Runge-Kutta/'Single-step'/'Multi-Stage' Methods

Idea: Compute intermediate 'stage values', compute new state from those:

$$\begin{aligned}
r_1 &= f(t_k + c_1 h,\; y_k + h(a_{11} r_1 + \cdots + a_{1s} r_s))\\
r_2 &= \quad c_2 \qquad a_{21} \qquad a_{2s}\\
&\ \vdots\\
r_s &= \quad c_s \qquad a_{s1} \qquad a_{ss}
\end{aligned}$$

$$y_{k+1} = y_k + h(b_1 r_1 + \cdots + b_s r_s)$$

$$\tilde{y}_{k+1} = y_k + h(\tilde{b}_1 r_1 + \cdots + \tilde{b}_s r_s)$$

Can summarize in a *Butcher tableau*:

$$\begin{array}{r|ccc}
c_1 & a_{11} & \cdots & a_{1s}\\
\vdots & \vdots & & \vdots\\
c_s & a_{s1} & \cdots & a_{ss}\\
\hline
\text{order of } y_{k+1} & b_1 & \cdots & b_s\\
\text{order of } \tilde{y}_{k+1} & \tilde{b}_1 & \cdots & \tilde{b}_s
\end{array}$$

'embedded pair'

Runge-Kutta: Properties

When is an RK method explicit?

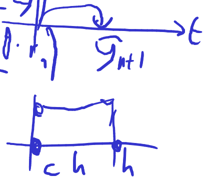
When is it implicit?

When is it *diagonally implicit*? (And what does that mean?)

Heun and Butcher

$$r_1 = f(y_k + h(0 \cdot r_1 + 0 \cdot r_2))$$

$$r_2 = f(y_k + h(1 \cdot r_1 + 0 \cdot r_2))$$



Stuff Heun's method into a Butcher tableau:

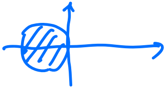
1. $\tilde{y}_{k+1} = y_k + 1hf(y_k)$
2. $y_{k+1} = y_k + \frac{h}{2}(f(y_k) + f(\tilde{y}_{k+1}))$.

#stages

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

RK4

F.E

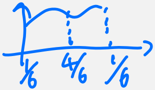


$\lambda = i$

What is RK4?

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

Simpson's rule



$$k_1 = f(t_n, y_n)$$

$$k_2 = f\left(t_n + \frac{h}{2},\ y_n + h\cdot\frac{k_1}{2}\right)$$

$$k_3 = f\left(t_n + \frac{h}{2},\ y_n + h\cdot\frac{k_2}{2}\right)$$

$$k_4 = f(t_n + h,\ y_n + h k_3)$$

$$y_{n+1} = y_n + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

Demo: Dissipation in Runge-Kutta Methods [cleared]

Multi-step/Single-stage/Adams Methods/Backward Differencing Formulas (BDFs)

Idea: Instead of computing stage values, use *history* (of either values of f or y–or both):

$$y_{k+1} = \sum_{i=1}^{M} \alpha_i y_{k+1-i} + h \sum_{i=1}^{N} \beta_i f(y_{k+1-i})$$

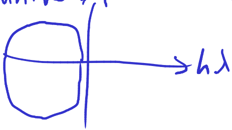
Method relies on existence of history. What if there isn't any? (Such as at the start of time integration?)

Not self-starting.

Stability Regions

$y' = \lambda y$ ← "universal" test ODE

$y' = Ay$



Why does the idea of stability regions still apply to more complex time integrators (e.g. RK?)

as long as the integrator "leaves the y whole" / only does linear combinations of y, then what diagonalizes A also diagonalizes the integrator.

Demo: Stability regions [cleared]

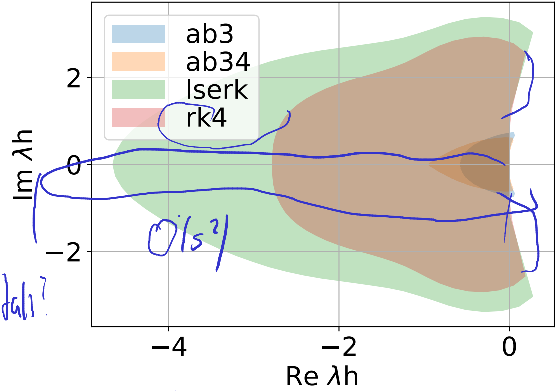
More Advanced Methods

Discuss:

- What is a good cost metric for time integrators?
- AB3 vs RK4
- Runge-Kutta-Chebyshev
- [LSERK](#) and [AB34](#)
- IMEX and multi-rate

stab?

- Parallel-in-time ("[Parareal](#)")



In-Class Activity: Initial Value Problems

In-class activity: Initial Value Problems

Outline

BVP Problem Setup: Second Order

Example: Second-order linear ODE

$$u''(x) + p(x)u'(x) + q(x)u(x) = r(x)$$

with *boundary conditions ('BCs')* at a:

- *Dirichlet* $u(a) = u_a$
- or *Neumann* $u'(a) = v_a$
- or *Robin* $\alpha u(a) + \beta u'(a) = w_a$

and the same choices for the BC at b.

Note: BVPs in time are rare in applications, hence x (not t) is typically used for the independent variable.

BVP Problem Setup: General Case

ODE:

$$\rightarrow \quad \boldsymbol{y}'(x) = \boldsymbol{f}(\boldsymbol{y}(x)) \quad \boldsymbol{f} : \mathbb{R}^n \to \mathbb{R}^n$$

BCs:

$$\rightarrow \quad \boldsymbol{g}(\boldsymbol{y}(a), \boldsymbol{y}(b)) = 0 \quad \boldsymbol{g} : \mathbb{R}^{2n} \to \mathbb{R}^n$$

$y' = f(y)$

$y(a) = 17$

$\cancel{y(b) = 12}$

(Recall the rewriting procedure to first-order for any-order ODEs.)

Does a first-order, scalar BVP make sense?

no, not well posed

Example: Linear BCs $B_a\boldsymbol{y}(a) + B_b\boldsymbol{y}(b) = \boldsymbol{c}$.
Is this Dirichlet/Neumann/...?

$\vec{y} = \begin{pmatrix} y \\ y' \\ y'' \end{pmatrix} \leftarrow$ could be anything

Does a solution even exist? How sensitive are they?

General case is harder than root finding, and we couldn't say much there.
$\to$ Only consider linear BVP.

pure.

Homogeneous

$\begin{cases} y' = Ay \\ B_a y(a) + B_b y(b) = c \end{cases} \xleftarrow{b(x)=0}$ $(*)\begin{cases} \boldsymbol{y}'(x) = A(x)\boldsymbol{y}(x) + \underline{\boldsymbol{b}(x)} \\ B_a\boldsymbol{y}(a) + B_b\boldsymbol{y}(b) = \underset{\sim}{\boldsymbol{c}} \end{cases}$ $\xrightarrow{c=0} \begin{cases} y' = Ay + b \\ B_a y(a) + B_b y(b) = 0 \end{cases}$

$\Downarrow$ y_h $\Downarrow$ y_b.

To solve that, consider *homogeneous IVP*

$$\boxed{\boldsymbol{y}_i'(x) = A(x)\boldsymbol{y}_i(x)}$$

$y = y_h + y_b$ solves $(*)$

with initial condition

$$\underline{\boldsymbol{y}_i(a) = \boldsymbol{e}_i}.$$

Note: $\boldsymbol{y} \neq \boldsymbol{y_i}$. $\boldsymbol{e}_i$ is the ith unit vector. With that, build the fundamental solution matrix

$$\underline{Y(x)} = \begin{bmatrix} | & & | \\ \boldsymbol{y}_1 & \cdots & \boldsymbol{y}_n \\ | & & | \end{bmatrix}$$

ODE Systems: Existence

$\int_D \delta_y(x) f(x)\, dx = f(y), \; y \in D.$

Let

$$Q := B_a Y(a) + B_b Y(b)$$

Then $(*)$ has a unique solution if and only if Q is invertible. Solve to find coefficients:

$$Q\boldsymbol{\alpha} = \boldsymbol{c}$$

$\begin{cases} y'(x) = Ay(x) + \delta_y(x) \\ B_a y(a) + B_b y(b) = 0 \end{cases}$

Then $Y(x)\boldsymbol{\alpha}$ solves $(*)$ with $\boldsymbol{b}(x) = 0$.

Define $\Phi(x) := Y(x)Q^{-1}$. So $\Phi(x)\boldsymbol{c}$ solves $(*)$ with $\boldsymbol{b}(x) = 0$.
Define *Green's function*

$$G(x,y) := \begin{cases} \Phi(x)B_a\Phi(a)\Phi^{-1}(y) & y \le x, \\ -\Phi(x)B_b\Phi(b)\Phi^{-1}(y) & y > x. \end{cases}$$

Then

$$\boldsymbol{y}(x) = \Phi(x)\boldsymbol{c} + \int_a^b G(x,y)\boldsymbol{b}(y)\mathrm{d}y.$$

Can verify that this solves $(*)$ by plug'n'chug.