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

$\vec{y}' = \vec{f}(\vec{y})$

Idea: Compute intermediate 'stage values':

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

Then compute the new state from those:

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

Can summarize in a Butcher tableau:

$$
\begin{array}{c|ccc}
c_1 & a_{11} & \cdots & a_{1s} \\
\vdots & \vdots & & \vdots \\
c_s & a_{s1} & \cdots & a_{ss} \\
\hline
 & b_1 & \cdots & b_s
\end{array}
$$

- When is an RK method explicit?

If only a_{ij} below the diagonal are non-zero.

- When is it implicit?

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

  if a_{ij} above the diag. are zero.

- Stuff Heun's method into a Butcher tableau:

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

  ↑ trapezoidal rule

0 ($t_k + 0 \cdot h$)	0	0
1 ($t_k + 1 \cdot h$)	1	0
	1/2	1/2

$r_1 = f(y_k)$

$r_2 = f(\tilde{y}_{k+1}) = f(y_k + h f(y_k))$

$= f(y_k + h r_1)$

- What is RK4?

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):

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

(one of these → hw) Extensions to implicit possible.

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

Demo: Stability regions

10 Boundary Value Problems for ODEs

BVP Problem Setup: Second Order

Example: Second-order linear ODE

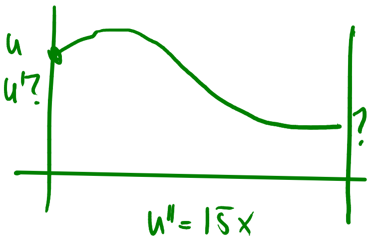
$$u''(x)+p(x)u'(x)+q(x)u(x)=r(x)$$

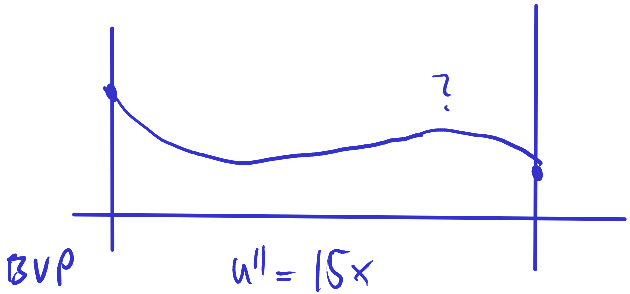
with boundary conditions ('BCs') at a:

- 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:

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

BCs:

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

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

- Does a first-order, scalar BVP make sense?

Example: Linear BCs

$$B_a \boldsymbol{y}(a) + B_b \boldsymbol{y}(b) = \boldsymbol{c}$$

- Is this Dirichlet/Neumann/...?

10.1 Existence, Uniqueness, Conditioning

Does a solution even exist? How sensitive are they?

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

$$(*)\begin{cases} \boldsymbol{y}'(x) = A(x)\boldsymbol{y}(x) + \boldsymbol{b}(x) \\ B_a\boldsymbol{y}(a) + B_b\boldsymbol{y}(b) = \boldsymbol{c} \end{cases}$$

To solve that, consider homogeneous *IVP*

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

with initial condition

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

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

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

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 coeffficients:

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

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

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

Define Green's function

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

Then

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

Conditioning:

Now easy. For perturbed problem with $\boldsymbol{b}(x) + \Delta\boldsymbol{b}(x)$ and $\boldsymbol{c} + \Delta\boldsymbol{c}$:

$$\|\Delta\boldsymbol{y}\|_\infty \leqslant \max\left(\|\Phi\|_\infty, \|G\|_\infty\right)\left(\|\Delta\boldsymbol{c}\|_1 + \int \|\Delta\boldsymbol{b}(y)\|_1 \mathrm{d}y\right).$$

- Did not prove uniqueness. (But true.)
- Also get continuous dependence on data.
- Can verify that above formula solves $(*)$ by plug'n'chug.

10.2 Numerical Methods

Shooting Method

Idea: Want to make use of the fact that we can already solve IVPs.
Problem: Don't know *all* left BCs.

Demo: Shooting Method

- What about systems?
- What are some downsides of this method?
- What's an alternative approach?