Numerical solution of ordinary differential equations

DE-1

Differential equation: function + its derivates in the equation.

$$\text{e.g.} \quad f'(x) = g(f(x), f'(x) \ldots, x)$$

Order: highest derivate

Ordinary: univariate   partial: multivariate

linear: $f(x)$, derivates on the first power, no multiplication

Homogeneous: no parts with x or constant

More function: set of differential equations

General solution: integration + constant

$$f(x) = \int f'(x)\,dx + C$$

Particular solution (initial condition: $f(x_0)$ known)

$$f(x) = \int_{x_0}^{x_r} f'(x)\,dx + f(x_0).$$

Boundary conditions: → eigen problems often

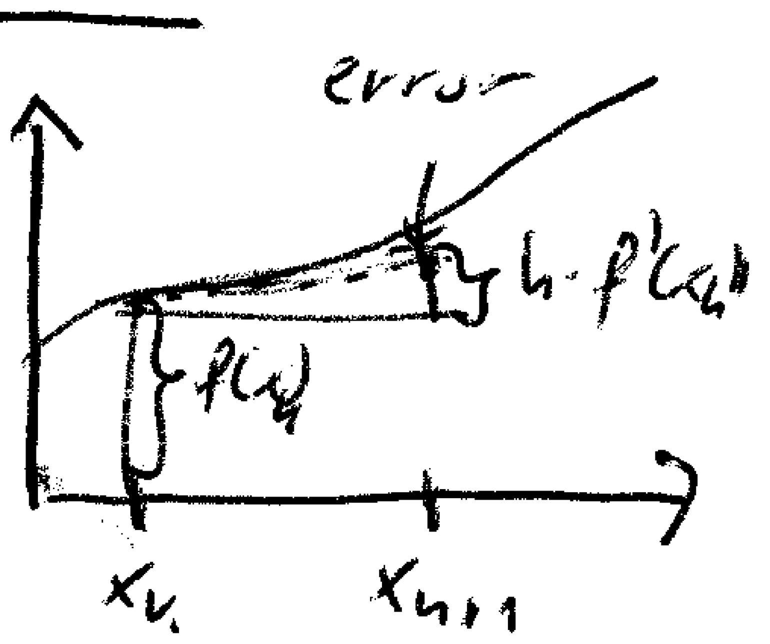
Old time: analytical sol. Nowadays: numerical

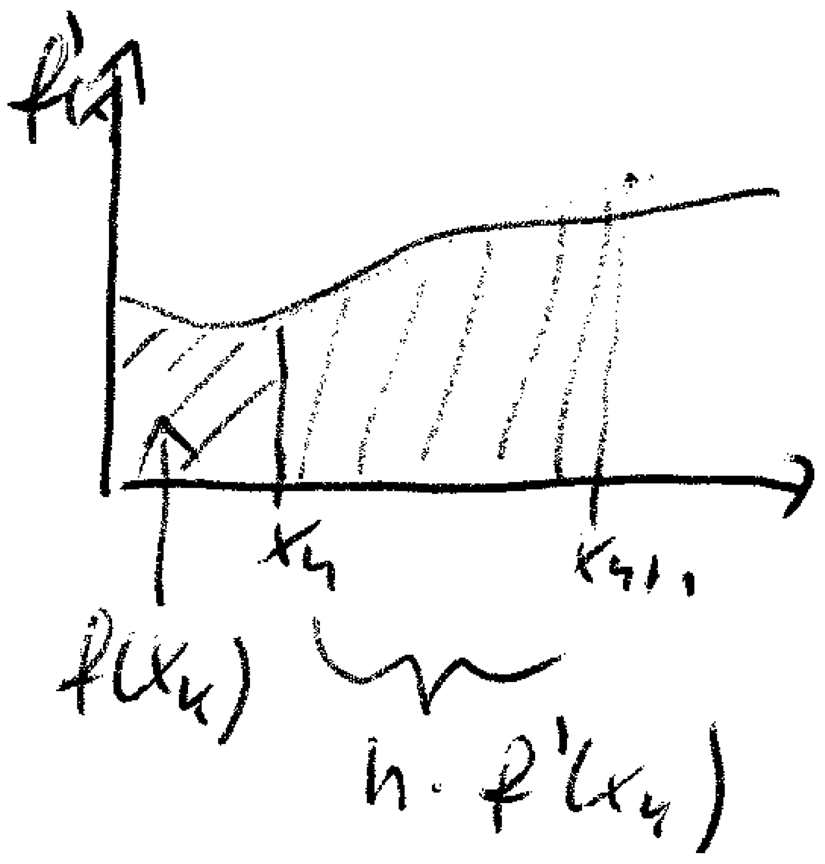
Higher order can be rewritten to first order ones, as:

$$f''(x) + f'(x) + q(x) = 0$$
$$g(x) = f'(x)$$
$$g'(x) = g(x) - q(x)$$

Methods using one starting points

Explicit Euler method:





$x_0 \to x_f$ interval

h stepsize $h = \dfrac{x_f - x_0}{n}$ ← n number of steps

$h = x_{k+1} - x_k$

$$f(x_{k+1}) = f(x_k) + h \cdot f'(x_k)$$

error: $\underbrace{\tilde{f}(x_{n+1})}_{\text{real}} - \underbrace{f(x_{n+1})}_{\text{calculated}} = \underbrace{\underbrace{\Delta f(x_n)}_{\text{error in previous steps}} + \underbrace{\delta(f(x_n) \to f(x_{n+1}))}_{\text{local step}}}_{\text{global error}}$

explicit Euler is bad!

Runge-Kutta methods

$y_{i+1} = f(x_{i+1})$

Use linear combination of different provisoric steps

$$y_{i+1} = y_i + h \cdot \sum a^{(i)} \cdot f^{1(i)} (x_i + \alpha^{(i)} \cdot h ; y_i^{(i)} (x_i + \alpha^{(i)} h))$$

e.g.: RK2 - improved Euler

$$k_1 = h \cdot f'(x_i, y_i)$$
$$k_2 = h \cdot f'(x_i + h ; y_i + k_1)$$
$$y_{i+1} = y_i + \frac{1}{2}(k_1 + k_2)$$

RK4 - (trapezoidal version)

$$y_{i+1} = y_i + k_1/6 + k_2/3 + k_3/3 + k_4/6$$
$$k_1 = h \cdot f'(x_i, y_i)$$
$$k_2 = h \cdot f'(x_i + \tfrac{h}{2} ; y_i + k_1/2)$$
$$k_3 = h \cdot f'(x_i + \tfrac{h}{2} ; y_i + k_2/2)$$
$$k_4 = h \cdot f'(x_i + h ; y_i + k_3)$$

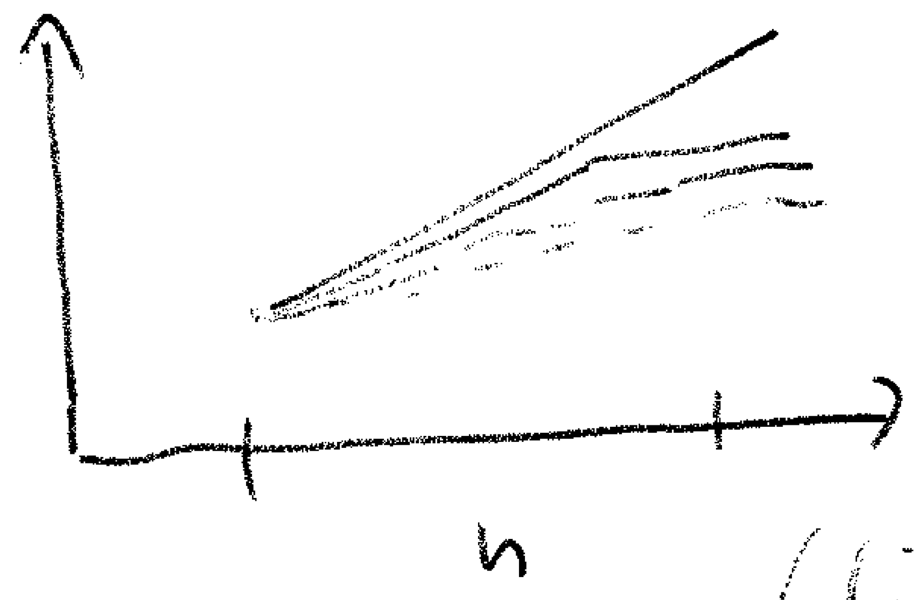
there are other „tangential" forms

How to determine h? $\simeq$ error^2 (repeat with $h/2$)

	global error	local error	no. f(x) calculation
exp Euler	$O(h)$	$O(h^2)$	1
imp. Euler	$O(h^2)$	$O(h^3)$	2
RK4	$O(h^4)$	$O(h^5)$	4

Runge-Kutta-Fehlberg method for error:

- Bulirsch-Stoer interpolation



do with $h, h/2, h/4 \ldots$

↓

interpolate to $h \to 0$

(like Romberg integration later)

Methods using more starting points

x_{i-2}, x_{i-1}, x_i and y_{i-2}, y_{i-1}, y_i are known

↓

fit a parabolic curve there ≈ Taylor expansion

(calculation of numerical derivatives backward)

3 point → 3-1=2 order polynomial

e.g. Adams-Bashfort method:

$$y_{i+1} = y_i + \frac{h}{12}(23y_i' - 16y_{i-1}' + 5y_{i-2}') + O(h^4) \quad *$$

implicit Euler:

$$y_{i+1} = y_i + f'(x_i + h, y_{i+1})$$

↑ obtained by solving non-linear equations or by rearrangement

~~more~~ first „more" starting points can be got by RK4

predictor-corrector methods

e.g. Adams-Bashfort-Moulton

(1) $\tilde{y}_{i+1}$ = as * prediction ≈ Taylor expansion

(2) $y_{i+1} = y_i + \frac{h}{12}(5\tilde{y}_{i+1}' + 8y_i' - y_{i-1}') + O(h^4)$ correction

Many different predictor-corrector methods:

- weight of previous steps in correction
- number of previous steps
- place of correction (e.g. impulse or acceleration)

↓

sees e.g. Gear-methods and tables

Differential equation sets (ordinary ones)

- paralel solution in a reasonable order
  e.g. $A(t)$, $B(t)$, $C(t)$ compounds, at first A, then B..
- total implicit schemes do not work (~~roots of~~ in each step
  x rootfinding in multidimensions is dangerous
- semi implicit works

$$f_j(x_{i+1}) = f_j(x_i) + h \cdot f_j'(f_1(x_{i+1}), f_2(x_{i+1}), \ldots f_j(x_i), \ldots f_n(x_i))$$

Stiff de sets

difference in the magnitudes, e.g:

mechanics: small-large particles, weak-strong springs
reactions: fast and slow reactions
stat. mechanics: simulation of intramolecular/intermolecular motions

how to solve:
- implicit methods
- more correction steps
- multi timestep integrations
- adaptive (h varying) methods

Direct solution of second order differential equations: DE-5

Störmer - 1907 (Verlet ~1960)

$h = x - x_0$ forward and backward Taylor series

$$y(x_0+h) = y(x_0) + y'(x_0)\cdot h + \frac{1}{2} y''(x_0) h^2 + \frac{1}{6} y'''(x_0) h^3 + O(h^4)$$
$$+\; y(x_0-h) = y(x_0) - y'(x_0)\cdot h + \frac{1}{2} y''(x_0) h^2 - \frac{1}{6} y'''(x_0) h^3 + O(h^4)$$

$$y(x_0+h) = -y(x_0-h) + 2y(x_0) + y''(x_0) h^2 + O(h^4)$$

symmetric for backward and forward

(pred. corr. not symmetric!)

importance in physics, stat. physics