8.12 Stiff equations

An ODE is <u>stiff</u> if some coeff. in it is large

$$x' = \underbrace{1000 f(t,x)}_{\text{faster time scale}} + \underbrace{g(t,x)}_{\text{slower} \sim}$$

- Stiff eqs arise in dynamics w/ multiple timescales (for example, chemical reactions)

$$A + B \rightleftharpoons C$$

$$2A \longrightarrow D$$

concentration $c_A, \dots, c_D$

$$\begin{cases} c_A' = \dots \\ \dots \\ c_D' = \dots \end{cases}$$

- Stiff eqs can arise from discretized PDEs (for example, heat eq. $\partial_t u = \partial_{xx} u$)

$$\vec{u}' = A \vec{u} \qquad A = \frac{1}{\Delta x^2} \begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & 1 & \ddots & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & 1 & -2 \end{pmatrix}$$

Some eigenvalues of A are $O(1)$

some others are $O\left(\frac{1}{\Delta x^2}\right)$

- Error estimate for Euler method is not effective.

$$\text{error} \le C(\cdots) h$$

Consider the ODE

$$x' = \lambda x, \qquad x(0) = 1 \qquad (\lambda \in \mathbb{C})$$

Exact sol'n $\quad x(t) = e^{\lambda t}$

If $Re(\lambda) > 0$, then the sol'n grows exponentially in time to ∞.
one cannot expect num. sol'n accurate if $Re(\lambda) > 0$ is large.

If $Re(\lambda) < 0$, then the sol'n decays exponentially in time to 0.
When $Re(\lambda)$ is very negative, it decays to zero very fast.
$\Rightarrow$ Need to capture this behavior by num. method.

- Forward Euler: $\quad x_{i+1} = x_i + h\lambda x_i = \underbrace{(1+h\lambda)}_{\phi(z) = 1+z} x_i, \quad x_0 = 1$

$$x_n = (1+h\lambda)^n$$

Suppose $\lambda \in \mathbb{R}$, $\lambda < 0$, then $|1+h\lambda| \le 1$ if $h \le \frac{2}{-\lambda}$

small if $|\lambda|$ is large.
$\rightarrow$ restrictive

If $h \le \frac{2}{-\lambda}$ is not satisfied, then

$1 + h\lambda < -1 \longrightarrow x_n$ grows to infinity w/ oscillation
(unstable)

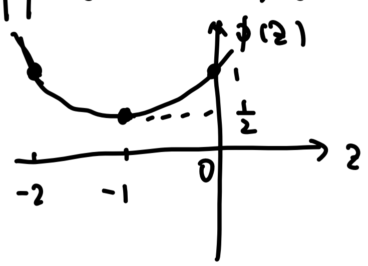
- Heun method: $\begin{cases} x^* = x_i + h\lambda x_i \\ x_{i+1} = x_i + \frac{1}{2} h (\lambda x_i + \lambda x^*) \end{cases}$

$$x_{i+1} = x_i + \frac{1}{2} h (\lambda x_i + \lambda (1+h\lambda) x_i)$$

$$= \underbrace{\left(1 + h\lambda + \frac{1}{2} h^2 \lambda^2\right)}_{\phi(z) = 1 + z + \frac{1}{2} z^2} x_i$$

"stability function"

Suppose $z \in \mathbb{R}$, $z < 0$



$|\phi(z)| \le 1 \Rightarrow -2 \le z \le 0$

$z = h\lambda$

$h \le \frac{2}{-\lambda}$ $\qquad$ still restrictive!

• Backward Euler: $x_{i+1} = x_i + h f(t_{i+1}, x_{i+1})$ (1st order implicit)

$$x_{i+1} = x_i + h\lambda x_{i+1}$$

$$(1-h\lambda)x_{i+1} = x_i$$

$$x_{i+1} = \frac{1}{1-h\lambda} x_i$$

$$\phi(z) = \frac{1}{1-z}$$

If $\mathrm{Re}(z) < 0$ then $\mathrm{Re}(1-z) = 1 - \mathrm{Re}(z) > 1$

$$\Rightarrow |1-z| > 1 \quad \Rightarrow \quad |\phi(z)| < 1$$

$\Rightarrow$ always stable for $\mathrm{Re}(\lambda) < 0$

• Generally explicit methods are not stable for stiff problems unless the fast time scale is resolved.

• Implicit methods tend to have better stability, but each time step is more expensive.

<u>Stability for Runge-Kutta methods</u> (explicit or implicit)

When applied to $x' = \lambda x$, one has

$x_{i+1} = \phi(h\lambda) x_i$ where $\phi(z)$ is its stability function.

The <u>stability region</u> of the method is $\{ z \in \mathbb{C} : |\phi(z)| \le 1 \}$.

The method is <u>A-stable</u> if its stability region contains $\{ z \in \mathbb{C} : \mathrm{Re}(z) < 0 \}$.

(for example, backward Euler is A-stable)

Another example: Crank-Nicolson method

$x_{i+1} = x_i + \frac{1}{2} h \left(f(t_i, x_i) + f(t_{i+1}, x_{i+1}) \right)$ (2nd order implicit)

$$x_{i+1} = x_i + \frac{1}{2}h(\lambda x_i + \lambda x_{i+1})$$

$$(1 - \frac{1}{2}h\lambda)\, x_{i+1} = (1 + \frac{1}{2}h\lambda)\, x_i$$

$$x_{i+1} = \frac{1 + \frac{1}{2}h\lambda}{1 - \frac{1}{2}h\lambda}\, x_i$$

$$\phi(z) = \frac{1 + \frac{1}{2}z}{1 - \frac{1}{2}z}$$

If $Re(z) < 0$ then

$$Re(1 + \frac{1}{2}z) = 1 + \frac{1}{2}Re(z)$$

$$Re(1 - \frac{1}{2}z) = 1 - \frac{1}{2}Re(z)$$ greater in $|\cdot|$

$$Im(1 + \frac{1}{2}z) = \frac{1}{2}Im(z)$$

$$Im(1 - \frac{1}{2}z) = -\frac{1}{2}Im(z)$$ same $|\cdot|$

$\Rightarrow |1 - \frac{1}{2}z| > |1 + \frac{1}{2}z| \Rightarrow |\phi(z)| < 1$

$\Rightarrow$ A-stable.

An RK method is <u>L-stable</u> if it's A-stable and $\lim_{z \to -\infty} \phi(z) = 0$.

(for example, backward Euler is L-stable; Crank-Nicolson is not).