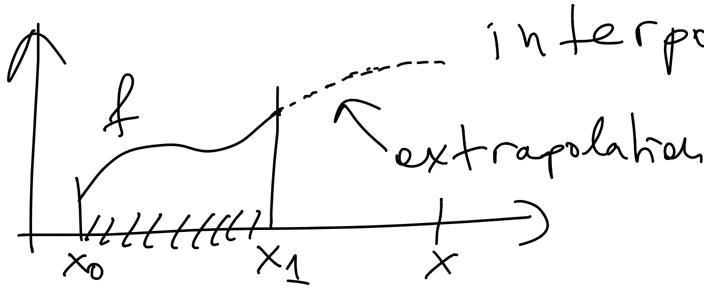
$$\begin{cases} y'(x) = f(y(x), x) \\ y(x_0) = y_0 \end{cases}$$

$|||$

unknown

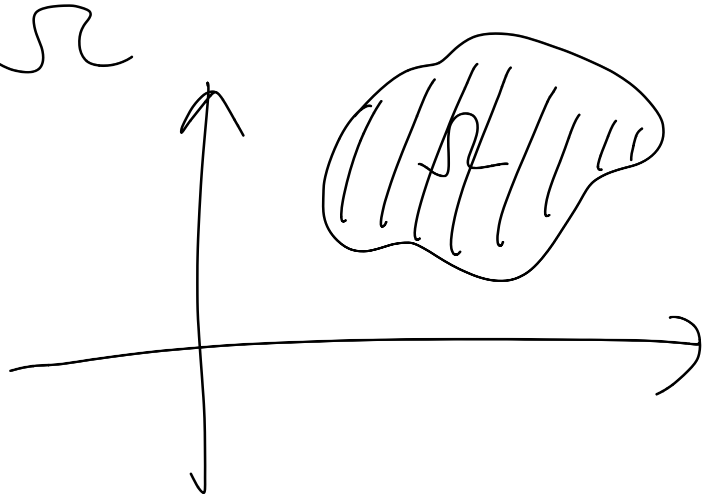
$$y(x) = \int_{x_0}^{x} f(y(x), x)\,dx + y_0$$

need to approximate r.h.s. of ODE by a polynomial & integrate it (extrapolation + interpolation)

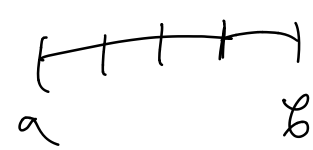


Aside: Quadrature in 2D/3D?

$$\underbrace{\iint}_{\Omega} f(x,y)\,dx\,dy$$



$$\int_a^b \cdot\, dx = \int_a^{x_1} + \int_{x_1}^{x_2}$$



If Ω is a rectangle

$$\int_a^b dx \int_c^d f(x,y)\,dy$$