§1.7 High-order Methods

- We've seen three single step methods so far:
  - (i) Forward Euler (explicit)
  - (ii) Backward Euler (implicit)
  - (iii) Trapezoidal method (implicit)

- These methods are in general derived by using Taylor series expansion.

- As seen in the Taylor series method, a higher-order method is to be achied by keeping more terms in the Taylor series.

- Therefore, we must compute higher derivatives by repeated differentiation of a given ftn of the IVP.

- This is impractical, and we seek for alternatives to obtain high-order accuracy without requiring to compute high-order derivatives.

- Two approaches are available;

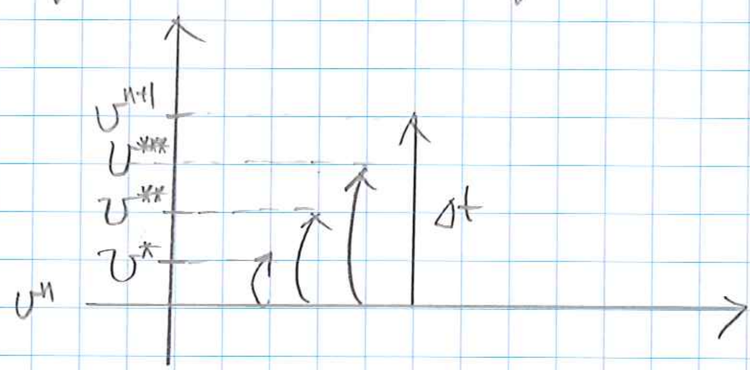
  intermediate updates

  - (i) single-step methods w/ multi-stages
    - (ex) pth order Runge-Kutta (RK)
  - (ii) linear multi-step method (LMM)

Runge-Kutta methods (RK)

→ Single step multi-stage methods to obtain high-order accuracy using intermediate multi-stage solutions, as opposed to calculate high-order derivatives explicitly in the Taylor series methods.

→ In the multi-stage approach, one evaluate intermediate solutions that are temporarily updated in order to achieve a desired order of solution accuracy within a single time step (i.e, $U^n \to U^{n+1}$)



→ Combine (linearly) $U^n, U^*, U^{**}, \cdots$ to finally update from

$$U^n \text{ to } U^{n+1}.$$

Ex Two stage RK2 (2^{nd} order in time)

$$\begin{cases} U^* = U^n + \frac{\Delta t}{2} f(U^n) & \cdots \text{ half time step update} \sim U^{n+\frac{1}{2}} \text{ using the forward Euler method.} \\ U^{n+1} = U^n + \Delta t f(U^*) & \cdots \text{ mid-pt or leapfrog method to update the full time step } \Delta t \text{ to } U^{n+1}. \end{cases}$$

→ If we combine the two into one, we can rewrite method as

$$\boxed{v^{n+1} = v^n + \Delta t\, f\left(v^n + \frac{\Delta t}{2} f(v^n)\right)} \quad \cdots \text{RK2}$$

→ This is a one-step explicit method

→ Let's check the order of accuracy:

$$E_{LT}^{n+1} = \frac{1}{\Delta t} E_{1step}^{n+1}$$

$$= \frac{1}{\Delta t}\left[u^{n+1} - N(u^n) \right]$$

$u(t^n) + \frac{\Delta t}{2} u'(t^n)$

$$= \frac{1}{\Delta t}\left[u^{n+1} - u^n - \Delta t\, f\left(u^n + \frac{\Delta t}{2} f(u^n)\right)\right]$$

$u' = f(u)$

$u'' = f'(u)u'$

$$= \frac{1}{\Delta t}\Big[\cancel{u(t^n)} + \cancel{\Delta t\, u'(t^n)} + \cancel{\frac{\Delta t^2}{2} u''(t^n)} + O(\Delta t^3)$$

$$- \cancel{u(t^n)}$$

$$- \Delta t \Big\{ \cancel{\underbrace{f(u(t^n))}_{u'(t^n)}} + \cancel{\frac{\Delta t}{2} \underbrace{u'(t^n) f'(u(t^n))}_{= u''}}$$

$$+ \frac{\Delta t^2}{4} (u'(t^n))^2 f''(u(t^n)) + O(\Delta t^3) \Big\} \Big]$$

$$= \frac{1}{\Delta t}\left[O(\Delta t^3) \right]$$

$$= O(\Delta t^2).$$

→ The method is 2nd-order accurate.

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Ex RK 2 in nonautonomous form ; $u'(t) = f(t, u(t))$

$$\begin{cases} v^* = v^n + \frac{\Delta t}{2} f(t^n, v^n) \\ v^{n+1} = v^n + \Delta t\, f(t^{n+\frac{1}{2}}, v^*) \end{cases}$$

→ This is again a second-order method as before.

→ To confirm this though, one now needs to conduct a Taylor series expansion in two variables :

$$f(x_0+\xi, y_0+\eta) = f(x, y) + \sum_{j=1}^{n} \frac{1}{j!}\left[\xi\frac{\partial}{\partial x} + \eta\frac{\partial}{\partial y}\right] f(x,y)\Big|_{x_0, y_0}$$

$$+ \frac{1}{(n+1)!}\left[\xi\frac{\partial}{\partial x} + \eta\frac{\partial}{\partial y}\right]^{n+1} f(x,y)\Big|_{x_0+\theta\xi,\ y_0+\theta\eta}$$

$$0 \le \theta \le 1.$$

Ex RK 4 (1 step w/ 4-stage, explicit) - most popular one

$$V_1 = v^n$$

$$V_2 = v^n + \frac{\Delta t}{2} f(t^n, V_1)$$

$$V_3 = v^n + \frac{\Delta t}{2} f(t^{n+\frac{1}{2}}, V_2)$$

$$V_4 = v^n + \Delta t\, f(t^{n+\frac{1}{2}}, V_3)$$

Finally,

$$v^{n+1} = v^n + \frac{\Delta t}{6}\left[f(t^n, V_1) + 2f(t^{n+\frac{1}{2}}, V_2) + 2f(t^{n+\frac{1}{2}}, V_3) + f(t^{n+1}, V_4)\right]$$

Rmk <u>Maximum order of the RK methods</u>

# of fn evaluations	1	2	3	4	5	6	7	8	9	11
Max order of method	1	2	3	4	4	5	6	6	7	8

- RK 4 has the most optimial feature in terms of having the same number of amount work and the resulting accuracy.
- Therefore RK4 is the most popular method.

<u>Ex. Heun's method</u> (2nd-order RK)

$$v_1 = v^n$$

$$v_2 = v^n + \Delta t\, f(t^n, v_1)$$

$$v^n = v^n + \frac{\Delta t}{2}\left[f(t^n, v_1) + f(t^{n+1}, v_2) \right]$$

Def. A general r-stage RK method:

$$\begin{cases} v_1 = v^n + \Delta t \sum_{j=1}^{r} a_{1j}\, f(t^n + \eta_j \Delta t,\, v_j) \\ v_2 = v^n + \Delta t \sum_{j=1}^{r} a_{2j}\, f(t^n + \eta_j \Delta t,\, v_j) \\ \vdots \\ v_r = v^n + \Delta t \sum_{j=1}^{r} a_{rj}\, f(t^n + \eta_j \Delta t,\, v_j) \\ \text{and finally} \\ v^{n+1} = v^n + \Delta t \sum_{j=1}^{r} b_j\, f(t^n + \eta_j \Delta t,\, v_j) \end{cases}$$

Note: The time stamp $t^n + \eta_j \Delta t$ is the temporal state of v_j, $j = 1, \cdots, r$.

Consistency Requirements ($\Leftrightarrow E_{LT}^{n+1} \to 0$ as $\Delta t \to 0$)

(1) $\sum_{j=1}^{r} a_{ij} = \eta_i$, $i = 1, 2, \cdots, r$

(2) $\sum_{j=1}^{r} b_j = 1$

(Proof is omitted here, but we roughly see that, if they are not true, then we fail to recover the soln of $u' \equiv 1 \equiv f(u)$)

Rmk: If the conditions for the consistency are met, then the method will be at least first-order accurate because $E_{LT}^{n+1} \to 0$ requires the method is at least $\sim O(\Delta t)$.

Def The Butcher Tableau for RK coefficients

$$
\begin{array}{c|cccc}
n_1 & a_{11} & a_{12} & \cdots & a_{1r} \\
n_2 & a_{21} & a_{22} & \cdots & a_{2r} \\
\vdots & & & & \\
n_r & a_{r1} & a_{r2} & \cdots & a_{rr} \\
\hline
 & b_1 & b_2 & & b_r
\end{array}
\qquad
\begin{array}{l}
\left.\begin{array}{l}
\rightarrow \sum_{j=1}^{r} a_{1j} = n_1 \\
\rightarrow \sum_{j=1}^{r} a_{2j} = n_2 \\
\\
\rightarrow \sum_{j=1}^{r} a_{rj} = n_r
\end{array}\right\} \text{consistency condition (i)} \\
\rightarrow \sum_{j=1}^{r} b_j = 1 \ \} \text{consistency condition (ii)}
\end{array}
$$

Ex RK 4

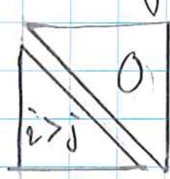
$$
\begin{array}{cc|cccc}
r=1 & 0 & 0 & 0 & 0 & 0 \\
r=2 & \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\
r=3 & \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\
r=4 & 1 & 0 & 0 & 1 & 0 \\
\hline
 & & \frac{1}{6} & \frac{3}{6} & \frac{3}{6} & \frac{1}{6}
\end{array}
\rightarrow \frac{1}{6} + \frac{3}{6} + \frac{3}{6} + \frac{1}{6} = \underline{1}
$$

Note that the elements on and above the diagonal are all zero.

$\rightarrow$ RK4 (explicit)

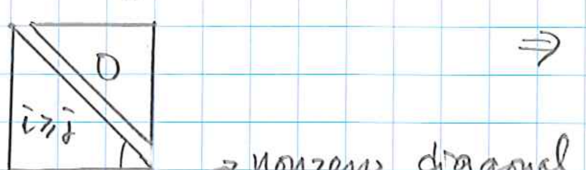
Rmk

(1) If $a_{ij} = 0$, $\forall j \geq i$ $\Rightarrow$ explicit RK



$\Rightarrow$ v_j is computed using only v_i, $i > j$

(2) If $a_{ij} = 0$, $\forall j > i$ $\Rightarrow$ implicit RK



$\Rightarrow$ v_j is computed using v_j itself as well.

Ex. Implicit RK2 (diagonally implicit RK, DIRK)

$$
\begin{cases}
U_1 = v^n \\
U_2 = v^n + \frac{\Delta t}{4}\left[f(t^n, U_1) + f(t^{n+\frac{1}{2}}, U_2) \right] \\
U_3 = v^n + \frac{\Delta t}{3}\left[f(t^n, U_1) + f(t^{n+\frac{1}{2}}, U_2) + f(t^{n+1}, U_3) \right] \\
\text{and finally} \\
v^{n+1} = U_3 .
\end{cases}
$$

$$
\begin{array}{c|ccc}
0 & 0 & & \\
\frac{1}{2} & \frac{1}{4} & \frac{1}{4} & \\
1 & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\
\hline
 & \frac{1}{3} & \frac{1}{3} & \frac{1}{3}
\end{array}
$$

nonzero diagonal

- We see that the consistency conditions

(i) $\sum_{j=1}^{r} a_{ij} = c_i$, $\forall i = 1, \dots, r$

(ii) $\sum_{j=1}^{r} b_j = 1$

- We also note that

$\frac{1}{6} + \frac{2}{6}$

(iii) $\underbrace{\sum_{j=1}^{r} b_j c_j = \frac{1}{2}}$ (i.e., $0 \cdot \frac{1}{3} + \frac{1}{2} \cdot \frac{1}{3} + 1 \cdot \frac{1}{3} = \frac{1}{2}$)

Rmk We say that a RK is 2nd order if (iii) is true, and hence DIRK is 2nd order.

Rmk Third-order RK requires two more conditions:

(iv) $\sum_{j=1}^{r} b_j n_j^2 = \frac{1}{3}$,

(v) $\sum_{i=1}^{r} \sum_{j=1}^{r} b_i a_{ij} n_j = \frac{1}{6}$.

Rmk Fourth-order RK needs additional four conditions, and higher order RKs requires an exponentially growing number of conditions.

Finding these conditions are done investigating E_T^{n+1} using Taylor series expansions.

One-step vs. multi-step methods (advantages of one-step)

(1) Self-starting: multi-step methods need some other methods (including one-step methods) to be used initially

(2) In one-step methods, Δt can be changed at any pt. in time $t = t^n$ because there is only v^n that is used for v^{n+1}.

However, in multi-step methods, one relies on the previous values of v^n, v^{n-1}, v^{n-2}, etc. to update v^n to v^{n+1}, where these previous values are assumed to be equally spaced in time.

Therefore one needs more care to change Δt in multi-step methods.

(3) If $u(t)$ becomes non-smooth at $t = t^{n*}$, one of the intermediate stages, then one-step method does not lose accuracy by treating $t = t^{n*}$ as an isolated singular (or discont) grid pt.

However, multi-step methods which use data from both sides of $t = t^{n*}$ in approximating derivatives, a loss of accuracy may occur.

Disadvantages of one-step methods

(1) Taylor series methods needs to compute high-order derivatives to get high-order methods

→ this can be cumbersome and expansive

(2) RK methods rely on entirely on "f" evalutions. If f evaluation becomes expansive when using multi-stage methods, RK methods become expansive to obtain high-order methods.

(ex) Implicit RK must evaluate f with newly iterated values each stage

→ expansive

Alternative for high-order methods.

→ Multi-step methods in which the ftn f evaluations are needed only once at each time step

→ The popular class of this approach is called the "linear multistep methods" (LMM)