LECTURE 2

IN THE LAST LECTURE WE STUDIED A-STABILITY

- EXPLICIT EULER IS NOT A-STABLE
- IMPLICIT EULER IS A-STABLE
- TRAPEZOIDAL METHOD IS A-STABLE

EXPLICIT RUNGE-KUTTA METHODS ARE NOT A-STABLE

DO EXPLICIT A-STABLE METHODS EXIST?

$\Downarrow$

YES $\Rightarrow$ EXPONENTIAL INTEGRATORS

WE CONSIDER

$$\begin{cases} y'(t) = A\,y(t) + g(y(t)) = f(y(t)) & t \in (0, t^*] \\ y(0) = y_0 \quad (t_0) \end{cases} \qquad (1)$$

$y(t) \in \mathbb{C}^N$ IS THE UNKNOWN, $A \in \mathbb{C}^{N\times N}$ CORRESPONDS TO THE LINEAR PART WHICH IS STIFF, $g(y(t)) \in \mathbb{C}^N$ IS THE NONLINEAR PART (NONSTIFF)

THIS IS A SYSTEM THAT ARISES, E.G., AFTER SEMIDISCRETIZATION IN SPACE OF SEMILINEAR DIFFUSION EQUATIONS.

WE ASSUME THAT (1) HAS EXISTENCE AND UNIQUENESS OF SOLUTION (f IS CONTINUOUS AND LIPSCHITZ).

THE EXACT SOLUTION OF (1) MAY BE EXPRESSED BY MEANS OF THE VARIATION-OF-CONSTANTS FORMULA

$$y(t) = e^{tA} y_0 + \int_0^t e^{(t-s)A} g(y(s))\,ds \qquad (*)$$

e^{tA} DENOTES THE MATRIX EXPONENTIAL

$$e^{tA} = \sum_{k=0}^{+\infty} \frac{(tA)^k}{k!}$$

LET'S PROVE THAT (*) IS INDEED THE SOLUTION OF (1)

$$y(t) = e^{tA} y_0 + \int_0^t e^{(t-s)A} g(y(s))\,ds$$

① $y(0) = y_0$ ✓ (SINCE $e^{0} = I$) $\qquad y'(t) = Ay(t) + g(y(t))$

② $y(t) = e^{tA} y_0 + e^{tA}\int_0^t e^{-sA} g(y(s))\,ds$

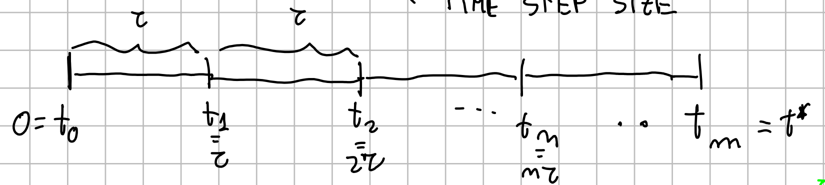
$$y'(t) = Ae^{tA} y_0 + Ae^{tA}\int_0^t e^{-sA} g(y(s))\,ds + e^{tA} \overbrace{\boxed{\frac{d}{dt}\int_0^t e^{-sA} g(y(s))\,ds}}^{e^{-tA} g(y(t))}$$

BY FUNDAMENTAL THM OF CALCULUS

$$= A\underbrace{\left(e^{tA} y_0 + \int_0^t e^{(t-s)A} g(y(s))\,ds\right)}_{y(t)} + \underbrace{e^{tA} e^{-tA}}_{=I} g(y(t))$$

$$= Ay(t) + g(y(t))$$

THE STARTING POINT FOR "STANDARD" EXPONENTIAL INTEGRATORS IS TO APPROXIMATE THE V.O.C. FORMULA. LET US INTRODUCE THE TIME DISCRETIZATION $t_n = n\tau$ ← TIME STEP SIZE



WE HAVE

$$y(t_{n+1}) = e^{\tau A} y(t_n) + \int_0^\tau \overbrace{e^{(\tau-s)A} g(\underbrace{y(t_n+s)}_{\approx g(y_n)})}^{\approx e^{\tau A} g(y_n)}\,ds$$

LAWSON INTEGRATORS

CALL $y_{n+1} \approx y(t_{n+1})$, $y_n \approx y(t_n)$ THEN WE GET

$$y_{n+1} = e^{\tau A} y_n + \left(\int_0^\tau e^{(\tau-s)A}\,ds\right) g(y_n)$$

TO WRITE INTEGRATOR IN A DIFFERENT FORM, WE INTRODUCE EXPONENTIAL-LIKE MATRIX FUNCTIONS CALLED φ - FUNCTIONS

$X \in \mathbb{C}^{N\times N}$

$$\varphi_\ell(X) = \begin{cases} e^{X} & \text{if } \ell = 0 \\ \dfrac{1}{(\ell-1)!}\displaystyle\int_0^1 e^{(1-\vartheta)X}\,\vartheta^{\ell-1}\,d\vartheta & \text{if } \ell > 0,\ \ell \in \mathbb{N} \end{cases}$$

THE φ - FUNCTIONS MAY BE DEFINED BY TAYLOR SERIES

$$\varphi_\ell(x) = \sum_{k=0}^{+\infty} \frac{X^k}{(\ell+k)!}$$

$$\varphi_1(X) = \sum_{k=0}^{+\infty} \frac{X^k}{(k+1)!} = \int_0^1 e^{(1-\vartheta)X}\,d\vartheta$$

$\vartheta = \frac{s}{\tau}$

$\tau\vartheta = s \rightarrow \tau d\vartheta = ds$

$$y_{n+1} = e^{\tau A} y_n + \left(\int_0^\tau e^{(\tau-s)A}\,ds\right) g(y_n)$$

$$= e^{\tau A} y_n + \tau \int_0^1 e^{(1-\vartheta)\tau A}\,d\vartheta\; g(y_n)$$

$$= e^{\tau A} y_n + \tau\,\varphi_1(\tau A)\, g(y_n)$$

$$\boxed{y_{n+1} = e^{\tau A} y_n + \tau\,\varphi_1(\tau A)\, g(y_n)}$$

THIS IS OUR FIRST EXPONENTIAL INTEGRATOR, WHICH IS CALLED EXPONENTIAL EULER METHOD

- IF $A \equiv \mathbb{O}$

$$y_{n+1} = e^{\mathbb{O}} y_n + \tau\,\varphi_1(\mathbb{O})\, g(y_n) = y_n + \tau g(y_n)$$

$e^{\mathbb{O}} = I$, $\varphi_1(\mathbb{O}) = I$

$\rightarrow$ EXPLICIT EULER FOR

OUR SYSTEM OF ODEs WAS $\begin{cases} y'(t) = g(y(t)) \\ y(0) = y_0 \end{cases}$

THIS IS THE UNDERLYING RUNGE-KUTTA METHOD (EXPLICIT)

- IF THE SYSTEM OF ODEs IS LINEAR

$$\begin{cases} y'(t) = Ay(t) + b \\ y(0) = y_0 \end{cases}$$

THEN EXPONENTIAL EULER IS EXACT

$$y_{n+1} = e^{\tau A} y_n + \tau \varphi_1(\tau A) b \qquad y_{n+1} \equiv y(t_{n+1})$$

IF $b=0$

$$\begin{cases} y'(t) = Ay(t) \\ y(0) = y_0 \end{cases}$$

$\Rightarrow$ WE ARE EXACT AND THEREFORE A-STABLE

$\Rightarrow$ WELL SUITED FOR STIFF PROBLEMS

$$y_{n+1} = e^{\tau A} y_n + \tau \varphi_1(\tau A) g(y_n) \qquad f(y(t)) = Ay(t) + g(y(t))$$

$$= y_n + \tau \varphi_1(\tau A) f(y_n)$$

$$\boxed{y_{n+1} = y_n + \tau \varphi_1(\tau A) f(y_n)}$$

$$= y_n + \tau \varphi_1(\tau A)(Ay_n + g(y_n))$$

$$= y_n + \tau \varphi_1(\tau A) A y_n + \tau \varphi_1(\tau A) g(y_n) \qquad x\varphi_1(x) = e^x - I$$

$$= y_n + (e^{\tau A} - I) y_n + \tau \varphi_1(\tau A) g(y_n)$$

$$= e^{\tau A} y_n + \tau \varphi_1(\tau A) g(y_n)$$

NOW WE PROVE THE CONVERGENCE OF THE EXPONENTIAL EULER METHOD (FIRST ORDER METHOD)

LEMMA 1 (DISCRETE GRONWALL LEMMA)

LET $\tau>0$, $t^*>0$, $0\le t_n = n\tau \le t^*$. ASSUME THAT THE SEQUENCE OF NON-NEGATIVE NUMBERS γ_n SATISFIES THE INEQUALITY

$$\gamma_n \le a\tau \sum_{j=1}^{n-1} t_{n-j}^{-\rho}\,\gamma_j + b\,t_n^{-\sigma}$$

FOR $\rho\ge 0$, $\sigma<1$, $a\ge 0$, $b\ge 0$. THEN THE ESTIMATE

$$\gamma_n \le c\,b\,t_n^{-\sigma}$$

HOLDS, WHERE C IS A CONSTANT DEPENDING ON ρ, σ, a, t^*.

THEOREM 1 (CONVERGENCE OF EXPONENTIAL EULER)

LET g BE DIFFERENTIABLE, UNIFORMLY BOUNDED AND UNIF. BDD DERIVATIVE. THEN, THE EXPONENTIAL EULER METHOD IS FIRST ORDER ACCURATE, THAT IS

$$\| y(t_n) - y_n \| \le C\,\tau$$

HERE C IS A CONSTANT THAT MAY DEPEND ON t^*, BUT NOT ON n. $0\le t_n \le t^*$

PROOF

FROM THE V.O.C. FORMULA WE HAVE

$$y(t_{n+1}) = e^{\tau A} y(t_n) + \int_0^\tau e^{(\tau-s)A} g(y(t_n+s))\,ds$$

FOR SHORTHAND NOTATION WE WRITE $h(t) \equiv g(y(t))$

$$y(t_{n+1}) = e^{\tau A} y(t_n) + \int_0^\tau e^{(\tau-s)A} h(t_n+s)\,ds$$

WE EXPAND h IN TAYLOR SERIES (WITH REMAINDER IN INTEGRAL FORM)

$$h(t_n+s) = h(t_n) + \int_0^s h'(t_n+\sigma)\,d\sigma$$

$$y_{n+1} = e^{\tau A} y_n + \tau\varphi_1(\tau A)\, g(y_n)$$

$$y(t_{n+1}) = e^{\tau A} y(t_n) + \int_0^\tau e^{(\tau-s)A} h(t_n+s)\,ds$$

$$= e^{\tau A} y(t_n) + \underbrace{\int_0^\tau e^{(\tau-s)A}\,ds}_{\tau\varphi_1(\tau A)}\, h(t_n) + \int_0^\tau e^{(\tau-s)A}\int_0^s h'(t_n+\sigma)\,d\sigma\,ds$$

$$= e^{\tau A} y(t_n) + \tau\varphi_1(\tau A)\, h(t_n) + \int_0^\tau e^{(\tau-s)A}\int_0^s h'(t_n+\sigma)\,d\sigma\,ds$$

$$y(t_{n+1}) - y_{n+1} = e^{\tau A}(y(t_n) - y_n) + \tau\varphi_1(\tau A)\big(h(t_n) - g(y_n)\big)$$
$$+ \int_0^\tau e^{(\tau-s)A}\int_0^s h'(t_n+\sigma)\,d\sigma\,ds$$

$$\varepsilon_{n+1} \doteq y(t_{n+1}) - y_{n+1} \qquad \varepsilon_n = y(t_n) - y_n$$

$$\delta_{n+1} = \int_0^\tau e^{(\tau-s)A}\int_0^s h'(t_n+\sigma)\,d\sigma\,ds$$

THEN WE GET

$$\boxed{\varepsilon_{n+1} = e^{\tau A}\varepsilon_n + \tau\varphi_1(\tau A)\big(h(t_n) - g(y_n)\big) + \delta_{n+1}} \qquad (R)$$

$\varepsilon_1 \quad (n=0)$

$$\varepsilon_1 = e^{\tau A}\varepsilon_0 + \tau\varphi_1(\tau A)\big(h(t_0) - g(y_0)\big) + \delta_1$$

$$\varepsilon_0 = 0, \quad h(t_0) = g(y(t_0)) = g(y_0), \quad \ldots = 0$$

$$= \delta_1$$

$$\varepsilon_2 = e^{\tau A}\varepsilon_1 + \tau\varphi_1(\tau A)\big(h(t_1) - g(y_1)\big) + \delta_2 \qquad h(t_1) = g(y(t_1))$$

$$= e^{\tau A}\delta_1 + \delta_2 + \tau\varphi_1(\tau A)\big(h(t_1) - g(y_1)\big)$$

$$e^{\tau A}\varphi_1(\tau A) = \varphi_1(\tau A)e^{\tau A}$$

$$\varepsilon_3 = e^{\tau A}\varepsilon_2 + \tau\varphi_1(\tau A)\big(h(t_2) - g(y_2)\big) + \delta_3$$

$$= e^{2\tau A}\delta_1 + e^{\tau A}\delta_2 + \delta_3 + \tau\varphi_1(\tau A)e^{\tau A}\big(h(t_1) - g(y_1)\big)$$
$$+ \tau\varphi_1(\tau A)\big(h(t_2) - g(y_2)\big)$$

YOU CAN PROVE THAT THE RECURSION (R) LEADS TO

$$\varepsilon_n = \tau \varphi_1(\tau A) \sum_{j=1}^{n-1} e^{(n-j-1)\tau A} \left(h(t_j) - g(y_j)\right) + \sum_{j=1}^{n} e^{(n-j)\tau A} \delta_j$$

$$\|\varepsilon_n\| \leq \tau \|\varphi_1(\tau A)\| \sum_{j=1}^{n-1} \|e^{(n-j-1)\tau A}\| \, \|h(t_j) - g(y_j))\| + \sum_{j=1}^{n} \|e^{(n-j)\tau A}\| \, \|\delta_j\|$$

① $\|\varphi_1(\tau A)\| \leq \varphi_1(\tau \|A\|) \underset{\varphi_1(t^* \|A\|)}{\leq} C(t^*)$

② $\|e^{j\tau A}\| \leq e^{j\tau\|A\|} \leq e^{n\tau\|A\|} = e^{t^*\|A\|} \leq C$

$\|e^{tA}\| \leq e^{t\|A\|} \leq e^{t^*\|A\|} \leq C(t^*, \|A\|)$

TERRIBLE

③ $\|h(t_j) - g(y_j)\| = \|g(y(t_j)) - g(y_j)\| \leq C \|y(t_j) - y_j\|$

SINCE g' UNIFORMLY BDD, THEREFORE LIPSCHITZ

④ $\|\delta_j\| = \left\| \int_0^\tau e^{(\tau - s)A} \int_0^s h'(t_{j-1} + \sigma) \, d\sigma \, ds \right\|$

$$\leq \int_0^\tau \underbrace{\|e^{(\tau-s)A}\|}_{\leq C} \int_0^s \|h'(t_{j-1} + \sigma)\| \, d\sigma \, ds \leq C\tau^2$$

$h'(t_{j-1}+\sigma) = g'(y(t_{j-1}+\sigma)) \cdots \leq C$

$A = \partial_{xx}$ ⊕ HOM. DIR. $\longrightarrow$ ✓ $\|e^{tA}\| \leq C$, $\|\varphi_1(tA)\| \leq C$

$$\|\varepsilon_n\| \leq \tau \|\varphi_1(\tau A)\| \sum_{j=1}^{n-1} \|e^{(n-j-1)\tau A}\| \, \|h(t_j) - g(y_j))\| + \sum_{j=1}^{n} \|e^{(n-j)\tau A}\| \, \|\delta_j\|$$

$$\leq C\tau \sum_{j=1}^{n-1} \|\varepsilon_j\| + C\tau^2 \underbrace{\sum_{j=1}^{n} 1}_{\leq \sum_{j=1}^{n} 1 = n = \frac{t^*}{\tau}} \leq C\tau \sum_{j=1}^{n-1} \|\varepsilon_j\| + C\tau$$

BY DISCRETE GRONWALL LEMMA $\quad \gamma_n = \|\varepsilon_n\|, \; a = C, \; p = 0,$
$\gamma_j = \|\varepsilon_j\|, \; b = C\tau, \; \sigma = 0$

$\Rightarrow \|\varepsilon_n\| \leq C\tau \iff \|y(t_n) - y_n\| \leq C\tau$

$\square$

CONNECTION OF EXPONENTIAL EULER WITH IMEX METHODS

$$\begin{cases} y'(t) = \underbrace{Ay(t)}_{\text{IM}} + \underbrace{g(y(t))}_{\text{EX}} = f(y(t)) \\ y(0) = y_0 \end{cases}$$

$$\frac{y_{n+1} - y_n}{\tau} = A y_{n+1} + g(y_n) \iff y_{n+1} = y_n + \tau A y_{n+1} + \tau g(y_n)$$

$$\iff \boxed{(I - \tau A) y_{n+1} = y_n + \tau g(y_n)}$$

BACKWARD-FORWARD EULER

(FIRST ORDER, A-STABLE)

$\to$ LINEAR SYSTEM

$\to y^{n+1} = y^n + \tau f(y^{n+1}) \Rightarrow$ NONLINEAR SYSTEM

$\to y^{n+1} = y^n + \tau f(y^n) \Rightarrow$ EXPLICT

$$\Rightarrow y^{n+1} = e^{\tau A} y^n + \tau \varphi_1(\tau A) g(y^n)$$

$$y_{n+1} = (I - \tau A)^{-1} y_n + \tau (I - \tau A)^{-1} g(y_n)$$

$(I - \tau A)^{-1}$ IS A $[0,1]$ PADÉ APPROXIMATION OF $e^{\tau A}$ AND $\varphi_1(\tau A)$

$$e^X \approx \frac{P_\ell(X) \to \text{POLY}}{S_d(X) \to \text{POLY}} = \frac{I}{(I - X)}$$