Runge-Kutta Methods

Numerical Methods II, A. Donev

I will mostly follow LeVeque sec. 5.7.

I already showed examples of 2nd order (trapezoidal, midpoint) and one 4th order (RK4) method.

A general RK method with r stages (so this is a multistage method) to solve the ODE:

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

with numerical approximation

$$u^k \simeq u(t_k) \underset{\uparrow}{=} u(k\tau)$$

for constant time step size τ

(Later we will talk about adaptive time stepping so τ will become τ_k)

Stage 1:

$$Y_1 = U^n + \tau \sum_{j=1}^{r} a_{1j} f(Y_j, t_n + c_j \tau)$$

This is implicit if any $a_{ij} \neq 0$

So the only explicit option is

$$Y_1 = U^n$$

Stage $k = 1, \ldots, r$

$$Y_k = U^n + \tau \sum_{j=1}^{r} a_{kj} f(Y_j, t_n + c_j \tau)$$

intermediate stage values (e.g., estimate of midpoint)

coefficients

Implicit if $a_{k\{j \geq k\}} \neq 0$

Diagonally implicit if only $a_{kk} \neq 0$

(means we only have to solve nonlinear equation for Y_k)

Finally, the time step update is:

$$U^{n+1} = U^n + \tau \sum_{j=1}^{r} b_j \underbrace{f(Y_j, t_n + c_j \tau)}_{\substack{\text{already evaluated} \\ \text{above if } a_{kj} \neq 0}}$$

So f is evaluated at r points

$$(Y_j, t_n + c_j \tau), \quad j = 1, \dots, r$$

The coefficients of a particular RK method are represented by a

Butcher tableau

$$\begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1r} \\ \vdots & \vdots & \ddots & \vdots \\ c_r & a_{r1} & \cdots & a_{rr} \\ \hline & b_1 & \cdots & b_r \end{array} \equiv \begin{array}{c|c} \vec{c} & \overleftrightarrow{A} \\ \hline & \vec{b} \end{array}$$

Explicit if A is lower triangular with zero diagonal

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E.g. the RK4 method I showed bases the $\vec{b}$ coefficients on Simpson's rule:

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

If only lower triangle and diagonal of $\overleftrightarrow{A}$ are non-zero, the method is diagonally implicit – DIRK

Example of 2nd order DIRK:

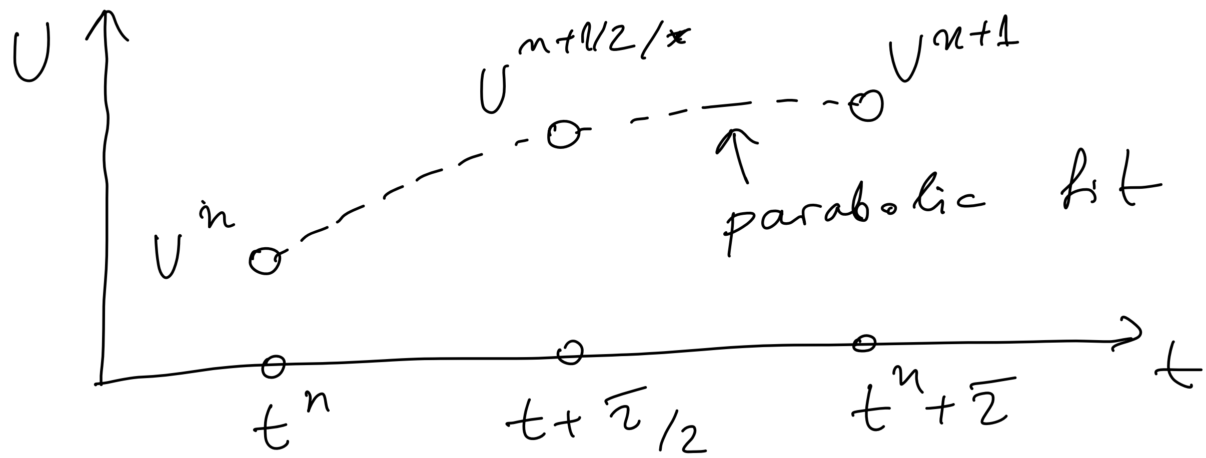
Trapezoidal Rule – Backwards Differentiation formula: TR – BDF2 (see 8.6 in LeVeque)

$$U^{n+1/2,*} = U^n + \frac{\tau}{4}\left(f(U^n) + f(U^{n+1/2,*})\right)$$

This is implicit trapezoidal to midpoint

$$U^{n+1} = \frac{1}{3}\left(4U^{n+1/2,*} - U^n + \tau f(U^{n+1})\right)$$

This update is based on a backwards differentiation formula:



$$u'(t^{n+1}) = f(u(t^{n+1}))$$

Let's fit a parabola through the tree points and differentiate that at t^{n+1} to estimate derivative to 2nd order:

$$u'(t^{n+1}) \simeq \frac{U^n + 3U^{n+1} - 4U^{n+1/2,*}}{\tau} = f(U^{n+1})$$

which gives the equation for U^{n+1}

This scheme has many nice properties and is often used, as we will explain later

Order conditions

① Consistency requires (first-order accuracy)

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

$$\sum_{j=1}^{r} b_j = 1$$

② Second-order requires also:

$$\sum_{j=1}^{r} b_j c_j = 1/2 \quad \text{(non-linear!)}$$

③ Third order requires also

$$\sum_{j=1}^{r} b_j c_j^2 = 1/3$$

$$\sum_{i,j=1}^{r} a_{ij} b_i c_j = 1/6$$

An example RK3 scheme that plays a special role in practice when solving hyperbolic PDEs (conservation laws) with the finite volume method: $f^n = f(U^n, t^n)$

$$U^* = U^n + \tau f^n \quad \text{(Euler step)}, \quad t^* = t^{n+1}$$

$$u^{**} = \frac{3}{4} U^n + \frac{1}{4} \big(\underbrace{U^* + \tau f^*}_{\text{second Euler step}} \big)$$

$$u^{n+1} = \frac{1}{3} U^n + \frac{2}{3} \big(\underbrace{U^{**} + \tau f^{**}}_{\text{third Euler step}} \big)$$

Observe that each stage is a convex combination of U^n and a forward Euler step. (this is important in the theory)

RK methods have been studied to death (still are...). Here are some important results

① An explicit r-stage RK method with order of accuracy r only exists if $r \le 4$

(This is why RK4 is special)

② The maximum order of accuracy is $2r$, for a fully implicit RK method (i.e., one has to solve at least r linear systems for all Y_k, $k = 1, \dots, r$)

Error control & adaptive time stepping

Sophisticated ODE schemes adjust the time step size to control the truncation error. The goal is to meet a certain specified relative or absolute error tolerance. This is not trivial to do, see HW3

E.g., absolute tolerance:

$$\| U^{N \leftarrow \text{final value}} - u(T) \| \leq \varepsilon$$

Here I will use $\Delta t \equiv \tau$ (more common notation)

Clearly this will be true if we spread the error uniformly over the time interval $[0, T]$

if we had $U^k = u(k\tau)$

$$e^k \approx \| \tilde{U}^{k+1} - u((k+1)\tau) \|$$

estimated from LTE

(A)

$$\|e^k\| \leq \varepsilon \frac{\Delta t_k}{T} \Rightarrow$$

$$\sum_{k=1}^{N-1} e^k \leq \sum_{k=1}^{N-1} \|e^k\| \leq \varepsilon \frac{\sum_{k=1}^{N-1} \Delta t_k}{T}$$

very pessimistic (safe) global error estimate

but $\sum \Delta t_k = T$

$$e_{global} \leq \varepsilon$$

as desired. This is not necessarily an optimal way to distribute the error but hard to do better.

We want to maximize Δt_k, i.e.,

$$\|e^k\| \approx \varepsilon \frac{\Delta t_k}{T}$$

How do we find a Δt_k that achieves this desired (max) error?

(B)

Option 1: Richardson extrapolation
(very important technique)
for ODEs / PDEs

Idea: Take first a step of duration Δt (or multiple steps), but then also run with half the time step size $\Delta t/2$.
Assume the method is of order p.

$U_{\Delta t}$ = solution with Δt

$U_{\Delta t/2}$ = solution with $\Delta t/2$

u = true solution, assuming we started with the correct solution

$$\begin{cases} u = u_{\Delta t} + C\,\Delta t^{p+1} + O\left(\Delta t^{p+2}\right) \\ u = u_{\Delta t/2} + C\left(\frac{\Delta t}{2}\right)^{p+1} + O\left(\Delta t^{p+2}\right) \end{cases}$$

same constant $C \sim u^{(p+1)}$
$\simeq u^{(p)} + O\left(\Delta t^{p+1}\right)$

©

$$\Rightarrow \quad u_{\Delta t} - u_{\Delta t/2} \approx C \cdot \Delta t^{p+1} \cdot \left(1 - \frac{1}{2^{p+1}}\right)$$

$$\Rightarrow C \approx \frac{2^{p+1}}{2^{p+1} - 1} \left(u_{\Delta t} - u_{\Delta t/2}\right)$$

$$U \approx U_{\Delta t} + e_k + O(\Delta t^{p+2})$$

$$e_k \approx \frac{2^{p+1}}{2^{p+1} - 1} \left(U_{\Delta t} - U_{\Delta t/2}\right)$$

So we <u>increased the order by one</u> via Richardson extrapolation.

This "trick" works for any method, for ODEs or PDEs, in space or in time, etc. <u>Remember it!</u>

Define $e_0^k = \frac{\Delta t_k}{T} \varepsilon$ ← allowed error for this time step

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This tells us that if we first run (once) Richardson extrapolation with step Δt_k and estimate the LTE e^k, and we then change to step $\widetilde{\Delta t}_k$:

$$\|\tilde{e}^k\| \simeq \left(\frac{\widetilde{\Delta t}_k}{\Delta t_k}\right)^{p+1} \|e^k\|$$

We want

$$\|\tilde{e}^k\| \simeq \varepsilon \frac{\widetilde{\Delta t}_k}{T} = \left(\frac{\widetilde{\Delta t}_k}{\Delta t_k}\right) e_0^k$$

$$\Rightarrow \quad \widetilde{\Delta t}_k = \Delta t_k \cdot \left(\frac{e_0^k}{\|e^k\|}\right)^{1/p}$$

But if the error was already small enough, $\|e_k\| < e_0^k$, that means we can increase the timestep so that the error is actually e_0^k:

(E)

$$\|\tilde{e}^k\| \simeq \left(\frac{\widetilde{\Delta t}_k}{\Delta t_k}\right)^{p+1} \|e^k\| \simeq e_0^k$$

$$\widetilde{\Delta t}_k = \left(\frac{e_0^k}{\|e_k\|}\right)^{1/(p+1)} \Delta t_k > \Delta t_k$$

$$\Rightarrow \|\tilde{e}^k\| \simeq e_0^k = \frac{\varepsilon\, \Delta t_k}{T} < \varepsilon \frac{\widetilde{\Delta t}_k}{T}$$

since $\Delta t_k < \widetilde{\Delta t}_k$

This leads to this adaptation strategy:

1. Set the target (absolute) error to

$$e_0^k = \frac{\Delta t_k}{T} \varepsilon$$

2. Use two different methods (both of order p or one p the other $p+1$) with known and proportional error estimates to estimate LTE e_k.

(3) Compute an improved estimate for U^{k+1} of order $p+1$ and return this as answer <u>if</u> $\|e_k\| < e^0_k$, and set

$$\Delta t_{k+1} = \Delta t_k \cdot \min\left\{ [5-10], \; [0.8-0.9] \left(\frac{e_0^k}{\|e^k\|} \right)^{\frac{1}{p+1}} \right\}$$

safety factors

(this time step was ok, so accept it, and increase time step size for <u>next</u> step)

(4) Otherwise (if $\|e_k\| \geq \varepsilon_0^k$), don't take the step and reduce the time step size

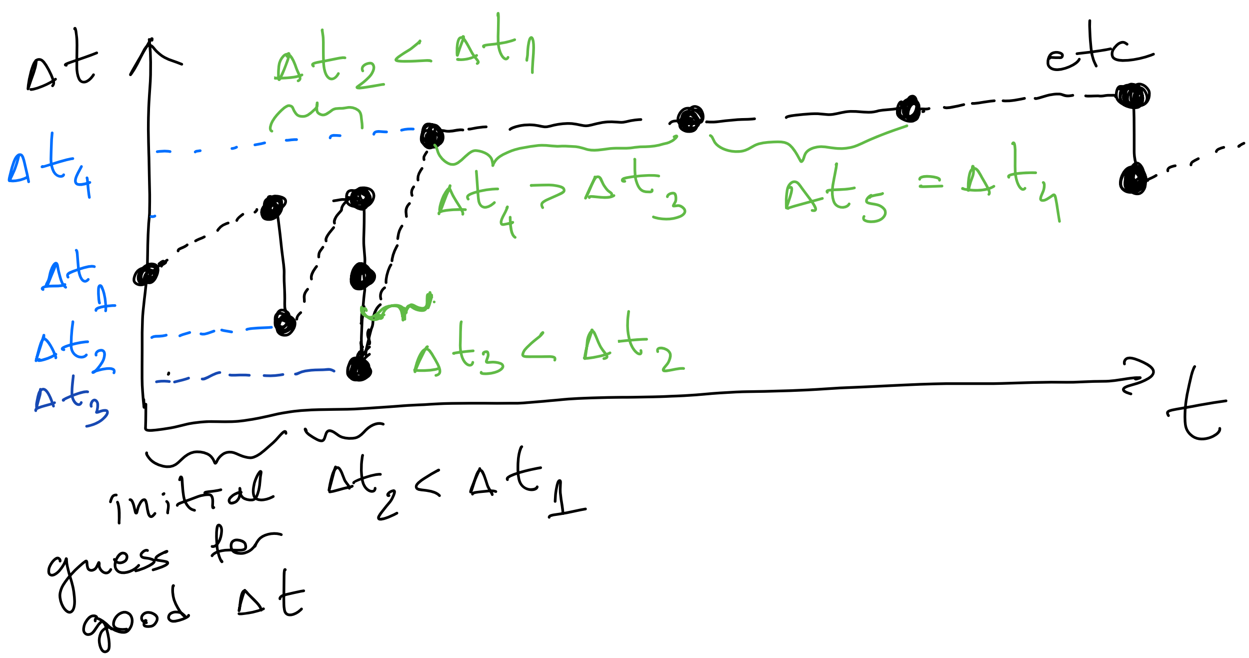
$$\Delta t_k \leftarrow [0.8-0.9] \left(\frac{e_0^k}{\|e_k\|} \right)^{1/p} \cdot \Delta t_k$$

and go back to step 1.

This is a very cautious method. It does not allow us to increase the error beyond what we estimate it to be with current Δt_k.

Important, the estimated error is for the solution of order p, even though we return a solution of order $p+1$. So this is quite pessimistic!

For homework, to debug, plot Δt



(H)

Embedded RK methods

Richardson extrapolation is expensive: each time step we need to take $3r$ stages instead of r to achieve error control.
In practice, we instead construct a set of $r+1$ (or $> r+1$ for very high order) stages that then let us compute both a solution of order p, and a solution of order $p+1$!

$$U_p^{n+1} = u(t_{n+1}) + O(\Delta t^{p+1})$$

$$U^{n+1} = U_{p+1}^{n+1} = u(t_{n+1}) + O(\Delta t^{p+2})$$

↖ best estimate we have

(I)

$$\| U_p^{n+1} - u(t_{n+1}) \| \simeq \| U_p^{n+1} - U_{p+1}^{n+1} \| + O(\Delta t^{p+2})$$

$$\| U_{p+1}^{n+1} - u(t_{n+1}) \| = \| e^k \| = O(\Delta t^{p+2})$$

$$\ll \| U_p^{n+1} - U_{p+1}^{n+1} \| = O(\Delta t^{p+1})$$

$$\Rightarrow \quad \| e^k \| \leq \| U_p^{n+1} - U_{p+1}^{n+1} \| = O(\Delta t^{p+1})$$

(pessimistic) error estimate of the method is formally of order p, though it may give a much <u>smaller</u> and <u>controlled</u> error in practice than the original method of order p

E.g. an RK2 embedded in an RK3 method

Bogački–Shampine RK23

(matlab solver ode23)

$$U^{n+1/2,*} = U^n + \frac{\Delta t}{2} f(U^n, t^n)$$

$$U^{n+3/4,*} = U^n + \frac{3\Delta t}{4} f\left(U^{n+1/2,*}, t^n + \frac{\Delta t}{2}\right)$$

$$U^{n+1} = U^{n+1}_{p+1} = U^n + \Delta t\left(\frac{2}{9} f^n + \frac{1}{3} f^{n+1/2,*} + \frac{4}{9} f^{n+3/4,*}\right)$$

third order estimate, only 3 function evaluations per step

2^{nd} order estimate:

$$U^{n+1}_p = U^n + \Delta t\left(\frac{7}{24} f^n + \frac{1}{4} f^{n+1/2,*} + \frac{1}{3} f^{n+3/4,*}\right) + \frac{1}{8}\Delta t f^{n+1} \leftarrow \text{reuse next step}$$

Aside: Fully implicit RK methods

As mentioned before, it is possible to get order of accuracy $2r$ with r stages if we use a fully implicit RK method.

For $r=2$, we can get such a 4th order method called the Gauss method, with tableau:

$$
\begin{array}{c|cc}
1/2 - \sqrt{3}/6 & 1/4 & 1/4 - \sqrt{3}/6 \\
1/2 + \sqrt{3}/6 & 1/4 + \sqrt{3}/6 & 1/4 \\
\hline
 & 1/2 & 1/2
\end{array}
$$

Gauss RK2

Consider ODE

$$x'(t) = f(x(t), t) \qquad (A)$$

This method arises by applying Gaussian quadrature with <u>two</u> points:

$$X^{n+1} = X^{n} + \int_{0}^{\Delta t} f(X(t),t)\,dt$$

$$\simeq X^{n} + \frac{\Delta t}{2}\sum_{i=1}^{r} w_i f\left(X\left(\frac{\Delta t}{2}\xi_i + \frac{\Delta t}{2}\right), \frac{\Delta t}{2}\xi_i + \frac{\Delta t}{2}\right)$$

where for $r = 2$

$$w_{1/2} = 1, \quad \xi_{1/2} = \pm\frac{1}{\sqrt{3}}$$

$$\frac{X^{n+1} - X^{n}}{\Delta t} = \frac{1}{2}\left[f\left(X\left(\underbrace{\frac{\Delta t}{2} - \frac{\Delta t}{2\sqrt{3}}}\right), \frac{\Delta t}{2} - \frac{\Delta t}{2\sqrt{3}}\right) + f\left(X\left(\underbrace{\frac{\Delta t}{2} + \frac{\Delta t}{2\sqrt{3}}}\right), \frac{\Delta t}{2} + \frac{\Delta t}{2\sqrt{3}}\right)\right] \quad B$$

Denoting

$$F_{1/2} = f\Big(X\big(\underbrace{\tfrac{\Delta t}{2} \mp \overbrace{\tfrac{\Delta t}{2\sqrt{3}}}^{\sqrt{3}\,\Delta t/6}}_{t_{1/2}}\big), \underbrace{\tfrac{\Delta t}{2} \mp \tfrac{\Delta t}{2\sqrt{3}}}_{t_{1/2}}\Big)$$

we have

$$X^{n+1} = X^n + \frac{\Delta t}{2}\left(F_1 + F_2\right)$$

which is the final step of the Gauss RK2 method.

To turn this into a solveable linear system, we need two more equations, i.e., the two stages of Gauss RK2.

These are

$$\begin{cases} X_1 \approx X(t_1) = X^n + \Delta t\left(\frac{1}{4}F_1 + \left(\frac{1}{4} - \frac{\sqrt{3}}{6}\right)F_2\right) \\ X_2 \approx X(t_2) = X^n + \Delta t\left(\left(\frac{1}{4} + \frac{\sqrt{3}}{6}\right)F_1 + \frac{1}{4}F_2\right) \end{cases}$$

Where do these come from?

We only need to know F_1 and F_2, i.e., X_1 and X_2, up to $O(\Delta t^3)$ since they are multiplied by Δt. So we need:

$$X_1 = X^n + \int_0^{(1/2-\sqrt{3}/6)\Delta t} \underbrace{f(x(t),t)}\, dt + O(\Delta t^3)$$

use linear fit through $(X_1,F_1),(X_2,F_2)$

we only need a first order approximation of this.

This calculation is done in Maple worksheet Euler RK2, and gives

$$X_1 = X^n + \frac{\Delta t}{4} F_1 + \left(\frac{1}{4} - \frac{\sqrt{3}}{6}\right)\Delta t \cdot F_2$$

as it appears in the first stage of Gauss RK2.

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