

STIFF ODE'S (NR § 16.6)

WE BEGIN BY CONSIDERING THE IMPORTANCE OF TIMESCALES:

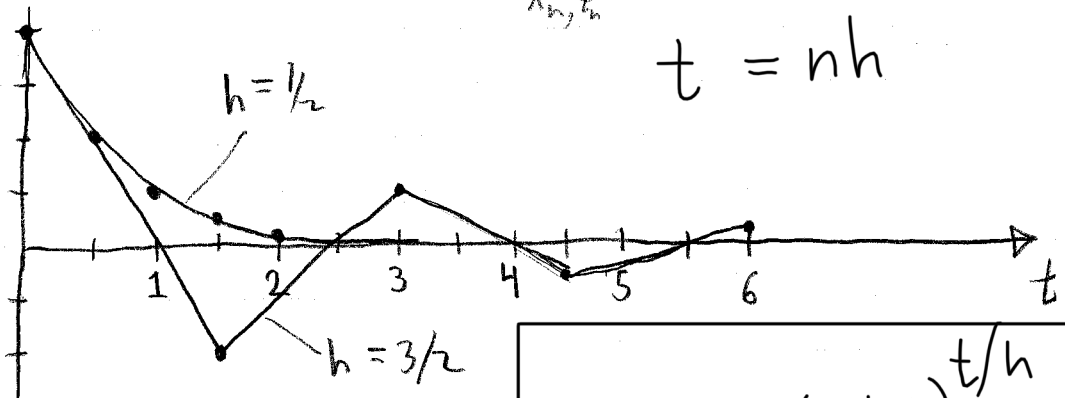
$$\frac{dx}{dt} = -kx$$

ANALYTICAL SOLN:  $x(t) = x(0) e^{-kt}$

EULER TIMESTEP:

$$X_{n+1} = X_n + h \left. \frac{dx}{dt} \right|_{x_n, t_n} = X_n (1 - hk)$$

$$t = nh$$



$$X_n = X_0 (1 - hk)^n = x(t) = x(0) (1 - hk)^{t/h}$$

SUPPOSE  $k=1$ .

$$h = \frac{1}{2}: X_n = \left(\frac{1}{2}\right) X_{n-1} \Rightarrow x(t) = x(0) \left(\frac{1}{2}\right)^{2t} = x(0) \left(\frac{1}{4}\right)^t$$

$$h = 1: X_n = 0 X_{n-1} \Rightarrow x(t) = x(0) 0^t$$

$$h = \frac{3}{2}: X_n = \left(\frac{1}{2}\right) X_{n-1} \Rightarrow x(t) = x(0) \left(\frac{1}{2}\right)^{2t/3}$$

$$h = 2: X_n = -X_{n-1} \Rightarrow x(t) = x(0) (-1)^{t/2}$$

ANALYTIC:  $x(t) = x(0) \left(\frac{1}{e}\right)^t; X_n = \left(\frac{1}{e}\right)^h X_{n-1}$

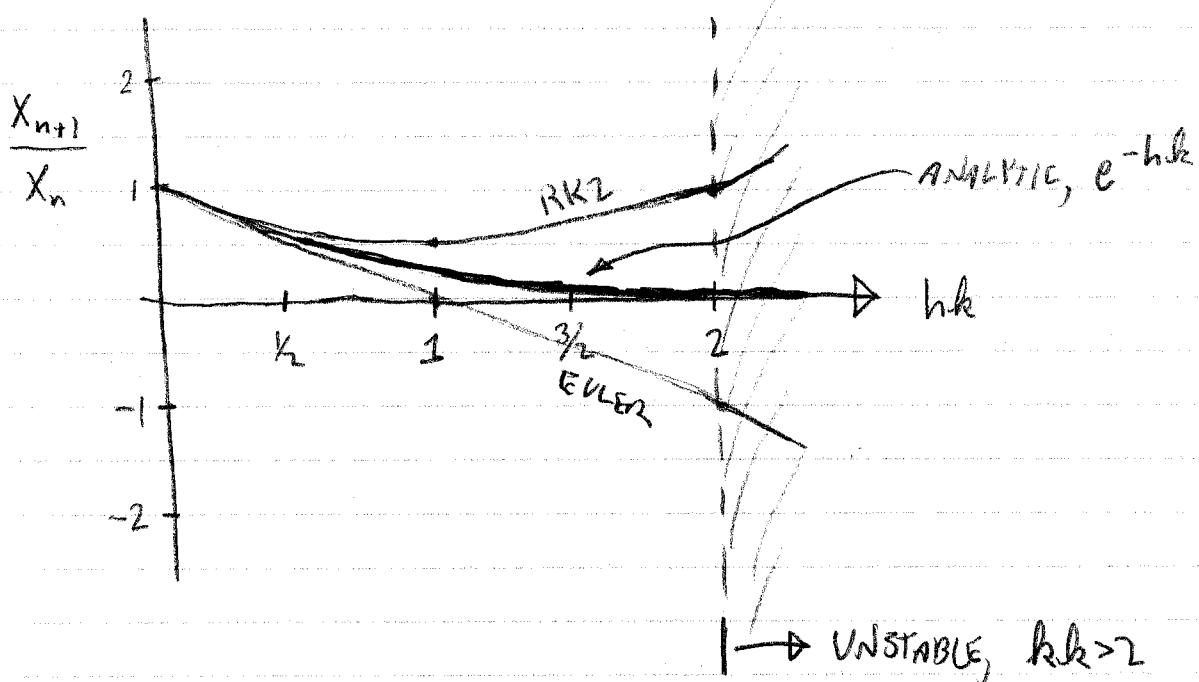
FOR  $hk > 2$ ,  $|X_n| > |X_{n-1}|$ .

THIS NUMERICAL INSTABILITY IS NOT CURED BY HIGHER ORDER SCHEMES!

E.G. RK2:

$$X_{n+\frac{1}{2}} = X_n + \frac{h}{2} \left. \frac{dx}{dt} \right|_{X_n, t_n} = X_n \left(1 - \frac{hk}{2}\right)$$

$$\begin{aligned} X_{n+1} &= X_n + h \left. \frac{dx}{dt} \right|_{X_{n+\frac{1}{2}}, t_{n+\frac{1}{2}}} \\ &= X_n + h \left[ -k X_n \left(1 - \frac{hk}{2}\right) \right] \\ &= X_n \left\{ 1 - hk + \frac{h^2 k^2}{2} \right\} \end{aligned}$$



SO WHAT?

A STIFF SET OF EQUATIONS HAS 2 (OR MORE) VASTLY DIFFERENT TIME SCALES.

- VARIATION ON THE SHORTEST TIMESCALE DIES OUT QUICKLY.
- AFTERWARD, THE BEHAVIOR IS DETERMINED BY THE LONGER TIMESCALE(S)
- NUMERICAL INSTABILITIES WILL RESULT UNLESS  $h$  IS KEPT SHORTER THAN THE SHORTEST TIMESCALE.

EXAMPLE

$$\frac{d}{dt} \begin{pmatrix} x \\ y \end{pmatrix} = a \begin{bmatrix} -(1+\epsilon)x + y \\ x - (1+\epsilon)y \end{bmatrix}, \quad 0 < \epsilon \ll 1.$$

SOLUTION:

$$\text{LET } u = x + y, \\ v = x - y$$

$$\dot{u} = a(-\epsilon x - \epsilon y) = -a\epsilon u$$

$$\dot{v} = a(-(2+\epsilon)x + (2+\epsilon)y) = -a(2+\epsilon)v$$

$$u = A e^{-a\epsilon t}, \quad v = B e^{-a(2+\epsilon)t}$$

$$\tau_u = 1/\epsilon a \quad (\text{SLOW}), \quad \tau_v \approx 1/2a \quad (\text{FAST})$$

$v$  DIES AWAY IMMEDIATELY, AND THEREAFTER WE COULD, IN PRINCIPLE, RESOLVE THE BEHAVIOR OF THE SYSTEM WITH LONG Timesteps  $1/2a \ll h < 1/a\epsilon$ .

IN REALITY, ALL THE SCHEMES WE'VE STUDIED WILL BE UNSTABLE UNLESS  $h \lesssim$  SHORTEST TIME CONSTANT.

IMPLICIT (BACKWARD) TIMESTEPS

AS BEFORE, CONSIDER THE ODE:

$$\dot{x} = -kx$$

EXPLICIT (FORWARD) EULER:

$$x_{n+1} = x_n + h \dot{x}_n = x_n - hkx_n$$

UNSTABLE FOR  $hk > 2$ .

WHAT IF, INSTEAD, WE COULD DO BACKWARD EULER:

$$x_n = x_{n+1} - h \dot{x}_{n+1}$$

(EQUIVALENTLY,  $x_{n+1} = x_n + h \dot{x}_{n+1}$ )

FOR OUR ODE, THIS WOULD BE

$$x_n = x_{n+1} (1 + hk)$$

$$x_{n+1} = \frac{x_n}{(1 + hk)}$$

- TO FIRST ORDER IN  $hk$ , SAME AS EXPLICIT EULER
- STABLE FOR ALL  $hk$ !

IMPLEMENTATION OF IMPLICIT EULER:

NEW NOTATION — Timestep INDEX IN SUPERSCRIPT.

$$\dot{\vec{x}} = \vec{f}(\vec{x}, t) \quad (\text{ODE})$$

$$\text{IMPLICIT STEP: } \vec{x}^{n+1} = \vec{x}^n + h \vec{f}(\vec{x}^{n+1}, t_{n+1}) \quad \star$$

SOLVE FOR  $\vec{x}^{n+1}$  BY TAYLOR EXPANSION:

$$\vec{f}(\vec{x}^{n+1}, t_{n+1}) \approx \vec{f}(\vec{x}^n, t_{n+1}) + \left. \frac{\partial \vec{f}}{\partial \vec{x}} \right|_{\substack{\vec{x}^n \\ t_{n+1}}} \cdot (\vec{x}^{n+1} - \vec{x}^n)$$

JACOBIAN MATRIX,  $J$

MORE EXPLICITLY:

$$f_j(\vec{x}^{n+1}, t_{n+1}) \approx f_j(\vec{x}^n, t_{n+1}) + \sum_k \left. \frac{\partial f_j}{\partial x_k} \right|_{\substack{\vec{x}^n \\ t_{n+1}}} (x_k^{n+1} - x_k^n)$$

PLUG BACK INTO  $\star$ , ISOLATE  $x_j^{n+1} - x_j^n$ :

$$\sum_k \left[ \delta_{jk} - h \left. \frac{\partial f_j}{\partial x_k} \right|_{\substack{\vec{x}^n \\ t_{n+1}}} \right] (x_k^{n+1} - x_k^n) = h f_j(\vec{x}^n, t_{n+1})$$

NEED TO INVERT THIS MATRIX

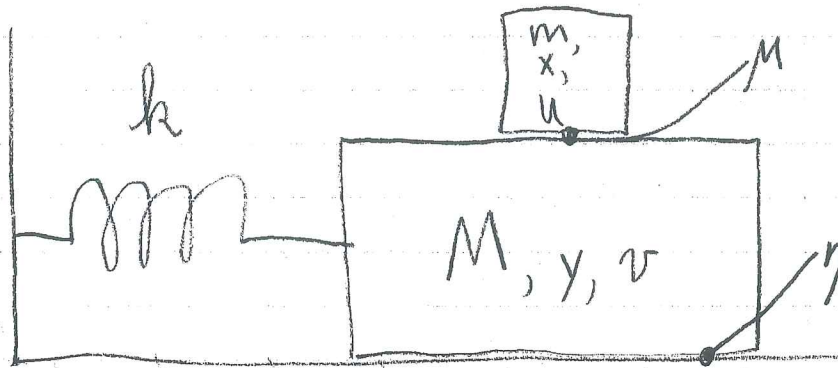
$$(\mathbf{I} - h\mathbf{J}) (\vec{x}^{n+1} - \vec{x}^n) = h \vec{f}(\vec{x}^n, t_{n+1})$$

$$\vec{x}^{n+1} = \vec{x}^n + h(\mathbf{I} - h\mathbf{J}(\vec{x}^n, t_{n+1}))^{-1} \vec{f}(\vec{x}^n, t_{n+1})$$

• IN ADDITION TO A ROUTINE FOR  $\vec{f}(\vec{x}, t)$ , WE NEED A ROUTINE FOR

$$J_{jk}(\vec{x}, t) = \frac{\partial f_j}{\partial x_k}(\vec{x}, t)$$

CLASS EXERCISE



FOR THE "FRICTION" FORCES, USE A LINEAR DAMPING, E.G.  
 $F = -\eta v$

① FOUR COUPLED ODE'S:

$$m \ddot{u} = -\mu(u-v), \quad \dot{x} = u$$

$$M \ddot{v} = -\eta v + \mu(u-v) - k y, \quad \dot{y} = v$$

② IDENTIFY THE UNITS OF ALL PHYSICAL PARAMETERS

$$M, m, k, \mu, \eta$$

③ IDENTIFY ALL THE TIME CONSTANTS FOR THE PROBLEM.

④ HOW CAN I CHOOSE THE PARAMETERS TO MAKE A VERY STIFF PROBLEM?

# NR § 5.7 NUMERICAL DIFFERENTIATION

MOTIVATION: A WAY TO AVOID DERIVING THE JACOBIAN ANALYTICALLY.  
(LSODE HAS THIS BUILT IN!)

APPROACH: FINITE DIFFERENCING

$$f(x+\delta) = f(x) + \delta f'(x) + \frac{\delta^2}{2} f''(x) + \frac{\delta^3}{6} f'''(x) + \dots$$

$$\frac{f(x+\delta) - f(x)}{\delta} = f'(x) + \frac{\delta}{2} f''(x) + O(\delta^2)$$

$$f'(x) = \frac{f(x+\delta) - f(x)}{\delta} - \underbrace{\frac{\delta}{2} f''(x) + O(\delta^2)}_{\text{TRUNCATION ERROR}}$$

WE CAN DO BETTER. CONSIDER:

$$f(x-\delta) = f(x) - \delta f'(x) + \frac{\delta^2}{2} f''(x) - \frac{\delta^3}{6} f'''(x) + O(\delta^4)$$

$$\frac{f(x+\delta) - f(x-\delta)}{2\delta} = f'(x) + \frac{\delta^2}{3} f'''(x) + O(\delta^3)$$

$$\star f'(x) = \frac{f(x+\delta) - f(x-\delta)}{2\delta} - \underbrace{\frac{\delta^2}{3} f'''(x) + O(\delta^3)}_{\text{TRUNCATION ERROR}}$$

CENTERED DIFFERENCING.

WE GET HIGHER ORDER ACCURACY FOR FREE — SAME NUMBER OF FUNCTION EVALUATIONS.

Q: WHAT HAPPENS AS  $\delta \rightarrow 0$  ?

A: TRUNCATION ERROR  $\rightarrow 0$   
WHAT ABOUT ROUND OFF ERROR?

## ROUNDOFF ERROR

SUBTRACTING 2 NUMBERS THAT ARE NEARLY EQUAL IS A RECIPE FOR DEATH BY ROUNDOFF ERROR!

EACH TIME WE REPRESENT A NEW RESULT AS A FLOATING POINT NUMBER, THERE IS A DISCRETIZATION ERROR. MULTIPLY BY  $(1+\eta)$ , WHERE  $\eta = \pm \epsilon$  AND  $\epsilon$  IS THE (FRACTIONAL) MACHING PRECISION ( $1.1 \times 10^{-16}$  FOR DOUBLE PRECISION).

FOR EXAMPLE, SUBTRACT TWO NUMBERS:

$$x-y \rightarrow [x(1+\eta) - y(1+\eta')] (1+\eta'')$$

↑                    ↑                    ↑                    INDEPENDENT ERRORS

$$\rightarrow x-y + \eta x + \eta' y + \eta''(x-y)$$

IF  $x \approx y$  THEN

$$x-y \rightarrow (x-y) \pm \sqrt{2} \epsilon x.$$

NOW CONSIDER OUR DIFFERENTIATION FORMULA (\*):

$$f'(x) \approx \frac{f(x+\delta) - f(x-\delta)}{2\delta} - \frac{\delta^2}{3} f'''(x) \pm \sqrt{2} \epsilon \frac{f(x)}{2\delta}$$

- WE HAVE 2 ERROR TERMS — ONE INCREASES AS  $\delta \rightarrow 0$ , AND THE OTHER DECREASES AS  $\delta \rightarrow 0$ .



FORMALLY, SINCE THE TRUNCATION AND ROUND-OFF ERRORS ARE UNCORRELATED, WE SHOULD ESTIMATE THE TOTAL UNCERTAINTY AS:

$$\Delta f' = \sqrt{\left(\frac{\delta^2}{3} f'''\right)^2 + \left(\frac{\epsilon f}{\delta \sqrt{2}}\right)^2}$$

MINIMIZE INSIDE OF THE  $\sqrt{\quad}$  WRT  $\delta$ :

$$\frac{d}{d\delta} \left( \frac{f'''^2}{9} \delta^4 + \frac{\epsilon^2 f^2}{2} \delta^{-2} \right) = 0$$

$$\Rightarrow \frac{4}{9} f'''^2 \delta^3 = \epsilon^2 f^2 \delta^{-3}$$

$$\delta = \left( \frac{9}{4} \frac{\epsilon^2 f^2}{f'''^2} \right)^{1/6} \quad \left( \frac{9}{4} \right)^{1/6} = 1.14 \quad \text{IGNORE!}$$

WE DON'T KNOW  $f'''$ . ESTIMATE: IF  $\lambda$  IS A CHARACTERISTIC LENGTH FOR OUR PROBLEM,

$$f''' \approx \frac{f}{\lambda^3}$$

SO WE WILL CHOOSE

$$\delta = \lambda \epsilon^{1/3}$$

AND

$$\Delta f' = \sqrt{\frac{f^2}{9\lambda^2} \epsilon^{4/3} + \frac{f^2}{2\lambda^2} \epsilon^{4/3}} = 0.8 \frac{f}{\lambda} \epsilon^{2/3}$$

$$\boxed{\Delta f' \approx f' \epsilon^{2/3}}$$

EQUAL IF  $\delta$  HAS ITS IDEAL VALUE.

THINK ABOUT THIS RESULT:  $\frac{\Delta f'}{f'} \geq \epsilon^{2/3}$

	MACHINE PRECISION	IDEAL ACCURACY OF CENTERED DERIVATIVE
SINGLE PRECISION	$6 \times 10^{-8}$	$1.5 \times 10^{-5}$
DOUBLE PRECISION	$1.1 \times 10^{-16}$	$2.3 \times 10^{-11}$

NUMERICALLY, INTEGRATION IS ACTUALLY EASIER (MORE ACCURATE FOR A GIVEN ORDER) THAN DIFFERENTIATION.

Q: WHAT HAVE WE FORGOTTEN IN OUR ERROR ANALYSIS?

WE MISSED SOMETHING IMPORTANT — BUT IT CAN BE FIXED.  
RECALL OUR CENTERED DERIVATIVE,

$$\frac{df}{dx} \approx \frac{f(x+\delta) - f(x-\delta)}{2\delta}$$

$$x+\delta \rightarrow (x+\delta)(1+\eta) \approx x+\delta + \eta x$$

$$f(x+\delta) \rightarrow f(x) + \delta f'(x) + \eta x f'(x)$$

$$f(x-\delta) \rightarrow f(x) - \delta f'(x) + \eta' x f'(x)$$

(I AM CONSIDERING ONLY THE ROUND-OFF ASSOCIATED WITH  $x+\delta$  AND  $x-\delta$  !)

$$\therefore \frac{f(x+\delta) - f(x-\delta)}{2\delta} \rightarrow f'(x) \left[ 1 + \frac{(\eta - \eta')x}{2\delta} \right]$$

↑  
HUGE ERROR!

SOLUTION: "LAUNDER"  $\delta$  AS FOLLOWS:

$$\frac{df}{dx} = \frac{f(x+\delta) - f(x-\delta)}{(x+\delta) - (x-\delta)}$$

THIS IS THE STANDARD IMPLEMENTATION.

DISCUSS

$$(x+\delta) - (x-\delta) \rightarrow 2\delta \left( 1 + \frac{(\eta - \eta')x}{2\delta} \right)$$