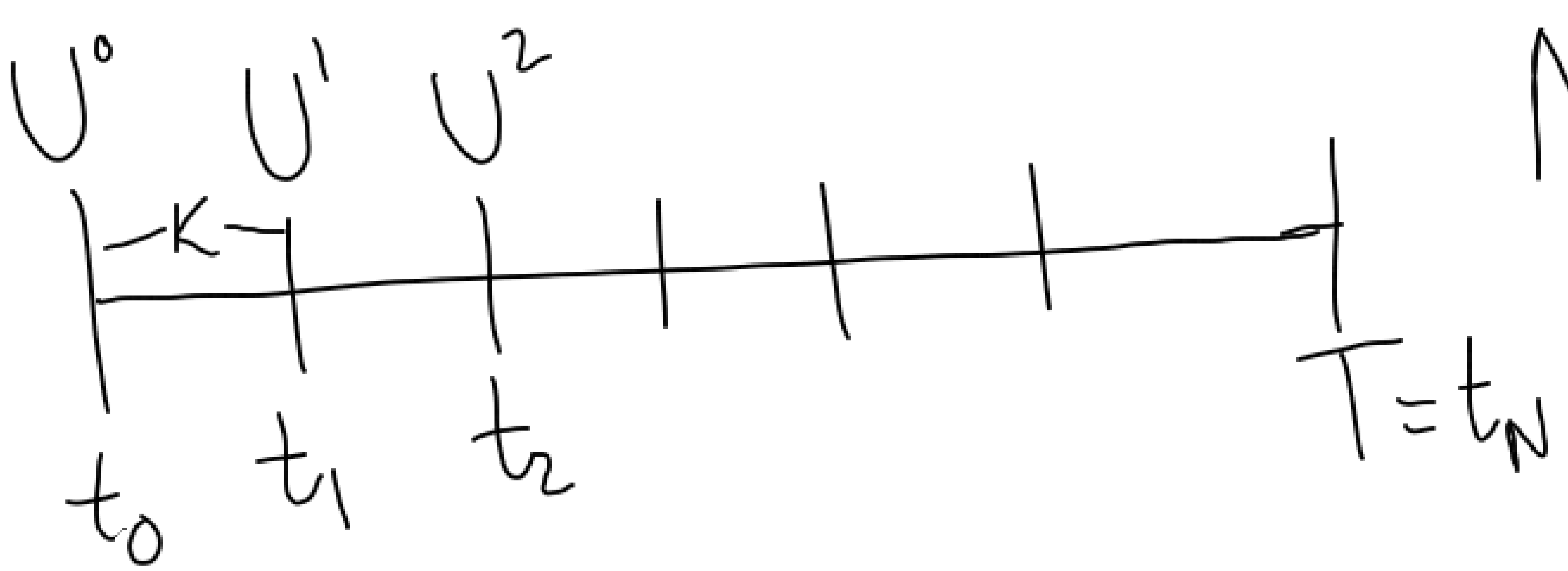
Numerical Methods For IVPs

$$u'(t) = f(u) \qquad u : \mathbb{R} \to \mathbb{R}^m$$

$$u(t_0) = \eta \qquad f : \mathbb{R}^m \to \mathbb{R}^m$$

$$t \in [t_0, T]$$

Discretize: $t_n = t_0 + nK$



$$N = \frac{T - t_0}{K}$$

$U^n \approx u(t_n)$

We will compute $U^1, U^2, \ldots$ marching forward in time.

Basic Methods

Explicit Euler

$$U^{n+1} = U^n + kf(U^n)$$

Conditionally stable (i.e. for small enough k)

i.e.: $$\frac{U^{n+1} - U^n}{k} = f(U^n)$$

Implicit Euler

$$U^{n+1} = U^n + kf(U^{n+1})$$

Unconditionally stable (for all k)

i.e. $$\frac{U^{n+1} - U^n}{k} = f(U^{n+1})$$

Implicit methods require solving a system of equations.

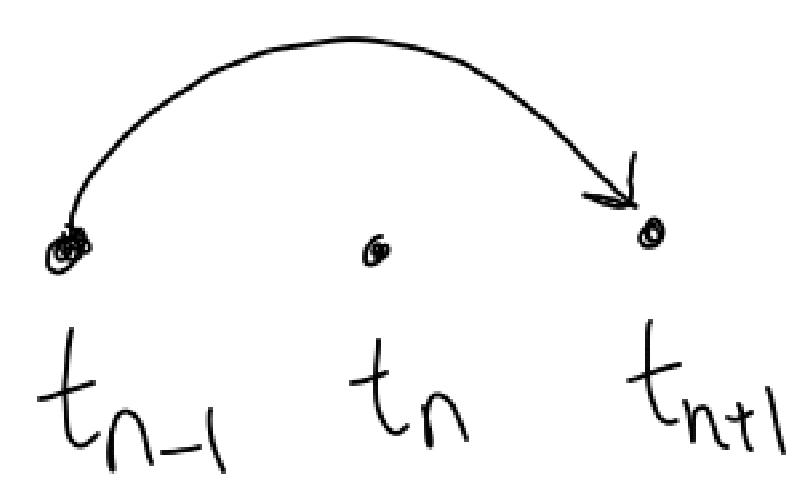
Trapezoidal method

$$U^{n+1} = U^n + \frac{k}{2}\left(f(U^n) + f(U^{n+1})\right)$$

2nd-order accurate

Leapfrog Method

$$U^{n+1} = U^{n-1} + 2kf(U^n)$$



How to achieve higher order accuracy

1. Use higher-order derivatives — Multi-derivative
2. Use more evalutions of f — Multi-stage or Runge-Kutta
3. Use more previous step values — Multistep

① Multiderivative

$$u(t_{n+1}) = u(t_n) + k u'(t_n) + \frac{k^2}{2} u''(t_n) + \frac{k^3}{6} u'''(t_n) + O(k^4)$$

$$U^{n+1} = U^n + k f(U^n) + \frac{k^2}{2} f' f(U^n) + \frac{k^3}{6}\left(f''(f,f) + f'f'f\right)$$

$$\frac{d^2}{dt^2} u_i(t) = \frac{d}{dt} f(u(t))_i = \sum_{j=1}^{m} \frac{\partial f_i}{\partial u_j} u_j'(t) = \sum_{j=1}^{m} \frac{\partial f_i}{\partial u_j} f_j$$

$$\frac{d^2}{dt^2} u(t) = f'f$$

$$\frac{d^3}{dt^3} u_i(t) = \frac{d}{dt} \sum_{j=1}^{m} \frac{\partial f_i}{\partial u_j} f_j = \sum_j \sum_l \frac{\partial^2 f_i}{\partial u_j \partial u_l} f_j f_l + \sum_j \sum_l \frac{\partial f_i}{\partial u_j} \frac{\partial f_j}{\partial u_l} f_l$$

$$\frac{d^3 u}{dt} = f''(f,f) + f'f'f$$

Pros / Cons

- \+ Only need 1 step
- − Need derivatives of f
- − May be costly for large m
- \+ Easy to adapt k

② Runge-Kutta

Example: $U^* = U^n + \frac{k}{2} f(U^n)$

(Midpoint method) $U^{n+1} = U^n + k f(U^*)$

Truncation error:

$$\frac{U^{n+1} - U^n}{k} = f\left(U^n + \frac{k}{2} f(U^n)\right)$$

$$\frac{u(t_{n+1}) - u(t_n)}{k} = f\left(u(t_n) + \frac{k}{2} f(u(t_n))\right) + \tau^n$$

$$f\left(u(t_n) + \frac{k}{2} f(u(t_n))\right) = f(u(t_n)) + \frac{k}{2} f'(u(t_n)) f(u(t_n)) + \frac{k^2}{8}\left(f''(f,f) + f'f'f\right) + O(k^3)$$

$$\frac{\cancel{u(t_n)} + \cancel{k u'(t_n)} + \frac{k^{\cancel{2}}}{2} u''(t_n) + \frac{k^{\cancel{3}\,2}}{6} u'''(t_n) + O(k^{\cancel{4}\,3}) - \cancel{u(t_n)}}{\cancel{k}}$$

$$= \cancel{f} + \cancel{\frac{k}{2} f'f} + \frac{k^2}{8}\underbrace{\left(f''(f,f) + f'f'f\right)}_{u'''} + O(k^3) + \tau^n$$

$$\tau^n = \frac{k^2}{24} u'''(t_n) + O(k^3)$$

2nd-order accurate

One-step error

$$\mathcal{L}^n = k\tau^n = O(k^3)$$

$Y_1 = U^n$

$Y_2 = U^n + \frac{k}{2} f(Y_1)$

$U^{n+1} = U^n + k f(Y_2)$

$$\begin{array}{c|cc} & 0 & 0 \\ & \frac{1}{2} & 0 \\ \hline & 0 & 1 \end{array}$$

General RK methods

$U'(t) = f(u,t)$

i-1 (explicit)

$$Y_i = U^n + k\sum_{j=1}^{\ell} a_{ij} f(Y_j, t_n + kc_j)$$

$$U^{n+1} = U^n + k\sum_{j=1}^{\ell} b_j f(Y_j, t_n + kc_j) \qquad A \in \mathbb{R}^{\ell\times\ell} \quad b \in \mathbb{R}^{\ell}$$

Pros/Cons

+ Only need 1 prev. step
+ Easy to adapt K
− Multiple evaluations of f per step

Butcher Tableau

$$\begin{array}{c|c} & A \\ \hline & b^T \end{array}$$

Kutta's method:

$$\begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 & 0 \\ 1/2 & 0 & 1/2 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ \hline & 1/6 & 1/3 & 1/3 & 1/6 \end{array}$$

$$\int_0^1 f(x)\,dx \approx \frac{1}{6}f(0) + \frac{1}{3}f\left(\tfrac{1}{2}\right) + \frac{1}{3}f\left(\tfrac{1}{2}\right) + \frac{1}{6}f(1)$$

③ Linear Multistep Methods

Example:

$$U^{n+1} = U^{n-1} + 2kf(U^n)$$

Pros/Cons

+ Only one evaluation of f per step
- Not self-starting (need multiple previous steps)
- Not trivial to adapt K